Coherence Effects in Heavy Ion-Atom Collisions

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ABSTRACT

A new approach to charge capture and ionization by highly stripped projectiles is described and shown to explain cross section systematics through the periodic table. Oscillations in cross section with respect to charge state observed around atomic number 70 are explained as an f-wave resonance in the target electron-projectile scattering. The ratio of $H_2$ to H cross sections for both light and heavy projectiles is shown to fit a two center coherent scattering model; independent scattering by the two centers is not a good assumption for velocities below 4 a.u. Similar coherence effects are predicted in stripping by molecular gases even in multi-electron processes where the independent atom model might be thought valid. Recent experiments on the forward peak of electrons ejected from the projectile show interesting structure which can be partly explained without invoking interference effects.


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1. INTRODUCTION

We shall survey a number of problems in the field of heavy ion-atom (or molecule) collisions where coherence or interference between quantal scattering amplitudes plays a significant role. In 2. we show how interference between short-range and long-range amplitudes explains anomalies in the variation of total cross sections with charge state. The ratio between capture from atomic and molecular targets is discussed in 3., and it is shown that a wide range of data is fitted by a two center scattering model. A similar model also predicts significant effects in stripping. In 4. we examine the forward peak in projectile ionization which is potentially a rich source of interference effects, though none have yet been clearly identified. Atomic units are used throughout.

2. SYSTEMATICS OF CHARGE CAPTURE BY HIGHLY STRIPPED IONS

We suppose that capture from a hydrogen atom by a highly stripped projectile at intermediate velocities (1 < v < 3)

\[ A^{+q} + H \rightarrow A^{+(q-1)} + H^{+} \]  

(1)

takes place in two stages. In the first, an amount of energy \( \Delta \) is transferred to the bound electron to remove it from the field of \( H^{+} \). Then the electron moves to the saddle point between \( H \) and \( A \), whence it may be captured by the heavy ion or escape depending on its acquired kinetic energy. The capture cross section

\[ \sigma_c = \sigma_L \exp(-2v/q^2) \]  

(2)

where \( \sigma_L \) is the binary encounter loss cross section, related to the e+\( A \) elastic scattering amplitude \( f \) by

\[ \sigma_L = \int_{\theta_o}^{\pi} |f|^2 \sin\theta d\theta, \cos\theta_o = 1 - \Delta/v^2. \]  

(3)
The second factor in (2) is calculated from classical transition state theory. If only the Coulomb field of A\(^{+q}\) is considered

\[ c_L = \frac{2\pi}{\Delta} \left( \frac{q}{\nu} \right)^2. \]  

To test (2), (4) empirical values of \( \Delta \) were calculated from a wide range of recent measurements\(^1\) and plotted against \( 1/\nu \) in Fig. 1, each point is an average over all available \( q \). Theoretically, one would expect \( \Delta = 1 \). The apparent discrepancy between light and heavy projectiles is entirely due to projectiles in low stages of ionization, and it can almost certainly be resolved by using a realistic \( e+A \) potential.

Improved calculations of \( f \) have been undertaken\(^2\) to explain the anomalies seen in the variation of \( \sigma_C \) with \( q \) for projectiles of atomic number \( Z = 70 \). In Fig. 2 we plot the Coulomb phase shifts \( \delta(\ell=2,3) \) in a Thomas-Fermi potential as a function of \( Z \) for \( q = 4, 6, 8 \) and \( \nu = 1.5 \). Phase shifts \( \delta(\ell \geq 4) \) are small, while \( \delta(0,1) \) are similar in behavior to \( \delta(2) \); dependence on \( \nu \), at least for \( 1 < \nu < 3 \), is slight. The uniquely rapid variation of \( \delta(3) \) for \( Z = 75, q = 6 \) (in fact, a shape resonance) largely accounts for the observed anomaly, as illustrated in Fig. 3. After the leading term (4), the most important contribution to \( \sigma_L \) is the Coulomb short range cross term, so that the effect is correctly described as interference.

