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C. O. Reinhold

Ronald E. Olson
Missouri University of Science and Technology, olson@mst.edu

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LETTER TO THE EDITOR

Theoretical description of the binary peak in clothed ion–atom collisions

C O Reinhold†, D R Schultz and R E Olson
Department of Physics, University of Missouri-Rolla, Rolla, MO 65401, USA

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Abstract. The impulse or binary encounter approximation for ion-atom collisions is extended to treat the non-Coulomb interaction between a clothed projectile ion and the target electrons. This model is shown to reproduce the unexplained enhancement of the zero-degree binary peak for partially stripped ions over that for equivelocity fully stripped ions that has recently been observed experimentally in $F^{q+}+H_2$, He collisions. Very good agreement is obtained between theory and experiment and, furthermore, this model is used to illuminate the underlying dynamics which leads to the observed enhancement.

We consider here the theoretical explanation of the recently observed anomalous behaviour of the binary peak resulting from collisions of F^{q+} with H_2 and He (Richard *et al* 1990). Certainly, the binary peak itself is a well known feature of the ejected-electron spectra arising from ion-atom collisions in which very close, binary collisions between the projectile and the target electrons occur (Rudd and Jorgensen 1963, Rudd *et al* 1966, Bonsen and Vriens 1970, Stolterfoht *et al* 1974, Stolterfoht 1978). For an electron at rest, energy and momentum conservation indicate that such so-called binary electrons would have an energy given by $E_b = 2m(\mu/m)^2v^2\cos^2\theta - U_i$, where m is mass of the electron, μ is the reduced mass of the electron-projectile system, v is the projectile velocity, θ is the electron ejection angle and U_i is the ionization potential of the target. In actuality, the binary peak possesses a width and its position is slightly shifted from E_b since the target electron is not initially at rest but has a distribution of velocities.

For bare ion impact at sufficiently high energies, the dependence of the binary peak on the projectile nuclear charge, Z, is well understood and its magnitude has been shown (Lee *et al* 1990, Toburen and Wilson 1979, Toburen *et al* 1980) to scale in direct proportion to Z^2. In contrast, understanding of the behaviour of the binary peak for clothed projectiles is at a much more primitive stage of development. For example, non-zero-degree measurements (Stolterfoht *et al* 1974, Toburen and Wilson 1979, Toburen *et al* 1980) have shown that the magnitude of the binary peak for clothed ion impact was not the same as that for equivelocity bare ions. Subsequently, an effective charge theory (Stolterfoht 1978, Toburen *et al* 1981) has been devised which, to some extent, has been able to explain these results.

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† Present address: Department of Physics, Univ. of Tennessee, Knoxville, TN 37996, USA.

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Quite recently, however, Richard *et al* (1990) have found that the zero-degree dependence of the binary peak magnitude on the projectile charge state cannot be explained in these terms. Specifically, these authors have found that instead of possessing a smaller binary peak, as would be expected on the basis of the effective charge theory, partially stripped ions produced a larger binary peak than that arising from equivelocity bare ions. No quantitative theoretical explanation of this anomalous behaviour was given. Thus, the study of this behaviour has become the main objective of other experimental (Quinteros 1990, Schmidt-Böcking 1990) and theoretical (Olson *et al* 1990) works, both because of its fundamental importance and for the practical use of the binary peak for the absolute normalization of electronic spectra.

It is shown here that this anomalous behaviour may be explained in terms of the static screening produced by a non-Coulomb potential used to represent the target-electron–projectile-core interaction. To this end, we utilize the impulse approximation, also known as the binary encounter approximation, originally introduced by Gryzinski (1959, 1965a, b, c) and subsequently developed by Vriens (1969), Gerjuoy (1966) and others, for Coulomb interactions. This approximation has been extended in a straightforward manner in this work to treat non-Coulomb interactions. In order to compare directly to the results of Richard *et al* (1990) we present calculations of the cross section, differential in both the angle and energy of the ejected electron, in the region of the binary peak for F^{q+} ions colliding with H_2.

In brief, the impulse approximation consists of the calculation of the elastic cross section as a function of impact energy for the scattering of an electron by the projectile core and its subsequent convolution with the momentum distribution of the target atom. Here, the elastic cross section has been obtained through a partial-wave expansion in which the electron–projectile-core interaction has been represented by the Hartree–Fock model potential of Garvey *et al* (1975). This form simulates the interparticle-separation-dependent screening of the nuclear charge by the electrons of the clothed ion, and has the correct asymptotic behaviour at both large and small separations. The non-Coulomb phaseshifts have been obtained by integration of the radial Schrödinger equation by the log-derivative method of Johnson (1973). The sensitivity of the cross sections to the choice of the H_2 momentum distributions has been checked and it is found that the forms given by Weinbaum (1933) or Wang (1928) yield almost identical results.

