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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

Study of the dependence of the electron emission spectra on the projectile charge in H^+, $He^{2+} + He$ collisions

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

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Abstract. The classical trajectory Monte Carlo method (CTMC) has been used to calculate doubly differential ionised-electron cross sections for the impact of He^{2+} and H^+ on He at collision energies of 50 and 100 keV amu^{-1}. The results exhibit the capture to the continuum peak and agree in both shape and magnitude with experimental data. The dependence of the cross sections on the projectile charge Z_P is analysed and it is found to be very asymmetric with regard to the capture to the continuum peak. This behaviour is in agreement with very recent experimental data. Large deviations from the Z_P^2 scaling predicted by first-order theories are found at large ejection angles.

The study of the dependence of the electronic spectra produced in ion–atom collisions on the projectile charge Z_P has been the central object of recent theoretical as well as experimental works. The aim of these studies is to show the importance of both the projectile and the target Coulombic centres in the collision dynamics. At high impact energies, Stolterfoht *et al* (1987) and Fainstein *et al* (1988) have recently analysed the behaviour of doubly differential ionisation cross sections (DDCS) in collisions of multiply charged ions on He. At intermediate impact energies, Reinhold *et al* (1987) have recently studied the dependence of singly differential ionised-electron cross sections (SDCS) on the projectile charge for the case of multiply charged ions on hydrogen targets. More recently, experimental data at intermediate impact energies for collisions of H^+ and He^{2+} with He have been reported by Irby *et al* (1988) and Bernardi *et al* (1988).

The main effects reported in the papers above are that, as the projectile charge is increased, the electronic spectra exhibit an enhancement at forward angles and a reduction at backward angles with respect to first-order scalings such as the Z_P^2 law predicted by the first Born approximation for direct ionisation. As has been recently proved by Bernardi *et al* (1988), the enhancement at forward angles is due to a very asymmetric dependence of the DDCS on Z_P around the capture to the continuum (CTC) peak (Crooks and Rudd 1970). In this work, we will present theoretical evidence of this enhancement by means of the classical trajectory Monte Carlo (CTMC) method, which is a valid theoretical method to deal with ion–atom collisions in the intermediate impact energy region (Abrines and Percival 1966, Olson and Salop 1977). For this purpose, we will compare our theoretical calculations with experimental data for the ratio between the DDCS for the $He^{2+} + He$ and the $H^+ + He$ systems at impact energies of 50 and 100 keV amu^{-1}.

The details of our calculations are almost the same as those of the papers of Olson *et al* (1987) and Irby *et al* (1988). In these papers, a three-body model considering

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effective charges was used, and the DDCS were calculated from the single-ionisation channel with the independent-electron model (IEM). In the present calculations we have included, also by means of the IEM, the transfer-ionisation and double-ionisation channels in the electronic spectra. The inclusion of these channels does not appreciably change the DDCS for the $H^+ + He$ system. However, significant differences were observed for the $He^{2+} + He$ system. We have compared our ratio between the CTMC total cross sections for free-electron production for these two systems with the corresponding experimental ratios (Shah and Gilbody 1985, Gibson and Reid 1986, Rudd and Jorgensen 1963, Rudd *et al* 1966, Rudd and Madison 1976) and we have obtained differences of only 5% and 10% at impact energies of 100 and 50 keV amu^{-1}, respectively. Moreover, we have observed a very good agreement between our calculations and absolute experimental DDCS at the impact energies considered here. A detailed comparison between our results and all the available experimental data will be presented in a forthcoming paper.

The main purpose of previous papers concerning CTMS DDCS (Olson *et al* 1987, Irby *et al* 1988) has been the study of saddle-point electrons; i.e. those electrons with post-collision velocities close to $v_{\mathrm{P}}/2$, v_{P} being the projectile velocity. The study of those electrons that are captured to the continuum of the projectile (i.e. those electrons scattered at small angles with a velocity close to v_{P}) has been delayed since the statistics of the calculations were insufficient. As is well known, the DDCS exhibit a sharp peak in this region, which is called the capture to the continuum (CTC) peak (Crooks and Rudd 1970).