3. ATOMIC VERSUS MOLECULAR TARGETS

A large body of data has now accumulated on process (1) with both H, H\(_2\) at the same values of \( q, \nu \). Thus the ratio

\[ R = \sigma(H_2)/2\sigma(H) \]  

can be compared with the oft-quoted value of unity, which indeed must be attained at high enough energies. Treating the molecular T-matrix as a sum
of atomic T-matrices with a phase difference appropriate to the equilibrium internuclear separation \( \rho \) we find to a good approximation that

\[ R = 1 + C \| \perp \]  \hspace{1cm} (6) \]

The transverse coherence factor

\[ C \perp = \langle T_A T_B \rangle / \langle T_A^2 \rangle \]  \hspace{1cm} (7) \]

where \( A, B \) refer to the two centers and the brackets to an average over impact parameters and molecular orientations. In a simple model

\[ T = \frac{1}{\sqrt{2}} \exp \left( -\frac{b}{b_0} \right), \sigma(H) = \pi b_0^2 \]  \hspace{1cm} (8) \]

\[ C \perp = \exp \left[ -\left( \frac{\rho}{2.7 b_0} \right)^2 \right] \]  \hspace{1cm} (9) \]

so that for \( b_0 > 1 \), \( C \perp = 1 \). The longitudinal coherence factor

\[ C \| = \frac{\sin X}{X}, X = \frac{\omega_0}{v} \]  \hspace{1cm} (10) \]

where \( \omega_0 \) is a mean energy transfer. The surprising feature of (5) - (10) is that for almost all available measurements \( C \perp = 1 \) and the scattering by the two centers is highly coherent. The simple argument that \( R = 1 \) is thus invalid and measurements which find \( R = 1 \) happen to be in a region where \( C \| \) is passing through zero.

In support of this contention, we have plotted \( R \) for all Oak Ridge data against \( 1/v \) in Fig. 4 (actually the ratio of \( \Delta s \), averaged over \( q \) as before). A reasonable fit is obtained with \( C \perp = 2, \omega = 4.5 \); this value of \( \omega \) corresponds to capture into the state \( n = 0.3q \) in reasonable agreement with most theories. The value of \( C \perp \) argues a T-matrix which peaks around \( b = 1 \), again not an unreasonable result. Similarly, the recent Belfast data with Li projectiles (Fig. 5) are fitted by \( C \perp = 2, \omega = 3.7 \) suggesting
that most capture is into the ground states of the ions. For some velocity 
> 4, we can expect $b_0 \to 0$, $C_+ \to 0$ and $R$ to turn over and $\to 1$, but Figs. 4 
and 5 show that this region has not yet been probed.

Another coherence effect has recently come to light in stripping 
processes

$$A^{+q} + B \to A^{+q'} + B'.$$

(11)

It might be thought that for $Q = q' - q > 1$, the cross section $\sigma_{\text{mol}}(Q)$ for a 
molecular stripper would be the sum of $\sigma_{\text{at}}(Q)$ for the constituent atoms.

In particular, the ratio

$$R(Q) = \sigma(Q)/\sigma(Q-1)$$

(12)

representing the probability of removing the last electron should be the 
same for both atom and molecule. However, we encountered great difficulty 
fitting $N_2$ and SF$_6$ stripping data (with Fe$^{+4}$ at 1.3 MeV/amu) by means of a 
theory which is quite successful for atomic strippers. This theory (A in 
Fig. 6) is consistently lower than experiment.$^4$ A direct calculation in 
which averaging over impact parameters and molecular orientations was carried 
out numerically, almost doubles $R$ and even overshoots experiment for $Q < 4$ 
($M$ in Fig. 6). The numerical calculations are roughly fitted by the ex-
pressions

$$R_{\text{at}}(Q) = (\frac{1}{2})^Q$$

(13)

$$R_{\text{mol}}(Q) = \left[\frac{1}{2}(1 + C_+ C_\|)\right]^Q$$

in the earlier notation. It should be borne in mind that the factors $C_+$, 
$C_\|$ fall off slowly with velocity, and that the average over molecular orien-
tations weights favorable orientations which enhance $\sigma(Q)$ by several decades.

