J. Phys. B: At. Mol. Opt. Phys. **23** (1990) 1203-1214. Printed in the UK

Neutralisation in $H^+ + H^-$ and ion pair production in H + H collisions

R Shingal† and B H Bransden

Physics Department, The University, Durham DH1 3LE, UK

Received 18 August 1989, in final form 13 November 1989

Abstract. Coupled-channel calculations are reported for neutralisation in $H^+ + H^-$ collisions and for ion pair production in H + H(1s) and H + H(2s) collisions for impact energies in a range from 0.15 to 50 keV, using a 23-state basis on each heavy particle. The results are compared with earlier calculations and with the available experimental measurements and, in particular, very good agreement is obtained with the most recent experimental data for neutralisation.

1. Introduction

The work reported in this paper is part of a project to carry out *ab initio* calculations of cross sections for collision processes in the two-electron-two-proton system, at low to intermediate impact energies. The semiclassical impact parameter method with rectilinear trajectories is employed (see, for example, Bransden 1983), using a two-centre expansion of travelling atomic orbitals, containing both real and pseudostates. Our first calculations (Shingal *et al* 1985, Shingal and Bransden 1987) were concerned with the neutralisation reaction

$$H^+ + H^- \rightarrow H + H. \tag{1}$$

Exchange effects were omitted, with the result that calculations were reported only for impact energies above 8 keV, where electron exchange was considered to have a small influence. In our more recent work, the wavefunction has been fully antisymmetrised in the electronic (space + spin) coordinates so exchange effects are fully included. It has been discovered that exchange is more important at higher energies than was previously estimated, so that in this paper new results are reported for the energy interval above 8 keV, in addition to extending the calculations to lower energies. The complete model, including full allowance for electron exchange and using plane wave translational factors has already been applied to excitation and ionisation in collisions between ground-state hydrogen atoms

$$H(1s) + H(1s) \rightarrow H(1s) + H(nl) \tag{2}$$

$$H(1s) + H(1s) \rightarrow H(1s) + H^+ + e^-. \tag{3}$$

† Present address: J R MacDonald Laboratory, Physics Department, Cardwell Hall, Kansas State University, Manhattan, Kansas 66506, USA.

0953-4075/90/071203+12$03.50

The calculated cross sections for the reactions (2) and (3) have been reported and discussed in a recent paper by Shingal *et al* (1989). In this paper, our results are given for the neutralisation reaction (1), in the impact energy interval between 150 eV and 50 keV. Some results are also given for the cross sections for double charge exchange

$$H_A^+ + H_B^- \rightarrow H_A^- + H_B^+. \tag{4}$$

In (4), the subscripts A and B label the two protons, which of course are distinguishable since the heavy particle motion is effectively classical.

Using the same theoretical model, cross sections for the H^- formation reactions

$$H(1s) + H(1s) \rightarrow H^+ + H^- \tag{5}$$

$$H_A(1s) + H_B(2s) \rightarrow H_A^+ + H_B^- \tag{6}$$

$$\rightarrow H_A^- + H_B^+ \tag{7}$$

have been computed for the same energy interval 150 eV to 50 keV. In these processes, it is important to emphasise the difference in mechanism between the neutralisation reaction (1) and the formation cross sections (6) and (7) on the one hand, and the formation reaction (5) on the other. The neutralisation reaction is dominated by transitions to the H(1s) + H ($n = 2$) and H(1s) + H ($n = 3$) configurations (Bates and Lewis 1955). These couplings are strong and occur through crossings at $R \simeq 12$ au ($n = 2$) and $R \simeq 36$ au ($n = 3$) and also through a broader coupling region ($n = 3$) between 15 and 20 au (Sidis *et al* 1983). It should therefore be relatively easy to calculate accurate cross sections for neutralisation and for the formation cross sections (6) and (7), provided the $n = 2$ and $n = 3$ hydrogenic states are represented in the trial wavefunction, and an H^- wavefunction is employed which is accurate at large distances. In contrast, the coupling between the H(1s) + H(1s) channels and the $H^+ + H^-$ channel is weak and is short range in nature. It follows that the calculation of accurate cross sections for the formation cross section (5) and for the double charge exchange cross sections (4) will require a much larger basis set than for neutralisation, and convergence may be more difficult to achieve.

