Close-coupling calculations of electron capture cross sections from the $n = 2$ states of H by protons and α particles

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Abstract. Cross sections for electron capture from the $n = 2$ excited states of atomic hydrogen in collisions with protons and α particles are calculated using the semiclassical close-coupling method where the time-dependent wavefunction is expanded in terms of travelling atomic orbitals on each collision centre. The results are compared with existing close-coupling calculations in which molecular orbital expansions were used. The dependence of the total and partial electron capture cross sections on the alignment of the initial excited 2p states is examined.

1. Introduction

Theoretical studies of charge transfer from the metastable H(2s) state to protons and other charged particles are needed for the interpretation of physical phenomena occurring in controlled fusion plasmas and astrophysical gases (Seaton 1960). Most earlier theoretical works on these collision systems used the simple Landau–Zener approximation (Salop 1976, Casaubon and Piacentini 1984), while others used close-coupling calculations with a small number of molecular orbitals (Blanco *et al* 1986, 1987).

In close-coupling calculations for collisions of ions with the excited states of atomic hydrogen, there are a number of complications intrinsic to molecular orbital expansion methods. First, the dipole coupling in atomic hydrogen between the 2s and 2p states due to their degeneracy must be treated appropriately at large internuclear distances. This treatment necessarily includes accounting for the Stark effect and the rotation of the internuclear axis. Second, each molecular state is a lengthy linear combination of atomic orbitals on the two centres, especially for $H^+ + H(n = 2)$ collisions. For example, at large internuclear separations, the molecular states $3d\sigma_g$ and $4f\sigma_u$ are given by (Fano and Fano 1972)

$$|3d\sigma_g> = \tfrac{1}{2}\left[\left(|2s^A> +|2p_z^A>\right) + \left(|2s^B> -|2p_z^B>\right)\right] \tag{1}$$

$$|4f\sigma_u> = \tfrac{1}{2}\left[\left(|2s^A> +|2p_z^A>\right) - \left(|2s^B> -|2p_z^B>\right)\right]. \tag{2}$$

Third, in the molecular orbital expansion method the results are very sensitive to the choice of electronic translational factor (ETF) as demonstrated in the recent calculations of Jouin and Harel (1991) for the total charge transfer cross sections in $\alpha+H(2s)$ collisions.

In this paper, we study the charge transfer cross sections for the collision of protons and α particles with the $n = 2$ states of H using travelling atomic orbitals in the close-coupling expansion. The close-coupling method has been applied in recent years to a

wide variety of atomic collisions in which the targets were initially in the ground state (Fritsch and Lin 1991). The method has also been used to calculate electron capture from laser excited target atoms in order to examine the dependence of electron capture cross sections on the alignment and/or orientation of the initial state (Shingal *et al* 1987, Fritsch 1987). The present calculation examines electron capture processes where long range couplings in both the initial and the final states are important. The results can also be used to check against the molecular orbital expansion calculations.

In section 2 we describe briefly the theoretical method and the basis sets used in the calculation. The results are presented in different subsections in section 3. Conclusions and a brief summary are given in section 4.

The present calculations were carried out on Sun SPARCstations.

2. Theoretical models and basis functions

The theoretical and computational methods used in the close-coupling approximation using atomic orbitals are quite standard; for examples, see Fritsch and Lin (1991). When applying the close-coupling methods to collisions with targets initially in excited states, the main difficulty lies in the large number of basis functions required. A further complication is the fact that each alignment or orientation of the initial state should be considered.

In this work, we assume straight-line trajectories for the motion of the nuclei. The time-dependent Schrödinger wavefunction is then expanded in terms of travelling atomic orbitals on each centre. These atomic orbitals are obtained by diagonalizing a given set of Slater orbitals on each centre. The resulting eigenenergies are typically accurate for the lower energy bound states; some of the higher energy states have positive eigenenergies and are called pseudostates.

In the present calculation, for p+H collisions, we use thirteen states on each centre which are constructed from six s, three p and one d Slater orbitals. These Slater orbitals are chosen such that both the $n = 2$ and $n = 3$ hydrogenic states are exactly reproduced.

For α+H collisions, the basis functions on α consist of the $n = 2$, 3, 4 and 5 atomic orbitals giving a total of 25 states. For the H^+ centre, the basis functions consist of the same thirteen states as above, reproducing the $n = 2$ and 3 hydrogenic states.

These basis sets were chosen because they are expected to contain the dominant capture channels in these collisions. No attempt was made to check the convergency of the calculation with respect to the basis sets. From our experience with other collision systems, we expect that the total electron capture cross sections presented are reliable.

