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Excitation and charge transfer in $He^+ + H$ collisions

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Abstract. We have performed a close-coupling calculation for the $He^+ + H$ collision in the energy range 2.5–25 keV amu^{-1} using the two-centre atomic orbital expansion method. The collision system was approximated in a one-electron model with proper accounting for the Pauli exclusion principle. From the calculated excitation cross sections, cross sections for Lyman-alpha and Balmer-alpha emission were determined and compared with available measurements. Detailed comparison is also made with the most recent theoretical results reported by Ermolaev *et al*. The overall better agreement between our calculation and the measurement is observed. On the other hand, the calculated total electron capture cross sections, which are much larger than the excitation cross sections, agree well with the results of Ermolaev *et al*, but differ from the measured values reported in Olson *et al* by 30–50%. We suspect the reliability of the latter experimental results.

1. Introduction

In a recent paper cross sections for excitation to the H(2p) and H(2s) states in $He^+ + H$ collisions have been determined by Geddes *et al* (1994) in the energy range 2.5–25 keV amu^{-1}. Measurements have been based on observations of both the spontaneous and electric field induced Lyman-alpha radiation emitted by the excited H atoms. Previous measurements by Young *et al* (1968) and by McKee *et al* (1977) were limited to energies below 7.5 keV amu^{-1}. In the overlapping energy region, the measured cross sections are in good agreement with each other.

There are only a few theoretical calculations for the studied processes. The Born and single-centre atomic state expansion method using only two and four states by Flannery (1969) are not expected to work in the low-energy region since electron capture channels were not accounted for. A much more serious theoretical calculation was carried out by Errea *et al* (1989). They performed a careful study for the present collision system using a molecular-state expansion method and optimized two-electron translation factors. Sixteen molecular states were included in their calculation. Their results, however, when compared to the experimental data of Geddes *et al*, show substantial discrepancies. Most recently, Ermolaev *et al* (1994) did a systematic study for the present collision system using a full two-electron formulation (Jackson *et al* 1992) as well as a pseudo-one-electron approximation. Their calculated excitation and electron capture cross sections agree better with the measurements than those obtained by Errea *et al* (1989). But the disagreement between the calculations and the measurements is still quite large. Further improvements are explored in the present paper.

In the experiment of Geddes *et al* (1994), the H(2p) and H(2s) excitation cross sections determined are apparent cross sections which include cascade contributions from the $n \geqslant 3$ states. In order to compare theoretical results with the experiment, excitation cross sections

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to $n \geqslant 3$ states should also be evaluated. From the calculated cross sections to the $n = 3$ states, one can also determine the Balmer-alpha emission cross sections which were reported by Donnelly *et al* (1991). The results from our calculation are found to be in good agreement with their measurement.

We also check the electron capture cross sections obtained from the present close coupling calculation which are five to ten times larger than the excitation to the $n = 2$ states in the energy region investigated. In comparing our results with the measurement reported in Olson *et al* (1977), we found that our results are 30–50% smaller. Since we have good agreement with experimental results for the smaller excitation channels, we suspect that the old experimental total electron capture cross sections are somewhat too large.

2. Theoretical model

In order to carry out calculations for $He^+ + H$ collisions using the close-coupling method, it is desirable to expand the time-dependent two-electron wavefunction in terms of two-electron atomic orbitals (Fritsch and Lin 1986, 1991) or two-electron molecular orbitals as done in Errea *et al* (1989). Since the dominant channels are the electron capture to $n = 2$ states, and excitation to $n = 2$ and $n = 3$ states are weak channels, it is clear that a relatively large number of basis functions should be included if the cross sections for the weaker excitation to the $n = 2$ and $n = 3$ states are to be calculated. Such an elaborate calculation can be done, but we show in this paper that a simpler one-electron model is adequate for the present collision system.