2. Theory

The theoretical model has been described earlier (Shingal *et al* 1985) and only brief details are given here for convenience. We are concerned with the solution of the time-dependent Schrödinger equation†

$$\left(-\tfrac{1}{2}\nabla_1^2 - \tfrac{1}{2}\nabla_2^2 - \frac{1}{r_{1A}} - \frac{1}{r_{2A}} - \frac{1}{r_{1B}} - \frac{1}{r_{2B}} + \frac{1}{r_{12}} - i\frac{\partial}{\partial t}\right)\Psi(\boldsymbol{b}, \boldsymbol{r}_1, \boldsymbol{r}_2 t) = 0 \tag{8}$$

where A and B label the two protons, 1 and 2 label the two electrons and $\boldsymbol{r}_1$, $\boldsymbol{r}_2$ are the position vectors of the electrons with respect to the mid-point of the internuclear line AB. For the reactions considered in this paper, only the $S = 0$ singlet state is concerned, so that a solution of (8) is required which is symmetrical in the spatial coordinates. The trial function divides into terms Ψ^+ and Ψ^- corresponding to states of gerade and ungerade symmetry respectively, and can be written in the form

$$\Psi^{\pm}_{\text{trial}}(\boldsymbol{b}, \boldsymbol{r}_1, \boldsymbol{r}_2, t) = (1 + P_{12})[\Phi^{\pm}(\boldsymbol{b}, \boldsymbol{r}_1, \boldsymbol{r}_2, t) \pm \Phi^{\pm}(\boldsymbol{b}, -\boldsymbol{r}_1, -\boldsymbol{r}_2, t)] \tag{9}$$

† Atomic units are used here and throughout.

where P_{12} is the spatial exchange operator which interchanges $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$. The functions $\Phi^{\pm}$ are expressed as two-centre travelling orbitals

$$\Phi^{\pm}(\boldsymbol{b}, \boldsymbol{r}_1, \boldsymbol{r}_2, t) = A_1^{\pm}(\boldsymbol{b}, t)\chi_1(\boldsymbol{r}_{B1}, \boldsymbol{r}_{B2}) \exp(-i\varepsilon_1 t + i\gamma(\boldsymbol{r}_1, \boldsymbol{r}_2)) + \sum_{i>1}^{m} A_i^{\pm}(\boldsymbol{b}, t)\phi_{1s}(\boldsymbol{r}_{B1})\phi_i(\boldsymbol{r}_{A2}) \exp(-i\varepsilon_i t + \bar{\gamma}(\boldsymbol{r}_1, \boldsymbol{r}_2)). \quad (10)$$

The function χ_1 is the wavefunction of the H^- ion while the functions ϕ_i are hydrogenic orbitals or pseudostate orbitals corresponding to internal energies ε_i. The factors γ and $\bar{\gamma}$ which ensure translational invariance are

$$\gamma(\boldsymbol{r}_1, \boldsymbol{r}_2) = \tfrac{1}{2}\boldsymbol{v} \cdot (\boldsymbol{r}_1 + \boldsymbol{r}_2) - \tfrac{1}{4}v^2 t \quad (11)$$

$$\bar{\gamma}(\boldsymbol{r}_1, \boldsymbol{r}_2) = \tfrac{1}{2}\boldsymbol{v} \cdot (\boldsymbol{r}_1 - \boldsymbol{r}_2) - \tfrac{1}{4}v^2 t. \quad (12)$$

The amplitudes $A_i^{\pm}(\boldsymbol{b}, t)$ satisfy coupled first-order differential equations of the usual form (Bransden 1983) and the cross sections are calculated from the asymptotic values $A_i^{\pm}(b, \infty)$ by integrating over the two-dimensional impact parameter space.

