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LETTER TO THE EDITOR

Reaction windows for electron capture by highly charged ions

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Abstract. It is pointed out that, when considering electron capture in collisions of highly charged ions with atoms or molecules, a qualitative discussion in terms of a common 'reaction window' is valid only when fully stripped ions are involved. In the case of partly stripped ions with well separated subshell levels it becomes essential to define individual reaction windows for the final states of the captured electron. These reaction windows generally appear at smaller internuclear separations than in the corresponding bare-ion case. The shift is particularly pronounced for final states of high angular momentum. This observation is supported by available experimental data.

Electron capture in slow collisions of highly charged ions with atoms or molecules has been discussed on several occasions in terms of the so-called reaction window (see for example Smith *et al* 1980, Kimura *et al* 1984, Cederquist *et al* 1985). This concept embraces the following understanding of the capture process: transitions in slow atomic collisions are strongly favoured if they may take place under quasi-adiabatic conditions, i.e. at level crossings of perturbed potential energy curves. Such level crossings appear frequently in collisions of highly charged ions with atoms or molecules because the potential energy curves belonging to rearranged configurations are strongly perturbed by the ion-ion Coulomb repulsion, while the potential energy curve belonging to the initial ion-atom configuration is only moderately perturbed. If, however, a potential energy curve crossing takes place at a very large value of the internuclear separation R , the active electron will have to tunnel through a wide potential barrier to rearrange the system. The effective coupling between the two states is therefore very small in the crossing region so that a transition, in spite of the energy degeneracy, becomes unlikely. The other extreme is a curve crossing at small internuclear separations. The interaction between the two states is then usually strong enough to generate an effectively avoided curve crossing. Only curve crossings that appear in a suitable intermediate range of internuclear separations are really efficient. This intermediate range of separations is now commonly referred to as the reaction window for the electron capture process.

The position of the reaction window depends modestly on the relative collision velocity, v . The adiabaticity at inner crossings becomes increasingly pronounced when v is reduced while the interaction time, and thus the transition probability at a distant crossing, becomes larger. The reaction window therefore shifts towards higher R values if v is reduced and vice versa.

A quantitative definition of the reaction window and its velocity dependence may be based on the Landau-Zener model in combination with Olson and Salop's (1976) analytic fit to the relevant coupling element (see, for example, Kimura *et al* 1984,

Meyer *et al* 1985). In accord with Kimura *et al* (1984) we define the reaction window in terms of the corresponding 'transmission coefficient'

$$T(R_c, v) = \sigma(R_c, v) / \pi R_c^2 \quad (1)$$

where σ is the Landau-Zener cross section pertaining to a potential curve crossing at the internuclear separation R_c

$$\sigma = 2\pi \int_0^{R_c} b \, db \, 2P(1-P). \quad (2)$$

Here, P is the Landau-Zener transition probability given by

$$P = \exp\{-\beta[1 - (b/R_c)^2]^{-1/2}\} \quad (3)$$

where

$$\beta = 2\pi |H_{12}(R_c)|^2 / [v(d\Delta E_{12}/dR)_{R_c}] \quad (4)$$

in terms of the coupling element H_{12} and the potential energy difference ΔE_{12} between the two crossing states. Here, and throughout, we use atomic units.

Substituting (2) and (3) in (1) we obtain

$$T(R_c, v) = G(\beta(R_c, v)) = 2 \int_0^1 dx \exp(-\beta x^{-1/2}) [1 - \exp(-\beta x^{-1/2})]. \quad (5)$$

The universal function $G(\beta)$ is readily computed. However, in order to obtain the separate dependence on R_c and v , as required in the reaction window, we need an explicit form of $\beta(R_c, v)$. In the range of interest for our present purpose it is sufficient to include the ion-ion repulsion term in an estimation of the angle of intersection of the potential energy curves, i.e.

$$d\Delta E_{12}/dR \approx (q-1)/R^2 \quad (6)$$

where q is the charge of the incident ion.

It is more difficult to obtain a satisfactory expression for the coupling element H_{12} . The case of fully stripped ions ($q=Z$) in collision with atomic hydrogen has been considered by Olson and Salop (1976), who devised an analytic fit to H_{12} data obtained by numerical solution of the one-electron two-centre problem. They obtained the following form

$$H_{12}^{\text{OS}} = (9.13/\sqrt{Z}) \exp(-1.324R_c/\sqrt{Z}) \quad (7)$$

which was found to be accurate to within 17% over the relevant range of R_c and Z . Noting that H_{12} should be squared and then exponentiated in equations (3) and (4), the 17% accuracy is not impressive, but for the present qualitative purpose it is acceptable.