3. Results and discussion

3.1. Electron capture from H(2s) and H(2p) states by protons

We first discuss the results for electron capture from H(2s). For this symmetric collision system, resonant charge transfer to the H($n = 2$) states is the dominant process. However, this is not a two-channel problem as in p+H(1s)→H(1s)+p. For the present system, both the entrance and the exit 2s states are strongly coupled to the 2p states. Earlier molecular orbital calculations by Blanco et al (1987) include only those states that converge to the H($n = 2$) thresholds, and no ETF were used in the calculation. In general, such results are expected to be less reliable than the present ones.

To describe electron capture from 2p states, we must first define the quantization axis. The beam is to be taken in the xz plane at an impact parameter $x = b$. The y axis is then
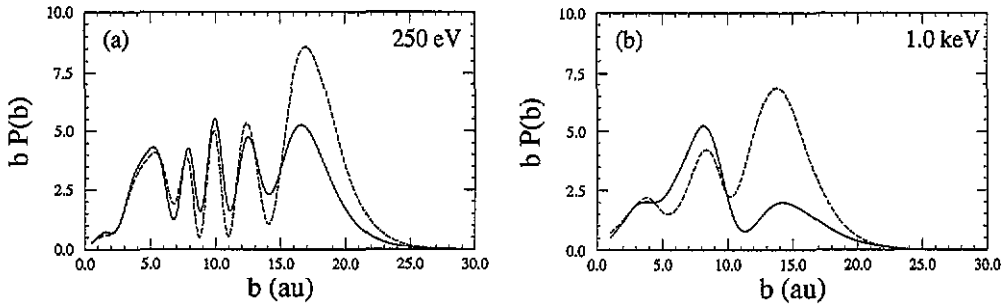
Figure 1. Comparison of $bP(b)$ plotted against b for total electron capture from 2s (full curves) and from $2p_z$ (broken curves) states for p+H collisions at (*a*) 250 eV, (*b*) 1.0 keV. Note the 'in-phase' oscillations of the probabilities in (*a*).

defined such that x, y and z form a right-handed coordinate system. Thus p_z states are aligned parallel to the beam; p_x states perpendicular to it and in the xz plane and p_y states perpendicular to both the beam and the plane.

In figure 1(*a*) we compare $bP(b)$ for electron capture from the 2s and $2p_z$ states of atomic hydrogen at 250 eV. Note that the two probabilities oscillate at essentially the same frequency. This oscillation is the result of 2s and $2p_z$ degeneracy at large internuclear distances. In figure 1(*b*) we show the same comparison at 1.0 keV. Here, the probabilities for capture no longer oscillate at the same frequency, and the capture probability from the $2p_z$ state is now much larger than from the 2s state.

We considered above electron capture from an initial state aligned along the direction of the incident beam. We now consider the situation in which the initial state is aligned perpendicular to the incident beam direction, i.e. along the x or y axis. We denote the probability amplitude for such alignments as $A_x(b)$ and $A_y(b)$, respectively, calculated for impact parameters $x = b$, as stated above. We note that such calculations provide all the information needed for evaluating both the differential and total electron capture cross sections, even for initial states aligned arbitrarily in the xy plane. For arbitrary alignments, the electron capture probability amplitude is a simple rotation of the amplitudes $A_x(b)$ and $A_y(b)$. For example, if $A_x(b)$ and $A_y(b)$ are the probability amplitudes for electron capture from initial $2p_x$ and $2p_y$ states, then the probability amplitude for electron capture from an initial state that is aligned along a direction that makes an angle ϕ with the x axis is given by

$$A(b, \phi) = A_x(b) \cos\phi + A_y(b) \sin\phi. \tag{3}$$

In figure 2(*a*) we compare electron capture probabilities versus the alignment of the initial state as a function of impact parameter. Recall that each of the $2p_x$, $2p_y$, and $2p_z$ orbitals has a dumbbell shaped density distribution along the x, y, and z directions, respectively, and that the projectile lies in the xz plane. At 100 eV, we note that electron capture at large impact parameters is more likely if the initial state is $2p_z$. The difference in electron capture probabilities from $2p_x$ and $2p_y$ states is small, and the probabilities oscillate at about the same frequency, cf figure 1(*a*). In figure 2(*b*) we show the same comparison at 2.25 keV. Electron capture from the $2p_z$ state is comparable to that from the $2p_x$ state, but electron capture from the $2p_y$ state is much smaller.