In figure 1 we display the results of this calculation of the doubly differential cross section for the ejection of electrons at zero degrees near the binary peak for 1.5 MeV u^{-1} F^{5+} and F^{9+} ions colliding with H_2. Also included in the figure are the experimental measurements of Richard *et al* (1990) which has been normalized to the theory at the peak of the F^{9+} spectrum. We note that the data of Richard *et al* (1990) being relative, were previously normalized to the impulse approximation of Lee *et al* (1990) which differs slightly from the impulse approximation used here (Bonsen and Vriens 1970) in the definition of the final electron energy in terms of the energy transfer. It should be emphasized that the normalization to the present theoretical result does not affect the relative magnitudes of the binary peaks and only amounts to a six per cent difference from the normalization published by Richard *et al* (1990).

The enhancement of the binary peak for the partially stripped ion relative to that for the fully stripped ion is clearly evidenced by both the experiment and the present theory. This trend is, as pointed out by Richard *et al* (1990), quite surprising since according to expectations based on the effective charge theory, the electrons of the partially stripped ion should screen the nuclear charge and cause a reduction of the

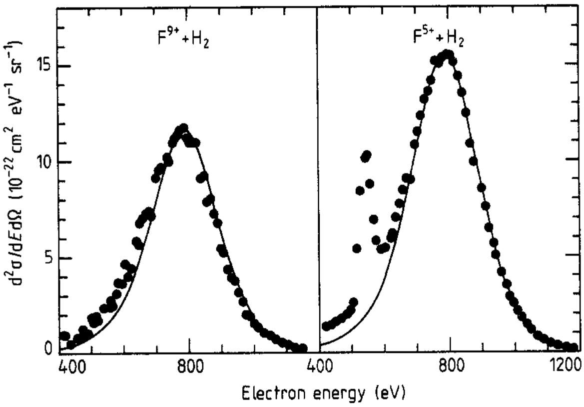

Figure 1. Comparison of the present theoretical calculations (full curve) and the experimental data of Richard *et al* (1990) for the doubly differential cross section for ejection of electrons at zero degrees as a function of the electron energy near the binary peak. The collision energy is 1.5 MeV u^{-1} and both the cross sections and the electron energy are given in the projectile reference frame. The relative experimental data have been normalized by a factor of 0.94 to the theoretical peak for F^{9+} projectiles. The KLL Auger line for F^{5+} impact is observed in the experimental data.

binary peak. Furthermore, if the effective charge is taken to be equal to the nuclear charge, since in a close, binary collision the projectile core of a partially stripped ion is exposed, then one might expect that both the fully and partially stripped ions would produce binary electrons in nearly equal amounts. Hence, a binary peak for the clothed ion would be at most as large as that for the bare ion. Thus, the effective charge model is found to be inadequate in this case.

This anomalous behaviour also occurs for other projectile charge states and impact energies, as illustrated by figure 2 in which the ratio of the binary peak magnitude for clothed ions to that for the fully stripped ion is plotted as a function of the charge state of the projectile. One clearly sees that the magnitude of the binary peak for

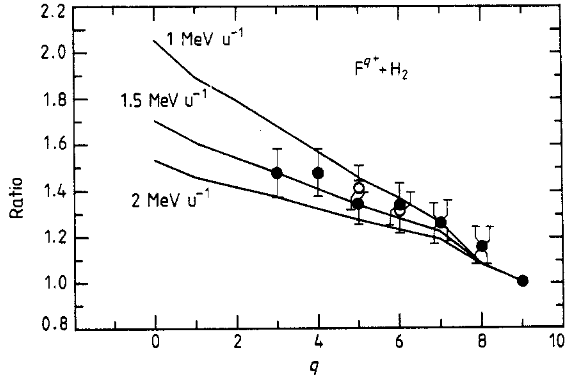

Figure 2. The ratio of the height of the binary peak for F^{q+} ions to the height of the binary peak for the F^{9+} ion at an ejection angle of zero degrees and for various impact energies. The theoretical calculations are compared with the absolute experimental data of Richard *et al* (1990) for 1 MeV u^{-1} (full circles) and 1.5 MeV u^{-1} (open circles).

partially stripped ions is larger than for the fully stripped ion and that the enhancement increases as the charge state is decreased. We note that close agreement between theory and experiment as to the value of the ratio is found and, in fact, on the basis of the theoretical calculations, the largest enhancement would come for neutral F. However, since multiple ionization for small values of q is known to be important, the model based on a static model potential could be insufficient for the smallest charge states. In addition, analogous calculations of the cross sections for $F^{q+}+He$ have yielded essentially the same good agreement between theory and experiment.