The wavefunction employed for the H^- ion has been described in Shingal and Bransden (1987) and includes both radial and angular correlations. The set of states and pseudostates consisted of the exact $n = 1$, 2 and 3 hydrogenic orbitals together with three s, three p and a single d pseudostate on one centre, together with a 1s hydrogen state on the other centre, 22 states in all. Parameters for the pseudostate set are given in table 1 of Shingal *et al* (1985). Two of the s and two of the p pseudostates together with the d pseudostate have positive energies and so allowance is made for coupling to the continuum. Indeed, for energies less than ~20 keV, the calculated ionisation cross section in the reaction $H(1s) + H(1s) \rightarrow H(1s) + H^+ + e^-$ agrees well with experiment (Shingal *et al* 1989). This set is, however, not large enough for the calculation of *detachment* which requires, in addition, positive energy pseudostates of the $H^-(nl, 1s)$ in which both electrons are centred on the same nucleus. The use of this basis set does not allow the calculation of cross sections for final channels containing excited atoms on both centres simultaneously, but these are not expected to be important at low energies because the covalent potential curve associated with $H(n \geq 2) + H(n \geq 2)$ does not cross the Coulombic curve for $H^+ + H^-$. In fact, applications of the CDW method (Moore and Banyard 1978) suggest that these channels do not contribute greatly to the total neutralisation cross section, even at high energies.

In all, 46 terms occur in the trial function which, using the gerade and ungerade symmetry, give rise to two sets of 23 coupled equations. The numerical methods employed to calculate the interaction and overlap matrices developed by one of us (RS) have been based on a two-dimensional numerical integration scheme employing prolate spheroidal coordinates. The computations were carried out on a CRAY-XMP at the Rutherford Appleton Laboratory's Atlas Centre.

3. Results and discussion

3.1. Neutralisation

Our calculated neutralisation cross sections are shown in tables 1, 2 and 3. At low energies the most important process is the capture of an electron into the $n = 2$ or $n = 3$ levels of the projectile, leaving the target in the ground state (table 1). At higher energies capture into the ground state by the projectile, leaving the target in the $n = 2$

Table 1. Calculated cross section for the reaction $H_A^+ + H_B^- \rightarrow H_A(nl) + H_B(1s)$ in units of 10^{-16} cm^2. The total cross section includes contribution from bound pseudostates.

E_{lab} (keV)	$\sigma_{H(1s)}$	$\sigma_{H(2s)}$	$\sigma_{H(2p)}$	$\sigma_{H(3s)}$	$\sigma_{H(3p)}$	$\sigma_{H(3d)}$	σ_{tot}
0.15	0.09	13.28	35.39	5.69	14.56	18.56	88.44
0.20	0.04	16.60	43.18	5.19	15.15	21.34	101.99
0.25	0.06	20.40	47.02	4.78	14.40	21.47	108.61
0.30	0.02	24.90	47.98	5.06	14.50	23.31	116.27
0.43	0.03	29.17	47.97	4.48	14.46	25.53	122.40
0.50	0.04	29.08	47.52	4.19	14.59	27.58	123.86
0.64	0.07	27.82	48.17	4.12	14.21	31.39	127.03
0.80	0.04	25.49	47.27	3.83	13.26	33.83	125.38
1.00	0.05	22.97	47.07	3.63	11.93	35.62	123.36
2.00	0.04	13.63	34.58	2.22	8.94	28.79	91.16
3.00	0.17	8.07	23.83	1.76	6.31	20.39	63.73
4.00	0.20	5.40	16.75	1.54	4.29	14.60	45.39
5.00	0.15	3.85	12.58	1.02	3.15	10.64	33.34
6.00	0.12	2.77	10.28	0.91	2.54	7.64	25.92
8.00	0.10	1.59	6.96	0.52	1.78	4.02	16.14
9.00	0.10	1.14	5.91	0.41	1.53	3.00	13.11
13.00	0.11	0.37	3.10	0.17	0.91	1.01	6.22
18.00	0.12	0.12	1.27	0.09	0.46	0.30	2.64
20.00	0.12	0.10	0.92	0.07	0.34	0.20	1.97
23.00	0.11	0.09	0.60	0.06	0.23	0.12	1.36
24.00	0.10	0.10	0.55	0.05	0.21	0.10	1.26
50.00	0.03	0.03	0.05	0.01	0.02	0.005	0.16

or $n = 3$ levels becomes increasingly important; the cross section for the two processes becoming approximately equal by an impact energy of 20 keV. The total cross sections shown in tables 1, 2 and 3 and figures 1 and 2 contain an allowance for capture into bound states with $n > 3$, obtained by adding the cross sections for populating the pseudostates of negative energy to those for $n \leqslant 3$. At low energies this correction is small but rises to ~8% at 9 keV and 12% at 24 keV.

