J. Phys. B: At. Mol. Opt. Phys. 22 (1989) L445-L449. Printed in the UK

LETTER TO THE EDITOR

Ionisation and electron transfer in $He^{2+} + H(1s)$ collisions

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Received 3 May 1989, in final form 31 May 1989

Abstract. Ionisation in collisions of alpha particles with hydrogen atoms has been investigated for impact energies lying between 2 and 900 keV amu^{-1}. The multistate semiclassical impact parameter model with a two-centre expansion in travelling atomic orbitals was employed. The computed ionisation cross sections are, in particular in the low-energy region, in good agreement with the recent experimental data of Shah *et al.* The total and partial charge transfer cross sections have also been calculated and found to be in harmony with the available theoretical and experimental data.

Cross sections for the ionisation process

$$He^{2+} + H(1s) \rightarrow He^{2+} + H^+ + e^- \tag{1}$$

in the simplest heteronuclear $He^{2+} + H(1s)$ collision system have been calculated in the impact energy range 2-900 keV amu^{-1}. This study was motivated by the discrepancies found in recent high precision measurements (Shah and Gilbody 1981, Shah *et al* 1988) of the cross section for the process (1) and the available theoretical results.

The standard semiclassical multi-state impact parameter model with an expansion in two-centre travelling atomic orbitals was employed. This basis set contained exact atomic states augmented by some bound and positive energy pseudo-states of the separated atomic species. The 22 atomic states given in table 1 of Shingal *et al* (1985) were placed on the target (hydrogen atom) centre. The He^+ ion was represented by 6s, 4p and 2d Slater-type orbitals. The parameters along with the energies are listed in table 1. The highest positive energy pseudostate for the s wave was excluded from the final calculation.

The total ionisation cross section for the process (1), computed by summing over all the partial cross sections for positive energy pseudostates, is displayed in figure 1 along with the experimental data of Shah and Gilbody (1981) and Shah *et al* (1988). In general, our calculated ionisation cross sections are in harmony with the experimental data over the energy range displayed. At higher impact energies, our computed ionisation cross section falls below the experimental data. Similar underestimation of the ionisation cross section in the corresponding energy region had been observed in p-H collisions using similar basis expansions (Fritsch and Lin 1983). In this energy region direct ionisation is dominant and pseudostates with higher partial waves such as f and g orbitals should be included in the basis expansion. We note that comparison with other high energy theories has already been made by Shah *et al* (1988).

Our major interest in ionisation cross sections is for the energy region below 40 keV amu^{-1}. In this region, we also show the 34-state triple-centre atomic-orbital

0953-4075/89/150445+05$02.50

Table 1. Parameters of the basis functions ϕ_i (for notation see equation (8) of Shingal *et al* (1985)).

j	p_j	λ_j	Level i	Eigenergies E_i
(a) $l=0$				
1	0	2.000	1s	−2.00
2	0	1.000	2s	−0.50
3	1	1.000	3s	−0.215
4	2	1.155	4s	0.077
5	2	1.666	5s	1.144
6	2	1.375	6s	8.44
(b) $l=1$				
1	1	1.000	2p	−0.50
2	2	1.155	3p	−0.20
3	1	1.666	4p	0.236
4	2	1.375	5p	2.417
(c) $l=2$				
1	2	1.666	3d	−0.222
2	2	1.275	4d	0.137

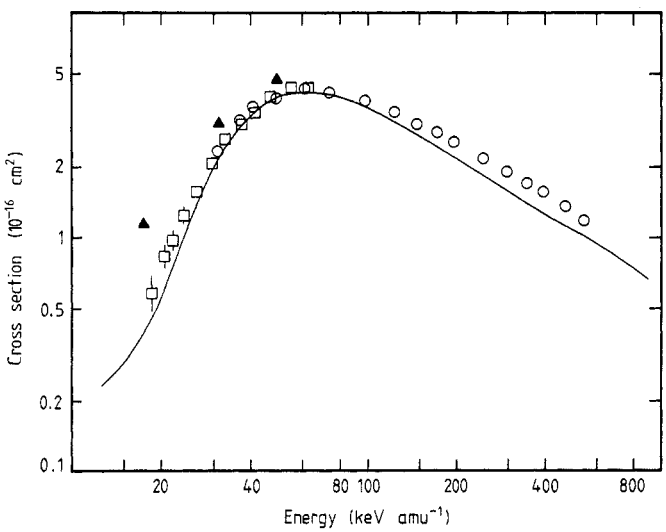

Figure 1. Cross sections for ionisation in $He^{2+}+H(1s)$ collisions. Experiment: □, Shah *et al* (1988); ○, Shah and Gilbody (1981). Theory: ——, present results; ▲, Winter (1988).

expansion results of Winter (1988). In his calculation, in addition to the $n=1$-3 atomic orbitals of the projectile and the $n=1$-2 atomic orbitals of the target, there are twenty atomic states at the third centre which is chosen to be the equiforce point (or the saddle point) of the two nuclei. The states at the third centre are the $n=1$-4 atomic states of the united atom ($Z=3$). These third-centre states are to represent ionisation at the end of the collision (Antal *et al* 1975, Winter and Lin 1984). In contrast to the direct ionisation and electron capture to the continuum, the ionisation at the third centre has been called saddle-point ionisation.