Figure 1 clearly shows that the CTMC approximation predicts the existence of the CTC peak. Moreover, our results are in good agreement with the experimental data of Gibson and Reid (1986). At large electron energies, the theoretical DDCS are too small in comparison with the experimental DDCS. However, new experimental data of Bernardi *et al* (1988) suggest that the data of Gibson and Reid at small angles and large electron energies are too large.

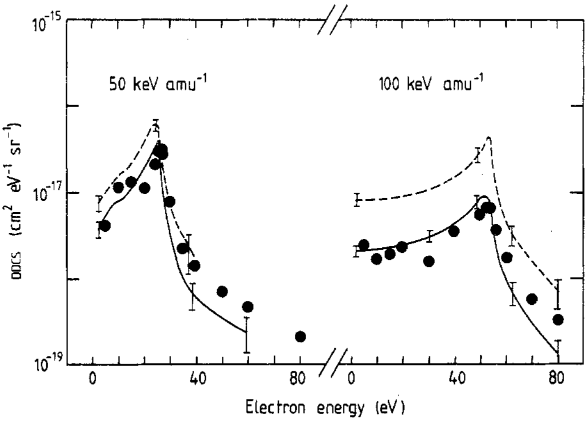

Figure 1. Present CTMC DDCS for ejection of electrons in collisions of H^+ (full curves) and He^{2+} (broken curves) projectiles with He targets at an ejection angle of one degree and impact energies of 50 and 100 keV amu^{-1}, as indicated. The results for H^+ projectiles are compared with the experimental data of Gibson and Reid (1986), denoted by full circles. The angular and energy acceptances of our calculations around the CTC peak were 2° and 2 eV, respectively. 10^6 trajectories were integrated to ensure the statistical errors shown in the figure.

Figure 2 shows our ratios between the DDCS for the $H^+ + He$ and $He^{2+} + He$ systems at 100 keV amu^{-1}. The arrows on the electron energy axis indicate the position where the electron velocity is equal to the projectile velocity v_P. We have not plotted our ratios at ejection angles smaller than 5° since the statistical errors of these ratios are too large. We compare our results with the experimental ratios of Bernardi *et al* (1988), who estimated errors of 10% for their data. There is a good agreement between our calculations and the data of Bernardi *et al*, except at 70° where our ratios are up to 50% smaller than the experimental data.

As may be clearly seen in figure 2, there is a sharp increase of the ratios at small angles and at the position where the electron velocity equals the projectile velocity. This behaviour is predicted by both the experimental data of Bernardi *et al* (1988) and our CTMC calculations. This enhancement indicates that the dependence of the DDCS on Z_P is very different on either side of the capture to the continuum (CTC) peak, and may be explained as follows. As is well known, the CTC peak is very asymmetric. The asymmetry of the peak can be explained as a Coulombic deformation produced by the target residual nucleus on the electrons that are in the continuum of the projectile. As the projectile charge is increased, the relative importance of the target residual nucleus decreases and it is expected that the CTC peak will become more symmetric (see figure 1).

As may be seen in figure 3, both theoretical calculations and experimental data also predict a sudden increase of the ratios around the CTC peak at 50 keV amu^{-1}. However, our results disagree in both shape and magnitude with the data of Bernardi *et al* (1988) (note that CTMC ratios have been multiplied by a factor of two in order to directly compare with experiment). We have not included correlation effects in our CTMC model and the impact energy of 50 kev amu^{-1} is the limit of the validity range of our calculations. However, we cannot explain the difference in the magnitude of the ratios due to the following facts. Firstly, the ratio between our calculated electron emission total cross sections for the He^{2+}, $H^+ + He$ systems is equal to 1.23, which is