The neutralisation cross section has been measured at laboratory impact energies between 60 eV and 4 keV by Peart *et al* (1985), between 5 eV and 4 keV by Szucs *et al* (1984), and between 2 keV and 80 keV by Schön *et al* (1987). The three sets of measurements are consistent but differ considerably from the earlier data of Rundel *et al* (1969), Moseley *et al* (1970), Gaily and Harrison (1970) and Peart *et al* (1976a). In figures 1 and 2 our calculated cross sections are compared with the more recent data.

In figure 1, curves are drawn illustrative of the data of Szucs *et al* (1984) and Peart *et al* (1985). In the former case the dispersion of the results is from ±16% at low energy to ±7.5% at high energy, while in the latter the systematic error was estimated at better than ±10%, with somewhat smaller statistical errors. Taking these errors into account, it is seen that the present results are completely consistent with the data of Peart *et al* (1985) below 2 keV, above which the calculated curve falls below the experimental curve. The data of Szucs *et al* (1984) lie slightly higher except below 0.4 keV where they agree closely with the present calculations and the data of Peart *et al* (1985). Also included in figure 1 are the data of Schön *et al* (1987) at 2.8 and 3.0 keV which are consistent with the present calculations. The data of Schön *et al* extend to 80 keV and this is shown in figure 2, where it is seen that the present calculated

Table 2. Calculated cross section for the reaction $H_A^+ + H_B^- \rightarrow H_A(1s) + H_B(nl)$ in units of 10^{-16} cm^2. The cross section for $nl = 1s$ is excluded in this table as it already appears in table 1. The total cross section includes contribution from bound pseudostates.

E_{lab} (keV)	$\sigma_{H(2s)}$	$\sigma_{H(2p)}$	$\sigma_{H(3s)}$	$\sigma_{H(3p)}$	$\sigma_{H(3d)}$	σ_{tot}
0.15	3.27	5.30	0.22	0.76	5.97	16.12
0.20	2.83	4.51	0.31	0.55	4.71	13.49
0.25	1.19	3.63	0.28	0.41	4.30	10.34
0.30	1.03	3.67	0.38	0.42	3.95	9.99
0.43	1.92	3.48	0.24	1.08	2.50	9.68
0.50	1.31	2.73	0.27	1.25	1.75	7.80
0.64	0.89	1.50	0.18	0.98	1.39	5.56
0.80	0.82	1.13	0.24	1.37	1.54	5.58
1.00	0.58	1.39	0.10	0.93	1.90	5.40
2.00	0.74	1.73	0.17	0.35	0.66	3.99
3.00	0.56	1.06	0.12	0.29	0.79	3.21
4.00	0.49	0.61	0.11	0.27	0.69	2.54
5.00	0.39	1.12	0.12	0.26	0.48	2.69
6.00	0.56	0.80	0.13	0.20	0.40	2.39
8.00	0.65	0.99	0.07	0.11	0.27	2.32
9.00	0.75	0.97	0.057	0.089	0.21	2.26
13.00	1.06	0.70	0.025	0.049	0.14	2.11
18.00	1.25	0.50	0.009	0.053	0.09	2.03
20.00	1.17	0.41	0.007	0.052	0.08	1.86
23.00	1.03	0.29	0.005	0.046	0.06	1.56
24.00	1.00	0.25	0.006	0.042	0.05	1.47
50.00	0.27	0.013	0.002	0.003	0.002	0.32

Table 3. Calculated total neutralisation cross section in collisions of protons with negative hydrogen ions in units of 10^{-16} cm^2. The total cross section includes contribution from bound pseudostates and is obtained by adding total cross sections for the configurations $H_A(1s) + H_B(nl)$ and $H_A(nl) + H_B(1s)$.

