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LETTER TO THE EDITOR

Electron emission from both target and projectile in $C^+ + He$ collisions

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Abstract. The first classical trajectory Monte Carlo calculation of the electronic spectra arising from both target and projectile ionisation is presented and compared with experimental measurements of the differential cross section for electrons emitted in $C^+ + He$ collisions. The theoretical treatment is based on an independent-electron model in which the interactions between the electrons are approximated by quantum model potentials. Good agreement is obtained between theory and experiment and structures appearing in the measurements can be explained in terms of the electron emission from either, or both, target and projectile. Further, the relative importance of the electron capture to the continuum and the electron loss to the continuum peaks is analysed for different impact energies and the conclusions obtained from this analysis are found to be in agreement with recent experimental works.

In the last decade, considerable experimental effort has been devoted to the separation of the electronic spectra arising from collisions between structured ions and atoms into target ionisation and projectile ionisation. The earliest studies consisted of comparisons of the total yield of electrons produced by structured projectiles with the yield of electrons produced by bare projectiles (see Kövér *et al* (1983) and Schader *et al* (1984, 1986) for reviews of these studies). Projectile ionisation was thereby inferred from the difference of these yields. However, real progress in the separation of the electronic spectrum into its target and projectile ionisation components has only been possible with the advent of coincident measurements.

These techniques have recently been utilised by DuBois and Manson (1986, 1989) to investigate the cross sections for electron emission coincident with projectile ionisation in $He^+ + He$, Ar collisions, over a wide range of ejection angles (20–150°). Also, coincident techniques have been used in studies of forward electron emission to understand the mechanisms that give rise to the well known cusp that is observed when the velocity of the ejected electrons is similar to that of the impinging projectile (Heil *et al* 1988, Sarkadi *et al* 1989, Kövér *et al* 1989a, b). As a result of these works, considerable insight has been obtained as to the relative contribution to the cusp of the electron capture to the continuum (ECC) and electron loss to the continuum (ELC) peaks.

Despite the available experimental information, there is a general lack of theoretical studies that analyse the relative importance of the emission of electrons from either the target or projectile at intermediate impact energies and for a broad range of electron

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ejection angles. To our knowledge, only a few theoretical works have been made on this subject, such as the first Born calculations of Manson and co-workers (Manson and Toburen 1981, DuBois and Manson 1986, 1989).

On the other hand, recent theoretical studies of the ionisation process in collisions of bare ions with atoms have shown the importance of regarding ionised electrons as electrons in the continuum of the combined target-nucleus-projectile Coulomb field (Olson 1986, Stolterfoht *et al* 1987, Fainstein *et al* 1988, Crothers and McCann 1983, Reinhold and Olson 1989). In fact, these studies have demonstrated the inability of one-centre formalisms such as the Born approximation to give an overall good description of the electronic spectra at intermediate impact energies. In this light, it is seen that it is important to consider electron emission from projectile and target within a two-centre formalism.

In this work, we extend the classical trajectory Monte Carlo (CTMC) method (Abrines and Percival 1966, Olson and Salop 1977, Reinhold and Falcon 1986) to include both target and projectile electrons within the independent-electron approximation (Hansteen and Mosebekk 1972, McGuire and Weaver 1977). To this end, electron-electron interactions are approximated by using the model potentials derived by Garvey *et al* (1975) by a variational procedure in a modified Thomas–Fermi model. Thus, it is assumed that the active electron interacts simultaneously with a target (t) core and a projectile (p) core through the two-centre potential

$$V(r) = V_t(r_t) + V_p(r_p) \tag{1}$$

with

$$V_{t,p}(r) = \frac{1}{r}[N_{t,p}S_{t,p}(r) - Z_{t,p}] \tag{2}$$

$$S_{t,p}(r) = 1 - [(\eta_{t,p}/\xi_{t,p})(e^{\xi_{t,p}r} - 1) + 1]^{-1} \tag{3}$$

where $Z_{t,p}$ and $N_{t,p}$ denote the nuclear charge and number of non-active electrons in the target core and the projectile core respectively, and $\eta_{t,p}$ and $\xi_{t,p}$ are the screening parameters derived by Garvey *et al* (1975), depending on $N_{t,p}$ and $Z_{t,p}$. A similar model with slightly different interactions has recently been used to account for target ionisation in collisions involving structured projectiles (Reinhold and Schultz 1989). The model potentials derived by Garvey *et al* (1975) were successfully utilised within the CTMC formalism for bare projectiles by Schultz *et al* (1989).

The result accounting for electron removal from both projectile and target within the two-centre field is obtained from the combination of two three-body calculations using the independent-electron model, which includes simultaneous ionisation, charge transfer and excitation for each centre. In the first calculation, the three bodies are the projectile (C^+), target core (He^+) and target electron (e) with the appropriate model potentials (C^+-e and He^+-e). In the second, they are the projectile core (C^{2+}), projectile electron (e) and target (He^0) with the corresponding interactions (C^{2+}-e and He^0-e).