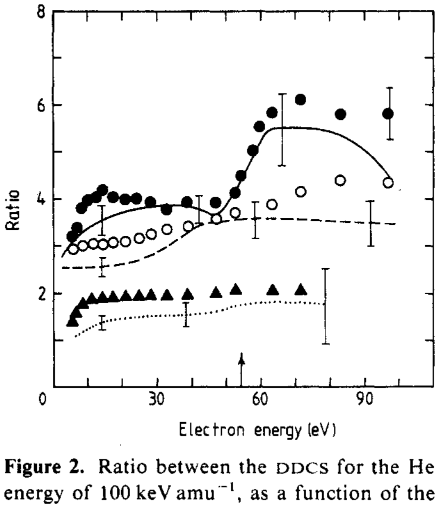

Figure 2. Ratio between the DDCS for the $He^{2+} + He$ and $H^+ + He$ systems at an impact energy of 100 keV amu^{-1}, as a function of the electron energy, for fixed electron angles. The arrow on the electron energy axis indicates the position where the electron velocity equals the projectile velocity. ●, ○, ▲: experimental data of Bernardi *et al* (1988) at ejection angles of 0°, 30° and 70°, respectively; ——, - - -, ...: present CTMC calculations at ejection angles of 5°, 30° and 70°, respectively.

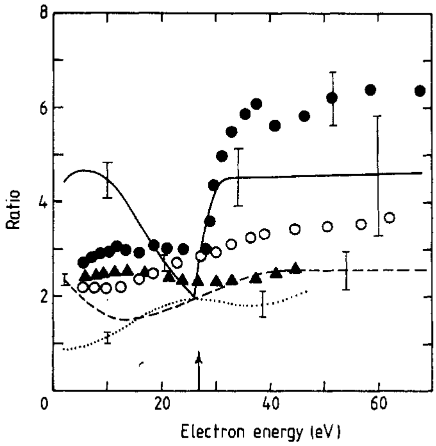

Figure 3. Ratio between the DDCS for the He^{2+} + He and H^{+} + He systems at an impact energy of 50 keV amu^{-1}, as a function of the electron energy, for fixed electron angles. The arrow on the electron energy axis indicates the position where the electron velocity equals the projectile velocity. The theoretical calculations have been multiplied by a factor of two in order to directly compare with experiment. ●, ○, ▲: experimental data of Bernardi *et al* (1988) at ejection angles of 0°, 30° and 50°, respectively; ——, - - -, ...: present CTMC calculations at ejection angles of 5°, 30° and 50°, respectively.

very similar to the mean experimental ratio 1.36 that can be obtained from the works of Shah and Gilbody (1985), Rudd and Jorgensen (1963), Rudd *et al* (1966), Rudd and Madison (1977) and Gibson and Reid (1986). Secondly, we have checked by means of the CTMC method that 85% of the total cross section at 50 keV amu^{-1} arises from electrons ejected at angles smaller than 50°. As the experimental ratios of Bernardi *et al* are always greater than two, it is expected that their ratio between total cross sections will also be greater than two. This would be very different from the mean experimental ratio 1.36 mentioned above. This conclusion contrasts with the fact that the ratios of Bernardi *et al* should be independent of any normalisation, since they were obtained under the same experimental conditions. Concerning the shape of the ratios, figure 3 shows that, while the ratios of Bernardi *et al* do not significantly change at small angles and small electron energies, the CTMC ratios decrease as the electron energy increases. We have observed that recent experimental data of Irby *et al* (1988) at 17° and an impact energy of 60 keV amu^{-1} exhibit a negative slope at small electron energies in agreement with our theoretical calculations.

Figures 2 and 3 also show that both experimental data and CTMC calculations predict large departures from first-order theories such as the first Born or the classical binary encounter approximations for direct ionisation. According to these theories, the ratio between the DDCS should be equal to four over the whole electronic spectrum. However, it may be clearly seen that the ratios depend on both the energy and the angle of the ejected electrons. We also note that the behaviour of the ratios around the CTC peak is very different from the Z_P^3 scaling (i.e. a ratio of nine) predicted by first-order theories for capture to the continuum of the projectile.

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