In order to understand the origin of this enhancement we have examined the elastic cross section and the classical deflection function for the scattering of an electron by (i) a partially stripped ion (F^{3+}), (ii) the fully stripped ion (F^{9+}) and (iii) a fully stripped ion of nuclear charge equal to the ionic charge of the clothed ion (Li^{3+}), as displayed in figure 3. The deflection function for F^{3+} is seen to be equal to that for Li^{3+} only for very large impact parameters, and lies near to that for F^{9+} at smaller impact parameters. Thus, as would be expected, F^{3+} behaves like an ion with Coulomb charge equal to +3 for distant collisions and similar to 9+ for close collisions.

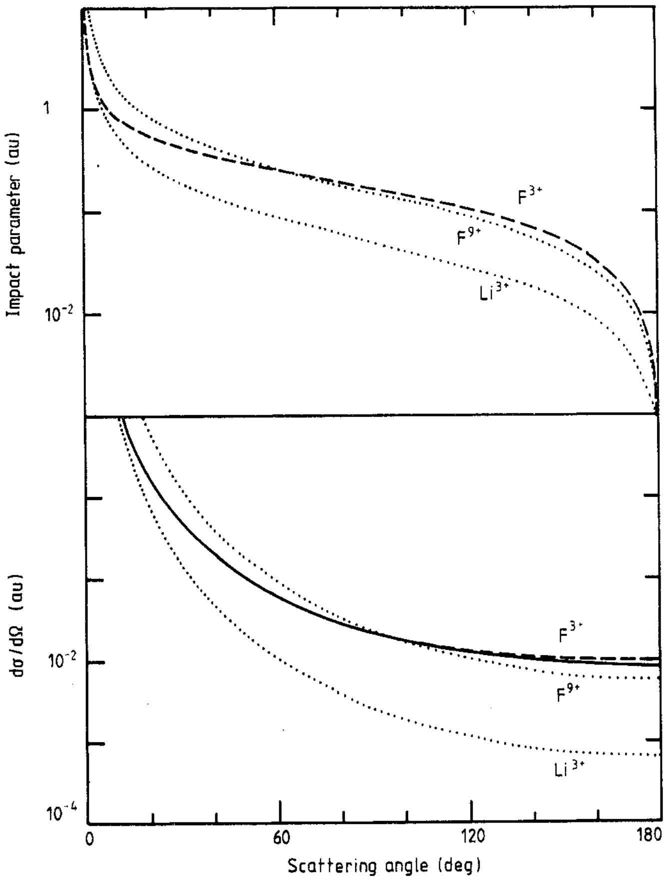

Figure 3. The classical deflection function (upper section) and the elastic differential cross section (lower section) for the scattering of an electron of energy 1.5 MeV u^{-1} from fully and partially stripped ions. The full and broken curves correspond to the quantum mechanical and classical results for F^{3+}, respectively.

Surprisingly though, for small impact parameters, the deflection function for F^{3+} exceeds that of the bare F^{9+} ion.

The consequence of this behaviour is manifested in the elastic differential cross section where an enhancement of the cross section for F^{3+} over that for F^{9+} is observed at large scattering angles. Further, since forward binary electrons originate in collisions leading to scattering angles near 180° in the projectile frame, this enhancement in the elastic cross section leads to the observed enhancement of the binary peak. We also note that for the F^{3+} ion, the classical and quantum mechanical elastic differential cross sections that we display in the figure are very similar, and thus, for this case, no quantum mechanical effect plays a dominant role. Hence, the observed behaviour of the binary peak magnitudes results simply from the differences in the two-body scattering dynamics for either bare or clothed ions. It is also clear from this analysis that it is not adequate to describe the forward binary peak for F^{3+} ions by means of a simple screened Coulomb potential with a static effective charge since the elastic cross section would always lie between the results for F^{9+} and Li^{3+}. Moreover, we emphasize that no contribution can occur due to head on projectile-electron-target-electron collisions since electrons originating through this mechanism would be detected at one fourth of the energy of the ion-induced binary peak (see expression for E_b above). Additionally, we have found that at 1.5 MeV u^{-1} the ratio of the binary peak magnitudes for the various F^{q+} ions with $q > 3$ is, quite simply, almost identical to the ratio of the elastic cross sections at 180°.

Summarizing, in this work we have extended the impulse approximation to treat non-Coulomb interactions between a clothed projectile and the target electrons. Utilizing this method we have analysed the behaviour of the binary peak for F^{q+} ions colliding with H_2 between 1 and 2 MeV u^{-1}. We find that very good agreement is obtained between this treatment and the enhancement of the forward binary peak observed by Richard *et al* (1990) for clothed ions over that for fully stripped ions. Furthermore, this model has allowed us to elucidate the underlying collision dynamics which lead to the enhancement. In particular, we find that an enhancement of the elastic cross section at backward angles in the projectile frame for the scattering of an electron from the statically screened projectile accounts for the binary peak enhancement.

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