In the present two-centre calculation, all the ionisation is represented by the pseudostates at the two centres. There is no account for the saddle-point ionisation directly. In contrast, in Winter's calculation, all the ionisation is from the saddle point and there is no account for direct ionisation and for capture to the continuum. Of course one recognises that the distinction of the three 'ionisation mechanisms' is not well defined. In the present problem the saddle point is not at the midpoint of the internuclear axis as in $H^+ + H$, instead, it is one third of the way from the target (H centre). One can argue that with the pseudostates used by Winter it is difficult to represent capture to the continuum since the saddle point is far from the projectile centre. On the other hand, in the present two-centre expansion, the saddle point is quite close to the target and part of the effect of the saddle point can be represented by orbitals at the target. The other *possible* limitation of Winter's calculation is due to the orbitals placed on the third centre. From the MO correlation diagram of $(HeH)^{2+}$ (see figure 1 of Winter and Hatton 1980), it is expected that the $3d\sigma$-$3d\pi$ and $3d\pi$-$3d\delta$ rotational couplings are to play an important role in the 'promotion' of the electron to the excited and continuum states. The pseudostates placed on the third centre have a maximum value of $n = 4$, which is probably not adequate. It would be desirable to include more diffuse pseudostates at the third centre. Similarly, the $n = 1$ and $n = 2$ states at the third centre are not expected to be important and can probably be dropped in the basis set.

As a 'byproduct' of the present investigation we also calculated partial and total capture cross sections in the energy region studied. In figure 2, we compare our calculated partial capture cross sections with 2s, 2p, 3p and (3s+3d) states of the projectile with experiments. The 3s and 3d states are considered together since they cannot be distinguished in photon measurements (Ciric *et al* 1985). We also compare the results with the data of Shah and Gilbody (1978) for impact energies in the range 2-10 keV amu^{-1}. We note that there is, in general, a good agreement with the experimental data. Furthermore, these cross sections are also in reasonable accord with the

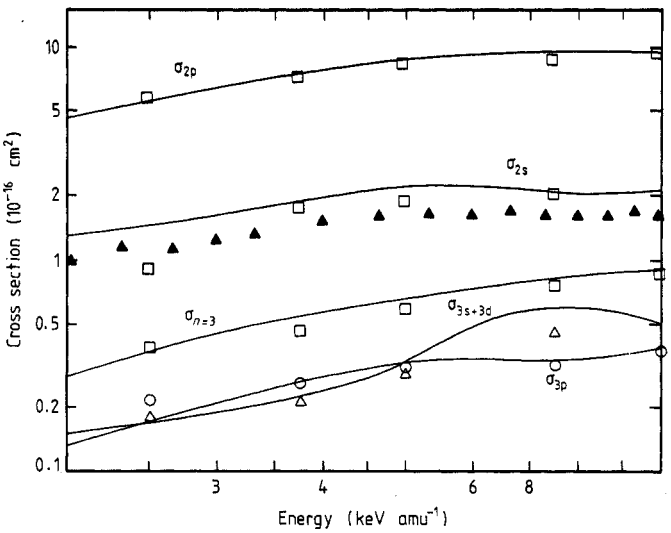

Figure 2. Partial cross section for capture to the $He^+(nl)$ state in $He^{2+} + H(1s)$ collisions. Experiment: □, ○, △, Ciric *et al* (1988); ▲, Shah and Gilbody (1978). Theory: ——, present results.

recent calculation of Fritsch (1988) who employed the exact $n = 1$-7 atomic states on the projectile. Thus, the cross section for electron transfer in the $He^{2+} + H(1s)$ collision seems to be independent of the choice of pseudostates and even a limited basis set on the projectile centre is sufficient to predict the $n = 2$ and $n = 3$ partial electron capture cross section. As a further illustration, in figure 3 we show that our calculated $He^{+}(2s)$ and total charge transfer cross section are also in agreement with experimental data from different groups in the energy range considered.

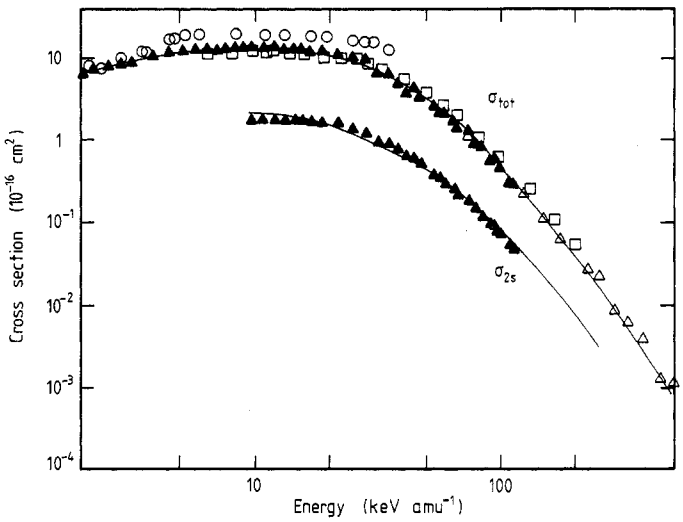

Figure 3. $He^{2+}(2s)$ and total capture cross section in $He^{2+} + H(1s)$ collisions. Experiment: ○, Bayfield and Khayrallah (1975); □, Olson *et al* (1977); ▲, Shah and Gilbody (1978); △, Hvelplund and Anderson (1982). Theory: ——, present results.

In summary, cross sections for ionisation and for partial and total charge transfer in $He^{2+} + H(1s)$ collisions have been calculated using two-centre atomic-orbital expansions including pseudostates for projectile energies from 2-900 keV amu^{-1}. From the good agreement between the calculated cross section and experimental data we conclude that the standard two-centre close-coupling calculations are adequate in describing the processes investigated.

This work is supported by the Division of Chemical Sciences, Office of Basic Energy Sciences, Office of Energy Research, US Department of Energy.

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