E_{lab} (keV)	σ_{tot}	E_{lab} (keV)	σ_{tot}
0.15	104.56	4.00	47.93
0.20	115.48	5.00	36.03
0.25	118.95	6.00	28.30
0.30	126.26	8.00	18.46
0.43	132.07	9.00	15.37
0.50	131.65	13.00	8.33
0.64	132.58	18.00	4.67
0.80	130.96	20.00	3.82
1.00	128.76	23.00	2.92
2.00	95.15	24.00	2.73
3.00	66.94	50.00	0.48

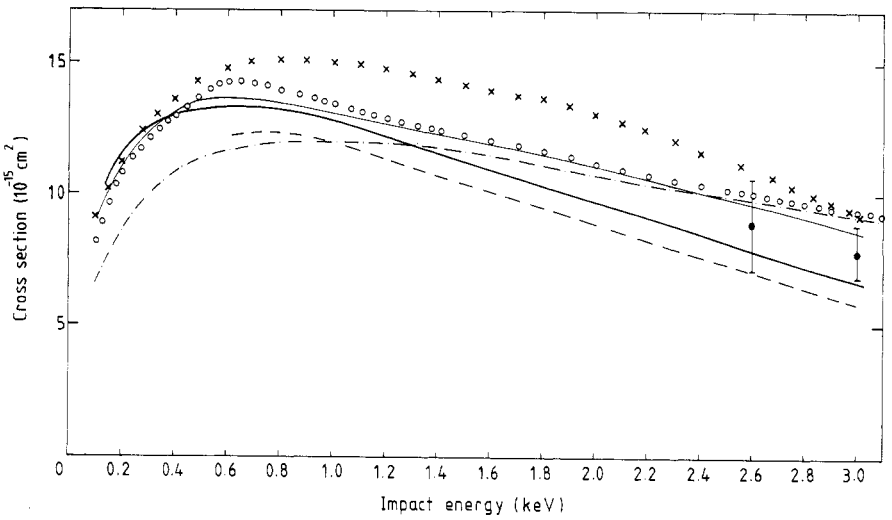

Figure 1. The cross section for neutralisation in the reaction $H^+ + H^- \rightarrow H + H$ at energies between 0.15 and 3 keV. ×××, curve illustrative of the data of Szucs *et al* (1984); ——, curve illustrative of the data of Peart *et al* (1985); ●, experimental data of Schön *et al* (1987); ——, present calculated cross section (two-electron model); — · —, calculated cross section of Borondo *et al* (1981, 1983) (two-electron model); ○○○, calculated cross section of Sidis *et al* (1981, 1983) (one-electron model); - - -, calculated cross section of Ermolaev (1988) (one-electron model).

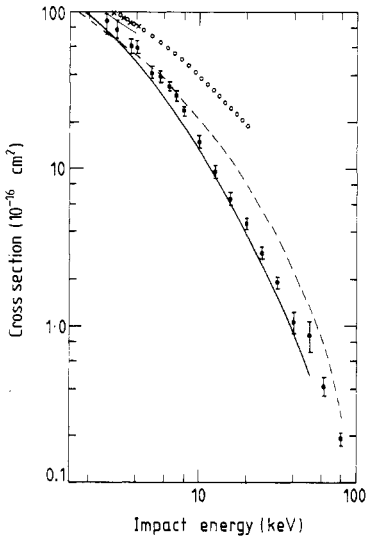

Figure 2. The cross section for neutralisation in the reaction $H^+ + H^- \rightarrow H + H$ at energies between 2 and 80 keV. Symbols as for figure 1.

cross sections, which extend to 50 keV, are slightly smaller than those measured. This may be because of the omission of final channels in which both the hydrogen atoms produced are in an excited state. However it can be stated that the general agreement with both the shape and magnitude of the cross section in the whole energy interval from 0.15 to 50 keV is very good.

The only other calculations treating the neutralisation reaction in a two-electron formulation are those of Borondo *et al* (1981, 1983) and our own earlier work—Shingal *et al* (1985). Shingal and Bransden (1987). Borondo *et al* employed a 12-state molecular orbital basis with no translational factors. The calculated cross sections included in figure 1 are somewhat too small at energies less than 1 keV, and while at higher energies up to 3 keV the agreement with the data is good, the lack of translational factors will limit the accuracy of the model at the higher energies. In an earlier work, which concerned the energy interval 8–50 keV, electron exchange was omitted. The new cross sections are slightly smaller than the old ones at the lower energies but slightly higher at the higher energies, for example the new (old) neutralisation cross sections are 18(26) at 8 keV and 0.5 (0.4) at 50 keV, in units of 10^{-16} cm^2.