It is clear from equation (7) that it is relevant to scale R_c with \sqrt{Z} . If we similarly scale the velocity by $(Z-1)^{-1}$ and insert equations (6) and (7) into (4), we find

$$\beta^{\text{OS}} = 524(\tilde{R}_c^2/\tilde{v}) \exp(-2.648\tilde{R}_c) \quad (8)$$

where the charge Z only appears implicitly through the reduced parameters

$$\tilde{R}_c = R_c/\sqrt{Z} \quad (9a)$$

$$\tilde{v} = v(Z-1). \quad (9b)$$

The transmission coefficient of the reaction window is therefore also independent of the ionic charge when expressed in terms of reduced parameters. The reaction window is shown in figure 1 as a function of the reduced internuclear separation for a selection of reduced impact velocities. The velocity dependence is in good accord with our discussion above. Note that the shape and width of the reaction windows is almost independent of velocity. The reaction window, as defined here, generally shows a narrow structure at very small separations ($\tilde{R}_c \ll 1$). Basically, it just reflects the divergence of equation (6) in the small R limit. Since this is an artefact of the model, we have excluded the region $\tilde{R} < 1$ in figure 1.

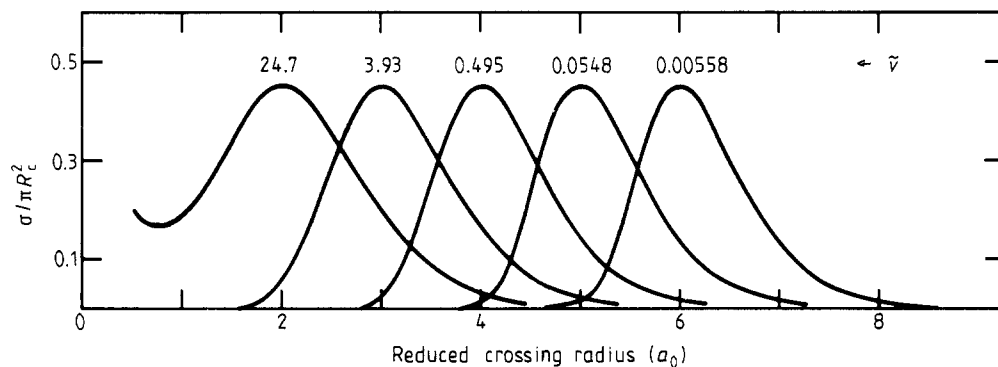


Figure 1. Reaction windows for a selection of reduced velocities \tilde{v} (au).

It appears that equation (7), and thus the reaction window, is independent of the quantum numbers characterising the final state. What matters is only the position of the crossing. However, for the following it is important to note that equation (7), as determined by Olson and Salop (1976) via the relation $\Delta\epsilon = 2H_{12}$, really represents the adiabatic energy splitting at a pseudocrossing between eigenstates of the molecular one-electron system and, more importantly, that states which exhibit this feature are of a very special type. Referring to prolate spheroidal coordinates, these strongly interacting molecular states in fact have only inner nodal surfaces. In a perturbed atomic picture (similar to a diabatic molecular picture at large separations) it is well known (Gershtein and Krivchenkov 1961) that the states of the one-electron two-centre system correspond to atomic one-electron states in a parabolic (Stark) representation. Molecular states with inner nodes only correspond, in particular, to the Stark states that are most strongly polarised towards the other centre. The strongly polarised states simply interact most effectively at large separation because of spatial overlap.

Returning now to equation (7), it is clear that the expression on the RHS represents the coupling to a particular Stark superposition of states from the degenerate manifold of states in the considered principal shell of the highly charged ion. The coupling to the residual space of states is much smaller and is implicitly ignored in the previous discussion. To be specific, we may refer to the parabolic representation of final states $\{\varphi_f^p(n_1, n_2, m)\}$, where n_1 and n_2 denote the number of parabolic nodal surfaces away from and towards the hydrogen nucleus. The situation may then be clarified by the following general expression

$$\langle \varphi_f^p(n_1, n_2, m) | H | \varphi_i(1s) \rangle = \delta_{n_1,0} \delta_{n_2,n-1} \delta_{m,0} H_{12}^{\text{OS}} \quad (10)$$

for the coupling between the initial state and an arbitrary final state in the n th principal shell. This more precise specification of the model is essential for the discussion of partly stripped incident ions.