While these predictions have not been confirmed experimentally, a definitive
test is not difficult to mount; more refined calculations are in progress.

4. THE FORWARD PEAK IN PROJECTILE IONIZATION

In (11) electrons ejected with velocities k close to that of the projectile v (the "forward peak") have two sources: (a) capture into the continuum which we shall not consider here, and (b) projectile ionization. Recent experiments reveal structures associated with (b) of two types. One type, for which no good explanation has yet been produced, is of small amplitude and rapidly varying with energy; the other consists of broad shoulders symmetric about k = v.

Looking for simple explanations to begin with, we apply the impact parameter Born approximation, making a multipole expansion of the field of B. For practical purposes, the cross section for ejecting an ns electron is

$$\sigma(ns-k') = 2\pi \left( \frac{Z_B}{v} \right)^2 \sum \frac{R_{\ell}^2}{(2\ell+1)} R_{\ell} = <ns|\ell|k'\ell>$$ (14)

where k' is the wavenumber in the projectile frame. For ions with between 4 and 10 electrons, the dominant process is found to be 2s-k'd, which is consistent with experiment. Now each partial wave has its own cusp shape F_\ell, e.g.

$$F_0 = (1+x^2)^{1/2} - x$$

$$F_1 = \frac{(1+2x^2)^{1/2}}{(1+x^2)} - 2x$$

$$F_2 = \frac{(4+20x^2 + 13x^4)}{4(1+x^2)^{3/2}} - \frac{13}{4} x$$

where x = |k-v|/vθ, θ = aperture of detector. F_0 is, of course, well known. If each cusp is normalized to unity at x = 0 and those for two successive stages of ionization subtracted, the resulting functions must be a
linear combination of $F_1-F_0$, $F_2-F_1$, etc. For $0^+4-0^+5$ only $F_2-F_1$ is possible, and a comparison of theory and experiment (Fig. 7) appears to give a satisfactory explanation of the "shoulders" referred to above. More extensive measurements should yield information on the matrix elements $R_1$, providing a probe of electron scattering by highly stripped ions.
REFERENCES

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   ions in O$_2$ show similar effects: H. D. Betz and A. B. Wittkower, Phys. 
   plotted R(Q) and noted that it was always - 0.6.

FIGURE CAPTIONS

Fig. 1. Variation of $\Delta$ defined in (4) with $1/v$ for different projectiles:
- Si, o Fe, x Mo, + Ta, $\Delta$ W, $\Box$ Au.

Fig. 2. Variation with atomic number $Z$ of $d$, $f$ phase shifts for scattering of electrons by a Thomas-Fermi field with long-range Coulomb interaction. The numbers beside each curve denote the charge state $q$. All results for a velocity $v = 1.5$.

Fig. 3. The capture cross sections for Ta ions at $v = 1.55$ are plotted against $q$. The dots are measurements and the solid line is the theory (2) with $\Delta = 1$.

Fig. 4. The ratio (5) of the $H_2$ to twice the $H$ cross sections is plotted versus $1/v$ for all the Oak Ridge data. Symbols have the same meaning as in Fig. 1.

Fig. 5. The ratio (5) is plotted versus $1/v$ for all the Belfast data:
- Li$^+$, + Li$^{+2}$, o Li$^{+3}$.

Fig. 6. The ratio (12) of successive stripping cross sections versus $Q$ the number of electrons removed. The dotted line is experiment and the solid lines are the two theories explained in the text.

Fig. 7. The functions $F_1 - F_0$ and $F_2 - F_1$ defined by (15), labelled 10, 21 respectively. The dotted line roughly follows the experimental $0^+4 - 0^+5$ difference, while the upper scale shows the electron energy in the projectile frame for ions of 2.5 MeV/amu and an aperture of 1 deg.