As a first test of the model, we have studied the $C^+ + He$ collision system assuming that the electrons in the K shell of C^+ do not play a significant role; i.e. only the $1s^2$ electrons of helium and the $2s^2$, 2p electrons of C^+ are considered to be active. The initial $He(1s^2)$ and $C^+(2s^2, 2p)$ configurations have been represented by microcanonical ensembles with binding energies of 0.904 au (experimental ionisation potential of He) and 1.07 au (weighted average of the Hartree–Fock orbital energies of the 2s and 2p sublevels of C^+).

The theoretical calculations are compared with non-coincident measurements of the energy and angular distributions of electrons emitted in collisions of carbon ions with helium atoms made at the Pacific Northwest Laboratory. The apparatus used for these measurements of doubly differential electron emission cross sections was first described by Criswell *et al* (1977) for the study of ionisation in collisions of low-energy protons with argon. In the present studies, a beam of singly charged carbon ions from a small tandem accelerator was collimated and passed through a gas beam target. The gas beam was produced by flowing the gas through a collimated hole structure (CMS) having channels with a length to diameter ratio of 100 to 1. A constant target density was maintained by continuously monitoring the driving pressure above the CMS by a capacitance manometer and controlling the pressure with a servo-driven valve. Electrons ejected in collisions between the carbon ions and target atoms were energy analysed by a cylindrical mirror electrostatic analyser (Toburen 1971). The analyser was collimated to approximately 10^{-4} sr and could be positioned for the measurement of electron spectra through the range of emission angles from 15 to 130°. The relative product of the solid angle and ion path length as observed by the detector was determined by analysis of the isotropic emission of Auger electrons from proton impact ionisation of the K shell of molecular nitrogen. The entire system is placed within a double-walled magnetic shield that, with the aid of a small Helmholtz coil, reduced the magnetic field in the region of the gas target and electron detector to less than about 2 mG.

Measurements of electron spectra were made at constant gas density for a range of carbon energies from 0.8 to 4.2 MeV and for emission angles from 15 to 130°, at 10° intervals for angles greater than 20°. Relative cross sections were obtained from a knowledge of the yield of electrons per unit charge of the transmitted ion beam, the transmission and detection efficiency of the electron analyser, and the relative acceptance angle of the analyser. Direct determination of absolute yields was precluded because of a lack of knowledge of the density profiles of the target gas. The relative yields obtained in these measurements were placed on an absolute scale by comparison to recent coincidence measurements in our laboratory of total cross sections for production of various target charge states in direct and transfer ionisation of helium. Measurements of single and double ionisation of helium by direct ionisation and simultaneous single and double ionisation with single electron capture are available for 25, 50 and 100 keV u^{-1} N^+ and C^+ ions. In addition, cross sections for single and double ionisation of helium were measured for simultaneous single and double electron loss from N^+ impact on helium. The latter data were used to estimate the contribution of electron loss for carbon ions as approximately 40% of the total electron yield; unfortunately the full set of partial cross sections does not yet exist for carbon ions. Thus, the integrated doubly differential cross sections have been normalised to the total yield of electrons at 100 keV u^{-1}. Based on this normalisation method, we expect the uncertainty in the accuracy of the differential cross sections to be ±35%.

In figure 1 we compare the theoretical and experimental total yield of electrons at an impact energy of 350 keV u^{-1} and ejection angles of 20° and 120°, as a function of electron energy. At 20° theory and experiment are in very good agreement whereas discrepancies can be seen in the low-energy portion of the 120° spectra. The reasons for these discrepancies could be theoretical or experimental. Regarding experiment, improper background subtraction or the nature of the electrostatic analysis (which is unreliable for electron energies below about 15 eV) could result in an overestimation of the yield of electrons. On the other hand, the CTMC method may underestimate the

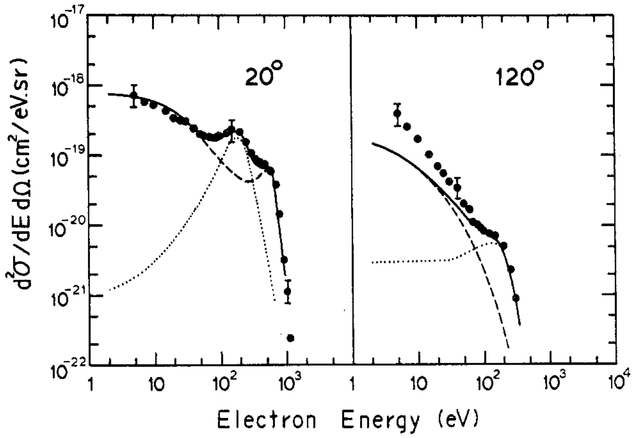

Figure 1. Doubly differential cross section for ejection of electrons in collisions of C^+ ions with He at an impact energy of 350 keV u^{-1} for ejection angles of 20°, and 120°, as a function of the electron energy. The theoretical total yield of electrons (full curve) is divided into electron emission from He (broken curve) and C^+ (dotted curve). The full circles are the present measurements of the total yield of electrons.

target electron emission spectra at large angles as has been discussed previously (e.g. Reinhold and Olson 1989). In fact, theory and experiment agree at 120° when the major contribution to the spectra consists of projectile electron emission.