Also included in figures 1 and 2 are the calculated cross sections of Sidis *et al* (1981, 1983) and of Ermolaev (1988). Both these calculations were based on a one-electron model, in the case of Sidis *et al* using a molecular orbital basis employing a common translational factor of the type introduced by Schneiderman and Russek (1969) and in the case of Ermolaev using a very large atomic pseudostate basis including plane wave translational factors. Both calculations agree with the low energy data but above ~4 keV, the calculated cross section of Sidis *et al* becomes too large, exceeding the data at 20 keV by more than a factor of two. This may be due to the use of a common translational factor, which does not lead naturally to the steep decrease in the exchange cross sections observed as the impact velocity increases (Hanssen *et al* 1984, Newby 1985).

A very full and interesting discussion of the one-electron approach has been given by Ermolaev (1988). In particular he has pointed out the difficulty in the full two-electron treatment of employing a large enough basis to examine detachment, and the effect of the detachment continuum on other cross sections. In contrast, a large basis to represent the continuum is comparatively easy to use within the one-electron model, which however has other difficulties.

3.2. Double charge exchange

As a byproduct of the calculation of neutralisation cross sections, the cross section (4) for double charge exchange is obtained. This cross section is almost two orders of magnitude smaller than that for neutralisation, and clearly depends strongly on correlation between the two electrons. For this reason accurate cross sections are difficult to calculate, and indeed a simple Landau-Zener approach (Brouillard *et al* 1979) leads to cross sections an order of magnitude greater than the experimental data. Measurements have been made by Peart and Forrest (1979) for impact energies between 0.088 and 1.14 keV, and by Brouillard *et al* (1979) between 0.06 and 0.4 keV. The data exhibit considerable structure at the lower energies. Between 0.15 and 1 keV comparison can be made with our calculated cross section and this is shown in figure 3. It is seen that although the calculated cross section is of the correct order of magnitude no detailed agreement is obtained. As already stated, for our main purpose of calculating neutralisation it was not considered necessary to employ basis states for which two electrons

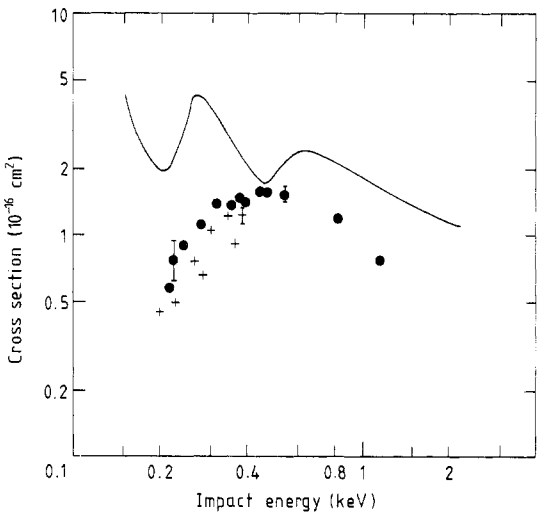

Figure 3. The cross section for double charge exchange in the reaction $H^+ + H^- \rightarrow H^- + H^+$. +++, Brouillard *et al* (1979); •••, Peart and Forrest (1979); ——, present calculated cross section.

are centred on each heavy particle, except for the H^- ground state, however such states are evidently necessary for accurate calculation of double charge exchange, detachment and the cross section for the formation of H^- in collisions of two ground-state hydrogen atoms. Specifically one would like to include states centred on A of the form $\phi_{1s}(r_{A1})\phi_i(r_{A2})$, with the appropriate phase factors, where the ϕ_i are positive energy pseudostates. These states, and similar states centred on B, would represent the continuum states of H^- of the form $H(1s)+e^-$ which is the dominant detachment channel.