When concerned with targets other than atomic hydrogen, Olson and Salop (1976) suggested a modification of the exponent in equation (7) by the multiplicative factor

$$\alpha = \sqrt{2I_t} \quad (11)$$

where I_t is the ionisation potential of the target. We also adopt this procedure, which seems reasonable since the exponential factor in the coupling element is determined by the tails of the atomic wavefunctions.

Let us now consider incident, partly stripped ions ($q < Z$). The final states on the projectile are then no longer degenerate in principal shells. This implies that there is a curve crossing for each particular subshell level. Crossings pertaining to sublevels of the same principal shell may, in typical cases, be spaced by a couple of atomic units (Larsen and Taulbjerg 1984). Aiming again at a definition of reaction windows on the basis of the Landau-Zener model we note that, while the angle of intersection of crossing potential energy curves remains well represented by equation (6), it is clear from the discussion of equation (10) that the Olson-Salop coupling element must be modified. In fact, it is entirely trivial to transform the coupling matrix as given by equation (10) into the spherical representation $\{\varphi_f^S(nlm)\}$. Thus we obtain

$$\langle \varphi_f^S(nlm) | H | \varphi_i(1s) \rangle = f_{nl} \delta_{m,0} H_{12}^{\text{OS}} \quad (12a)$$

where

$$f_{nl} = \langle \varphi_f^S(nl0) | \varphi_f^P(0, n-1, 0) \rangle \quad (12b)$$

are elements of the unitary matrix that transforms between parabolic and spherical representations. Explicit values for these matrix elements are given by Omidvar (1967) for selected values of n . A simpler closed form may, however, be derived following Park (1960). As also noted by Burgdörfer (1983), it is possible to relate the parabolic and spherical representations by a simple Clebsch-Gordan transformation involving the pseudospin $j = (n-1)/2$. In the specific case of equation (12) we find

$$f_{nl} = (-1)^{n+l-1} (2l+1)^{1/2} \Gamma(n) [\Gamma(n+l+1) \Gamma(n-l)]^{-1/2} \quad (13)$$

which is well defined even if one refers to non-integer effective values of n (Larsen and Taulbjerg 1984). An explicit evaluation of equation (13) shows that the overlap factor is sensitive to l and becomes quite small when l approaches its maximum value.

Including the α factor to allow for targets other than atomic hydrogen, we finally obtain the following generalisation of equation (7)

$$H_{12} = (9.13 f_{nl} / \sqrt{q}) \exp(-1.324 R_c \alpha / \sqrt{q}) \quad (14)$$

which represents the coupling between the initial state and a final state with quantum numbers n and l on a partly stripped ion of charge q .

A comparison with numerical values (Larsen and Taulbjerg 1984, Gargaud and McCarroll 1985, McCarroll 1986) indicates that equation (14) has a tendency to slightly overestimate the coupling element. This might suggest a moderate reduction of the numerical factor in equation (14) but the available data are too scarce to quantify this effect. For the present qualitative purposes we therefore conform with equation (14) as it stands, but note that it would be too optimistic to expect it to retain the same degree of accuracy as in the simpler case represented by equation (7).

The coupling element in equation (14) depends explicitly on the final state, but it is easy to show that the scaled expression (8) remains valid in this general case if equations (9) are replaced by

$$\tilde{R}_c = R_c(\alpha/\sqrt{q}) \quad (15a)$$

$$\tilde{v} = v[(q-1)\alpha^2/|f_{nl}|^2]. \quad (15b)$$

The reaction windows exhibited in figure 1 therefore remain valid in the general situation if rescaled units are used according to equations (15). However, it must be noted that the velocity scaling factor in equation (15b) depends on n and l . Since $|f_{nl}|^2 < 1$, it is clear that reaction windows belonging to resolved subshells appear at smaller values of the internuclear separation than the corresponding reaction window in the bare-ion case $Z = q$. Since $|f_{nl}|^2 \ll 1$, for high values of l , the shift towards smaller separations is particularly important in this limit.