Nevertheless, it should be noted that both theory and experiment predict similar structures in the electronic spectra. These features can be explained in terms of structures already known in collisions involving bare projectiles. For example, at large ejection angles (e.g. 120°) both theory and experiment display a shoulder at an electron energy of approximately $E_p = 0.5v_p^2$ au (i.e. 190 eV), v_p being the projectile velocity. Separation of the electronic spectra into projectile (C^+) and target (He) electron emission, indicates that the shoulder is due to the yield of electrons arising from C^+.

As is well known (Toburen and Wilson 1979, Kövér *et al* 1983, Schader *et al* 1984, 1986), the electronic spectrum arising from projectile ionisation displays a peak at electron energies close to E_p, almost independent of the ejection angle. This peak, or ridge, is usually referred to as the electron loss to the continuum (ELC) peak. At very small ejection angles, it is found to become a very sharp cusp-like feature. Interestingly, conservation of momentum and energy in the laboratory reference frame indicates that the backward ELC peak arises from a binary collision between projectile electrons and the target core. That is, the backward ELC peak is the well known binary peak due to projectile ionisation transformed to the target reference frame. In other words, the binary peak for electron emission from the projectile is found at backward angles in the laboratory frame, whereas for target electron emission it is found at forward angles. The backward peak was first pointed out by Wilson and Toburen (1973) and Burch *et al* (1973).

Similarly, at small ejection angles (e.g. 20°), both theory and experiment exhibit very clearly a peak as well as a shoulder at electron energies of approximately 190 and 650 eV, respectively. In this case, separation of the electronic spectra into target and projectile ionisation indicates that while the peak consists of C^+ electrons, the shoulder is composed of electron emission from He. In fact, the structure around 190 eV is the forward ELC peak which, in contrast to the backward ELC peak, is formed

not in binary collisions but arises from electron emission in soft collisions. On the other hand, the shoulder is the well known binary peak for target electron emission, which is found at an energy of approximately $E_b = 2v_p^2 \cos^2\theta - U_i$, where θ and U_i are the ejection angle and the ionisation potential, respectively.

At very small ejection angles (figure 2), another structure arising from target electron emission becomes increasingly important: i.e. the electron capture to the continuum (ECC) peak. This cusp-like feature occurs when target electrons are emitted and focused into the continuum of the projectile (Reinhold and Olson 1989). However, we note that, at an impact energy of 350 keV u^{-1}, this peak is much smaller than the ELC peak. In contrast, this situation is reversed at a smaller impact energy of 100 keV u^{-1}. Thus, our calculation of the forward electron spectra at these two impact energies confirms theoretically the recent experimental conclusions obtained by Kövér *et al* (1989) as to the changing importance of ECC and ELC according to the impact energy. In fact, since the mechanisms leading to the ECC and ELC peaks are strongly related to the electron capture and direct ionisation processes, this conclusion can be explained in terms of the dependence of the cross sections for these processes on the impact energy. That is, for low impact energies, where the capture channel is the most significant, the ECC peak should dominate. However, at higher energies, where the capture probability is negligible compared with that for ionisation, the largest portion of the forward cusp is due to ELC.

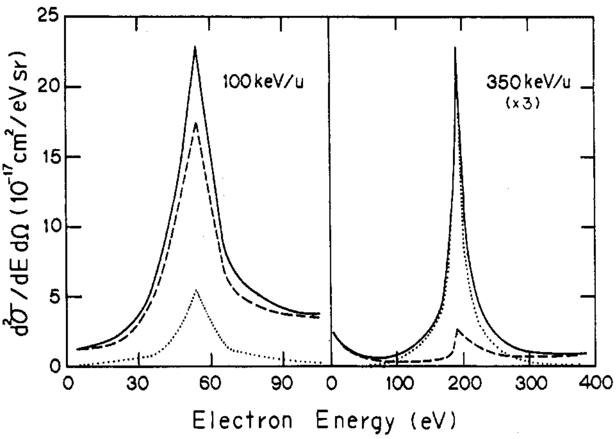

Figure 2. Doubly differential cross section for ejection of electrons in collisions of C^+ ions with He at an ejection angle of 1° for impact energies of 100 and 350 keV u^{-1}, as a function of the electron energy. The theoretical total yield of electrons (full curve) is divided into electron emission from He (broken curve) and C^+ (dotted curve), i.e. into the ECC and ELC contributions, respectively.

In summary, we have extended the CTMC two-centre formalism to treat electron removal from both projectile and target within an independent-electron approach. This treatment has been demonstrated to yield reasonable agreement with experiment as well as to provide insight into the formation of the different structures appearing in the electronic spectra. Further developments are in progress to study coincident charge-state yields within (i) the current model and (ii) a treatment explicitly including the interactions between projectile electrons and target electrons.

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