3.3. Formation of H^-

As noted earlier, the formation cross sections for H^- in the $H(1s)+H(2s)$ collision are dominated by a curve crossing near $R = 12$ au between the $H^+ + H^-$ potential curve and the $H(1s)+H(n=2)$ curves. This is a strong process, and the cross sections may be expected to be given accurately by our theoretical model. By time reversal invariance, the formation cross sections in the singlet state are just those listed for neutralisation with a final $H(2s)+H(1s)$ state in tables 1 and 2. For comparison with experiments, which have been performed with unpolarised beams, the cross sections required are one-quarter of those listed in the tables.

In figure 4, our calculated cross sections are shown compared with the data of Fussen *et al* (1982) and the theoretical predictions of Sidis *et al* (1983) for reaction (7) and with the data of Hill *et al* (1979) for reaction (6). For reaction (7) the agreement with the data of Fussen *et al* is very good. The theoretical cross section of Sidis *et al* (1983) is in harmony with our own for energies below about 2 keV, but decreases more slowly with increasing energy.

For reaction (6) the calculated cross section is larger than the data of Hill *et al* by up to 40%. The data of Hill *et al* only extend down to an energy of ~5 keV, but at much lower energies (160–800 eV) Claeys *et al* (1977) have investigated this reaction

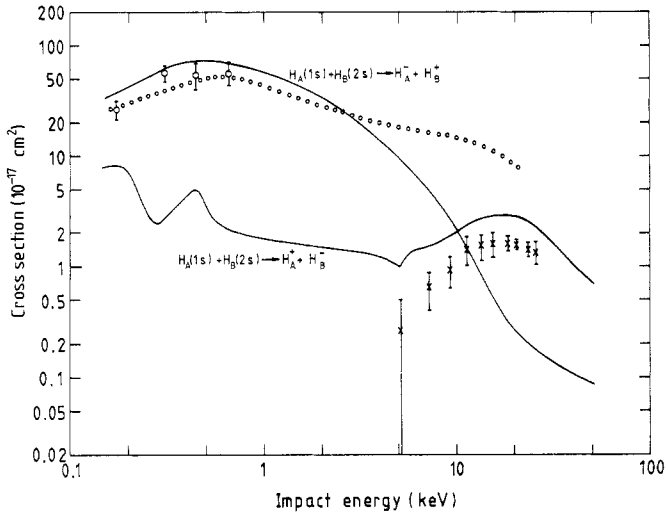

Figure 4. Formation cross sections for H^- from the H(1s) + H(2s) channel. ——, present calculated cross sections; ∘∘∘, calculated cross section of Sidis *et al* (1981, 1983) (one-electron model); ⊽, data of Fussen *et al* (1982); ⊼, data of Hill *et al* (1979).

experimentally and predict that the cross section has an upper limit of 2.8×10^{-17} cm^2. This value is in fact not far from the average of the calculated cross section in this energy region. Further experimental and theoretical investigation is required.

Because the cross section for the formation reaction $H_A(1s) + H_B(1s) \rightarrow H_A^+ + H_B^-$ is small and the initial and final levels are far apart in energy, it is expected that the cross section will be sensitive to the size of the basis, and as the impact energy increases a good representation of the continuum by the included pseudostates will be necessary. In the one-electron model Ermolaev (1988) has examined the convergence of the detachment and neutralisation cross sections and has shown that the inverse cross section $H_A^+ + H_B^- \rightarrow H_A(1s) + H_B(1s)$ (which is related to the formation cross section by time reversal invariance) was particularly sensitive to an increase of basis from 29 terms to 36 terms for impact energies in excess of ~10 keV. For this reason, with the particular basis employed in the present work, which was designed to give a good account of the most important neutralisation channels, we believe that meaningful cross sections can only be computed for impact energies less than ~5 to 10 keV.