3.2. Total electron capture cross sections from H(2s) by protons

We have calculated the total charge transfer cross sections to each individual H(nl) final state for the collision of protons with the metastable H(2s) state. These cross sections are
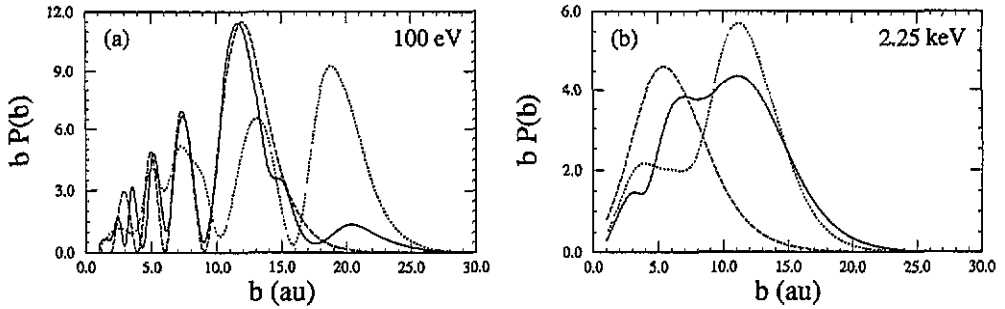
Figure 2. Comparison of $bP(b)$ plotted against b for total electron capture from $2p_x$ (full curves), $2p_y$ (broken curves) and $2p_z$ (dotted curves) for p+H collisions at (a) 100 eV and (b) 2.25 keV. Note that the probabilites for the $2p_x$ and $2p_y$ initial states again oscillate 'in phase' in (a).

of interest in astrophysical and thermonuclear plasma applications. The results are shown in table 1. Note that at low velocities, the 2s and 2p states are dominantly populated, with only a small fraction going to the $n = 3$ states. As the velocity increases, however, electron capture to the $n = 3$ states becomes quite significant. At $v = 0.4$ au, where the cross section for electron capture to the $n = 3$ states peaks, the cross sections for electron capture to $n = 2$ and $n = 3$ final states are about equal.

Table 1. Partial electron capture cross sections to H(nl) substates for p+H(2s) collisions. The cross sections are given in units of 10^{-16} cm^2.

v (au)	2s	2p	$n = 2$	3s	3p	3d	$n = 3$
0.1	40.25	72.98	113.23	0.15	1.21	1.83	3.20
0.2	25.11	35.37	60.48	1.11	4.46	2.00	7.58
0.3	5.51	20.81	26.33	4.81	9.47	5.63	19.92
0.4	7.34	10.72	18.06	3.70	12.38	8.59	24.67
0.6	2.93	3.68	6.61	1.42	2.57	1.21	5.21
0.8	1.14	1.89	3.03	0.45	0.26	0.16	0.87

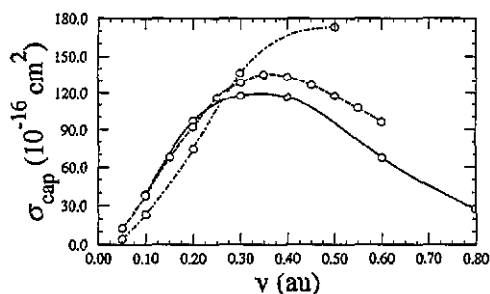### 3.3. Total electron capture cross sections from H($n = 2$) states by protons

To calculate the total electron capture cross sections from a target atom initially in 2s or $2p_z$, due to the cylindrical symmetry of the collision geometry, the cross section can be obtained by integrating the electron capture probabilities over the impact parameter directly. To obtain total electron capture cross sections for collisions in which the system is not cylindrically symmetric, say p+H($2p_x$), we need to integrate over the entire impact parameter plane. Using equation (3) for $A(b, \phi)$, the cross section for electron capture from a perpendicularly polarized initial state is

$$\sigma_\perp = \int\int |A(b, \phi)|^2 b\,db\,d\phi$$

$$= \tfrac{1}{2}\left(2\pi \int |A_x(b)|^2 b\,db + 2\pi \int |A_y(b)|^2 b\,db\right)$$

$$= \tfrac{1}{2}\left(\sigma_x + \sigma_y\right) \tag{4}$$

where the last line defines σ_x and σ_y. We see then that the cross sections for perpendicularly polarized initial states are obtained by integrating the probability amplitude over b as if
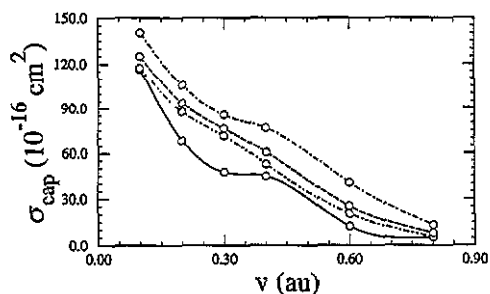
Figure 3. Total electron capture cross sections from the excited states of H in p+H collisions: from 2s (full curve), from $2p_z$ (chain curve), from a $2p_\perp$ (double chain curve); and from an unpolarized 2p state (broken curve).