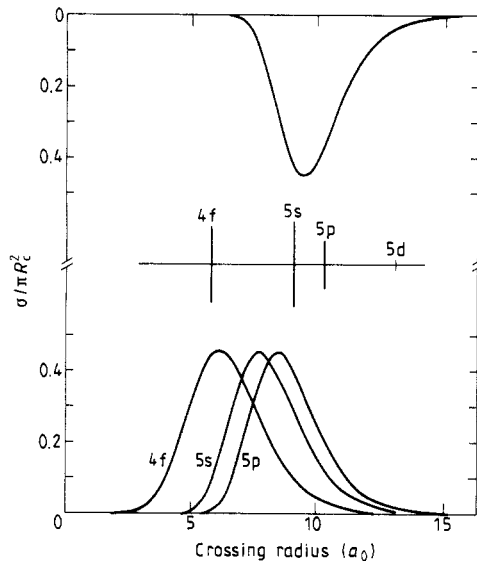


Figure 2. Specific reaction windows for capture to 4f, 5s and 5p in collisions of partly stripped 8+ ions with neon at an impact velocity of 0.158 au. The common reaction window pertaining to fully stripped 8+ ions at the same impact velocity is shown in the upper part. The position of the relevant curve crossings for the Ar^{8+} -Ne system is shown in the centre of the figure. The height of the full bars represents the experimental value of the corresponding partial capture cross sections (Nielsen *et al* 1985).

Reaction windows for $\text{Ar}^{8+} \rightarrow \text{Ne}$ at 1 keV are shown in figure 2 as a particularly illuminating example. The upper part of the figure shows the common reaction window that results if the fractional factors f_{nl} are ignored, as in previous discussions. The crossings that actually take place in the vicinity of the reaction window are marked by bars in the centre of the figure. The height of the bars is determined by the experimental value of the corresponding partial capture cross sections (Nielsen *et al* 1985). The following two observations are especially important. First of all, the 4f crossing appears far outside the common reaction window which would suggest that the 4f capture cross section should be very small. This is in clear contradiction with the data. Secondly, the 5d cross section was not big enough to be determined experimentally although, from its position in the wing of the reaction window, it would have been expected to be about a quarter of the cross section at maximum transmission.

Individual reaction windows, properly obtained using equation (14) as the coupling element, are shown in the lower part of figure 2. The 5d curve would appear between

the 5s and 5p curves. It can be seen that the shifted reaction windows are in very good accord with the data. In particular, we note that the 4f crossing takes place at the maximum of the 4f reaction window. The 5d window is shifted enough to reduce the value of the expected cross section to about $\frac{1}{15}$ of the maximum cross section, which is compatible with the data.

In conclusion, we remark that it is essential for the present discussion that the crossings due to individual l levels are well separated. Otherwise a coherent treatment is required and we will have to rely on a numerical solution of the relevant coupled-state equations.

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References

- Burgdörfer J 1983 *Z. Phys. A* **309** 285
Cederquist H, Andersen L H, Bárány A, Hvelplund P, Knudsen H, Nielsen E H, Pedersen J O K and Sørensen J 1985 *J. Phys. B: At. Mol. Phys.* **18** 3951
Gargaud M and McCarroll R 1985 *J. Phys. B: At. Mol. Phys.* **18** 463
Gershtein S S and Krivchenkov V D 1961 *Sov. Phys.-JETP* **13** 1044
Kimura M, Iwai T, Kaneko Y, Kabayashi N, Matsumoto A, Ohtani S, Okuno K, Takagi S, Tawara H and Tsurubuchi S 1984 *J. Phys. Soc. Japan* **53** 2224
Larsen O G and Taulbjerg K 1984 *J. Phys. B: At. Mol. Phys.* **17** 4523
McCarroll R 1986 private communication
Meyer F W, Howald A M, Havener C C and Phaneuf R A 1985 *Phys. Rev. Lett.* **54** 2663
Nielsen E H, Andersen L H, Bárány A, Cederquist H, Heinemeier J, Hvelplund P, Knudsen H, MacAdams K B and Sørensen J 1985 *J. Phys. B: At. Mol. Phys.* **18** 1789
Olson R E and Salop A 1976 *Phys. Rev. A* **14** 579
Omidvar K 1967 *Phys. Rev.* **153** 121
Park D 1960 *Z. Phys.* **159** 155
Smith D, Adams N G, Alge E, Villinger H and Lindinger W 1980 *J. Phys. B: At. Mol. Phys.* **13** 2787