In figure 5, we show our calculated formation cross sections up to $E = 10$ keV, compared with the experimental data of Gealy and van Zyl (1987), Hill *et al* (1979) and McClure (1968). The calculated cross section is of the correct order of magnitude in the interval 0.2 to 4 keV, but shows oscillations which are not present in the experimental data, while above 4 keV the calculated cross section becomes too small. Also shown are the results of a MO basis calculation, including translational factors, by Borondo *et al* (1987), which appears to decrease at low energies much too rapidly. Recently Hahn and Dalgarno (1989) have made a very interesting estimate of the cross section by making a closure evaluation of the Green function occurring in the exact T-matrix element. The results depend on an energy parameter, and for one value adopted ($\Delta E = 1.5$) the calculated curve gives a reasonable representation of the data, showing in particular the relatively flat behaviour below 1 keV. Hahn and Dalgarno

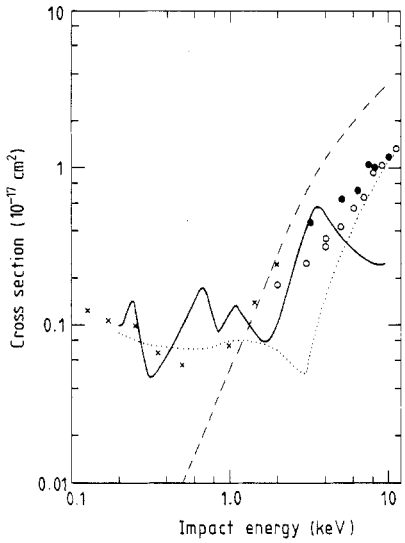

Figure 5. Formation cross section for H^- from the H(1s) + H(1s) channel. •••, experimental data of McClure (1968); ∘∘∘, experimental data of Hill *et al* (1979); ×××, experimental data of Gealy and van Zyl (1987); ——, present calculated cross section; - - -, calculated cross section of Borondo *et al* (1987); ·····, calculated cross section of Hahn and Dalgarno (1989) with $\Delta E = 1.5$ au.

obtained evidence that intermediate continuum states are important for this reaction. Such states are represented in our basis, and as we remarked earlier, the calculated ionisation cross section from the H(1s) + H(1s) channel agrees well with experiment for $E \leqslant 20$ keV. However it is likely that a more complete representation will be necessary for an accurate coupled-channel calculation of the small formation cross sections, in particular by adding the term representing continuum states of H^-, which are missing from the present basis. Qualitatively, the present calculations support a mean value of the cross section of about 10^{-18} cm^2 in the energy interval 0.1 to 1 keV, in harmony with the data. However since this cross section is very small compared with the cross sections for the major reaction paths, it will not be determined to high accuracy. For this reason, although the cross section may well oscillate as a function of energy, too much reliance should not be placed on the particular oscillations shown in the figure.

4. Conclusion

The present coupled-channel calculations include a proper treatment of both exchange and translational invariance, and employ a 23-state basis on each heavy particle. This model provides a good description of the neutralisation reaction (9), and the formation reactions (6) and (7), as reported in this paper, and the excitation and ionisation reactions (2) and (3) as reported earlier (Shingal *et al* 1989). The attempt to calculate double charge exchange and the formation of H^- from the H(1s) + H(1s) channel is less successful, and the detachment cross section

$$H^+ + H^- \rightarrow H^+ + H(1s) + e^-$$

cannot be calculated at present, because the basis does not contain a description of the continuum H^- state.

Although Ermolaev (1988) has shown that detachment can be calculated very successfully within a one-electron model, for such a fundamental system, it is important to extend the two-electron calculation to this process, and to improve the description of double charge exchange and formation. This will require the additional terms in the basis set. This must be carefully chosen so as to give an economical description of the parts of the continuum which are under-represented at present. For example, Sidis *et al* (1981, 1984) and subsequently Fussen and Claeys (1984), showed that within a single electron model a *single* pseudostate could be devised to represent the detachment channel. In the calculation of Fussen and Claeys very good agreement was obtained with the experimental data of Peart *et al* (1976b, c) up to impact energies of 20 keV and reasonable agreement between 20 and 100 keV. In the present two-electron model it may be possible to employ, in a similar way, a very small number of such pseudostates to represent detachment, so that the total basis set remains of manageable size. This is under investigation.

Acknowledgments

We wish to thank Dr D R Flower and Dr A M Ermolaev for interesting discussions, Professor A Dalgarno for helpful correspondence and for sending us details of his work in advance of publication, and the staff of the RAL Atlas Centre for their assistance in the use of the CRAY-XMP. This work was supported, in part, by the Science and Engineering Research Council.

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