Figure 4. Total electron capture cross sections for α+H(2s) collisions: present results (full curve), Jouin and Harel (1991) (broken curve), Blanco *et al* (1987) (chain curve).

there were cylindrical symmetry. This result applies equally well to any initial state linearly polarized in a direction perpendicular to the incident beam.

In figure 3 we show the total electron capture cross sections for initial 2s and 2p states. For the 2p states, we differentiate among initial states which are aligned along the direction of the beam ($2p_z$), aligned perpendicular to it ($2p_\perp$), and those which are not aligned (2p). The cross section for the unpolarized initial 2p state is obtained from

$$\sigma(2p) = \tfrac{1}{3}\sigma(2p_z) + \tfrac{2}{3}\sigma(2p_\perp).$$

In the energy region shown, the incident projectile velocity is comparable to or higher than the orbital velocity of an electron in the $n = 2$ state, and the total electron capture cross sections drop rapidly with the collision velocity. Over the velocity region covered, electron capture from the H(2p) state is more likely than from the H(2s) state. However, according to perturbation theory, the cross section for electron capture from H(2s) is expected to become larger than from H(2p) at higher velocities. Presumably this occurs at higher velocities than covered in our calculations.

We do not anticipate that electron capture cross sections from aligned H(2p) states can be measured. However, electron capture from aligned Na(3p) states in collisions with protons have been measured recently (Dowek *et al* 1990). The dominant electron capture channels in H^++Na(3p) are the $n = 2$ states of H, similar to the present p+H(2p) collisions. In the experiment of Dowek *et al* (1990), for protons on aligned Na(3p) states it was found that within the velocity range of 0.14–0.28 au, the electron capture cross section is larger if the initial state is aligned parallel to the incident beam direction than if it is aligned perpendicular to it. From figure 3, this is also the case for p+H(2p) collisions despite the fact that H(2p) and H(2s) are degenerate, while for Na, the 3s and 3p states are separated by an energy of 2.10 eV. Apparently the Stark mixing of H(2s) and H(2p) states does not affect the dependence of electron capture cross sections on the alignment of the initial state.

3.4. Electron capture from H(2s) by α particles

We also investigate electron capture from H(2s) by α particles. In the velocity region of 0.1 to 0.8 au, the dominant process is electron capture to the $n = 3$ and $n = 4$ states, where $n = 3$ is the larger of the two. The calculated total electron capture cross sections are shown in figure 4 and are compared to results from Jouin and Harel (1991) and to results from Blanco *et al* (1987). The latter two calculations are based on the molecular orbital

expansion method, and they differ in the choice of electronic translational factors. It is argued by Jouin and Harel (1991) that their optimized ETFs are superior to those used by Blanco *et al* (1987). Our results agree with those of Jouin and Harel (1991) in the lower velocity region ($v < 0.25$), but are smaller in the higher velocity region. We believe that the present results are more reliable since the atomic orbital expansion method is expected to be more accurate than the molecular orbital expansion method in the higher velocity region.
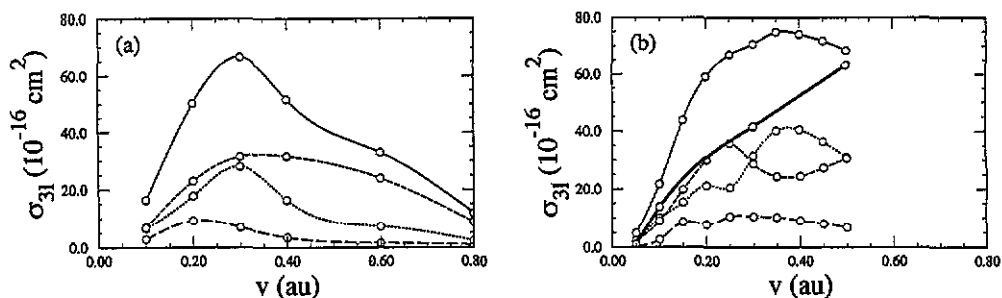
Figure 5. Comparison of the partial electron capture cross sections to the various $n = 3$ states of He$^+$ for He^{2+}+H(2s) collisions: to 3s (long broken curves), to 3p (dotted curves), and to 3d (short broken curves). Results from the present calculations are shown in (*a*) and from Jouin and Harel (1991) in (*b*). The thin full curves are for total electron capture to the $n = 3$ states, and the thick full curve in (*b*) is for the total electron capture cross section to the $n = 3$ states calculated by Blanco *et al* (1987).
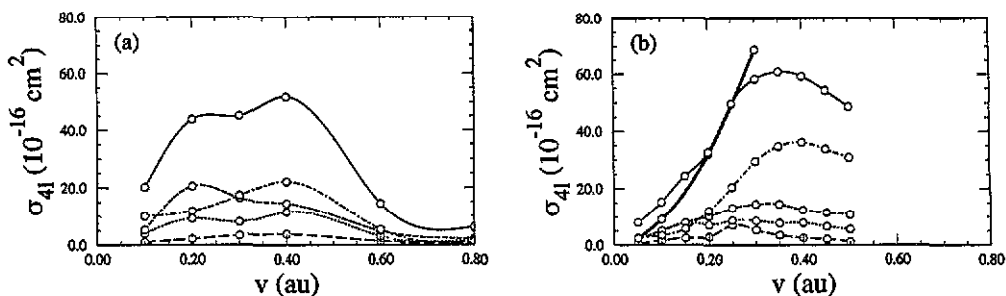
Figure 6. Comparison of partial electron capture cross sections to the various $n = 4$ states of He$^+$ for He^{2+}+H(2s) collisions: to 4s (long broken curves), to 4p (dotted curves), to 4d (short broken curves), and to 4f (chain curves). Results from the present calculations are shown in (*a*) and from Jouin and Harel (1991) in (*b*). The thin full curves are for total electron capture to the $n = 4$ states, and the thick full curve in (*b*) is for the total electron capture cross section to the $n = 4$ states calculated by Blanco *et al* (1987).

In figures 5 and 6 we compare the partial cross sections of the different $n = 3$ and $n = 4$ substates obtained from the present calculation to those from Jouin and Harel (1991). It is obvious that the discrepancies among the subshell cross sections are larger. We are confident that the results from our calculations are reliable since similar subshell cross sections have been calculated for collisions with atoms in the ground state, and the results have been shown to be in good agreement with experiment (see Fritsch and Lin (1991) for examples).
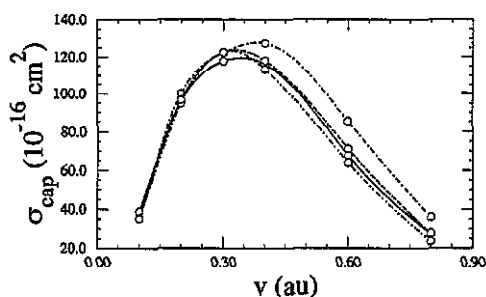
Figure 7. Total electron capture cross sections from the excited states of H in α+H collisions: from 2s (full curve), from $2p_z$ (chain curve), from $2p_\perp$ (double chain curve), and from an unpolarized 2p state (broken curve).

3.5. Electron capture from aligned 2p states in α+H collisions

In figure 7 we show the dependence of the total electron capture cross sections on the alignment of the initial 2p states. We note that over the energy region considered, the electron capture cross section for a 2p state aligned parallel to the beam direction is larger than for a 2p state aligned perpendicular to the beam direction. For electron capture from Na(3p) by α particles in the velocity range of $v = 0.1$ to 0.45 au, it has been found that the reverse is true (Aumayr *et al* 1992). The significance of this difference is not clear. For α+Na(3p), the dominant electron capture channels are $n = 4$ states, with small contributions from the $n = 5$ states. For the present system, both the $n = 3$ and $n = 4$ channels are nearly equally populated. In figure 7, we also show the total electron capture cross sections from an unpolarized initial 2p state and from the 2s initial state.

4. Summary and conclusions

Electron capture cross sections from the $n = 2$ excited states of atomic hydrogen in collisions with protons and α particles are studied in the velocity range of $v = 0.1$ to $v = 0.8$ au using the close-coupling expansion method with travelling atomic orbitals. The results are compared to the results of previous calculations based on molecular orbital expansions. It is found that the total electron capture cross sections are in reasonable agreement, but prominent discrepancies exist for the partial cross sections. The effect of the alignment of the initial state on the total electron capture cross sections is also examined and the results compared to similar collisions with aligned Na(3p) targets. We find no simple rule or interpretation of the dependence of electron capture cross sections on the alignment of the initial states from the data available to date.

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