The dominant process in $He^+ + H$ collisions in the 2.5–25 keV amu^{-1} region is electron capture to the $n = 2$ states, although in the higher energy region, electron capture to $n = 1$ is also important. To perform a one-electron model calculation, the electron in He^+ is to be treated as a spectator. This model is adequate if the collisions at very small impact parameters (i.e. less than the radius of the He^+ ion) are not important in determining the total cross sections for each process. Thus the model is expected to be adequate for treating electron capture to the excited states and for the excitation processes. If the electron is captured to the $n = 1$ state, then the one-electron model is limited since the Pauli exclusion principle restricts the two electrons to forming the $1s^2(^1S^e)$ singlet state only. In order to account for this fact, we did two calculations within the one-electron model. The first is to simulate the spin singlet case where electron capture to the 1s state is allowed. The second is to simulate the spin triplet case where electron capture to the 1s state is not permitted. The only difference in the two calculations is that the 1s state on the projectile in the second calculation is not included in the basis set. The final results are obtained by summing over the two processes weighted by $\frac{1}{4}$ for the singlet and $\frac{3}{4}$ for the triplet, respectively.

In this model, the electron and He^+ ion interaction is represented by a model potential which has the form

$$V_P(r) = -Z_0/r + (Z_1 + Z_2 r)\exp(-Z_3 r)/r \tag{1}$$

where $Z_0 = -Z_1 = 1$, $Z_2 = -0.6535$, and $Z_3 = 2.697$. This potential gives good ground-state and singly-excited-states energies for He and has been used in many previous calculations involving He atoms (Bransden *et al* 1984, Shingal 1988).

We used the two-centre atomic orbital expansion method as described in detail in Fritsch and Lin (1991) to solve the time-dependent Schrödinger equation,

$$\left(i\frac{\partial}{\partial t} - H\right)\Psi(r, t) = 0 \tag{2}$$

with

$$H = -\tfrac{1}{2}\nabla_r^2 + V_P(r_P) + V_T(r_T) \tag{3}$$

where V_P is the potential given in (1) and V_T is the Coulomb potential due to the target, and r_P and r_T are the distances of the electron measured from the projectile and the target, respectively.

Table 1. Basis set used for H^++H collision in the present calculation. Slater orbitals of the form $r^n \exp(-\lambda r)Y_{lm}(\hat{r})$ are used on both centres. The corresponding energies resulting from diagonalizing the one-centre Hamiltonian are also given.

Centre H				Centre He			
l	n	λ	ϵ (au)	l	n	λ	ϵ (au)
0	0	2.000	−0.5000	0	0	1.950	−0.9033
	0	1.000	−0.1250		0	1.300	−0.1574
	0	0.500	−0.0555		0	0.800	−0.0612
	1	0.500	0.0128		1	0.900	0.0630
	1	1.000	0.3394		1	0.500	0.6536
	1	1.500	1.7704		2	0.500	4.3852
	2	0.333	11.1751				
	2	0.800		1	1	1.200	0.1276
					1	0.800	−0.0551
1	1	0.500	−0.1250		1	0.433	0.0202
	1	1.000	−0.0556		2	0.433	0.3166
	1	0.200	−0.0312		3	1.000	1.6297
	2	1.200	0.0013				
	2	0.333	0.2217	2	2	1.200	−0.0556
	3	0.500	1.6139		2	0.600	−0.0306
					2	0.100	−0.0195
2	2	1.200	−0.0556		3	2.000	0.0315
	2	0.666	−0.0245		3	0.300	0.3200
	2	0.333	0.0803		4	0.500	1.2354
	3	0.500	0.7051				

The atomic orbitals used in the present calculation include both bound states and pseudostates (31 states on the target and 34 states on the projectile). They are listed in table 1. We have extracted cross sections for electron capture to $n = 1$, 2 and 3 states and excitation cross sections to $n = 2$ and 3 states. The results are discussed in the following sections.

3. Results and discussion

3.1. Excitation to 2s and 2p states

In figure 1 we show the calculated H(2p) and H(2s) excitation cross sections along with the calculations by Ermolaev *et al* (1994) and the experimental data of Geddes *et al* (1994). Note that the linear scaling was used in all figures. We show two theoretical curves, the dotted lines are the 'true' H(2p) and H(2s) excitation cross sections, and the full curves include the contribution of the cascade from the $n = 3$ states. We did not calculate excitation cross sections to higher n states but the contribution from these higher states are not expected

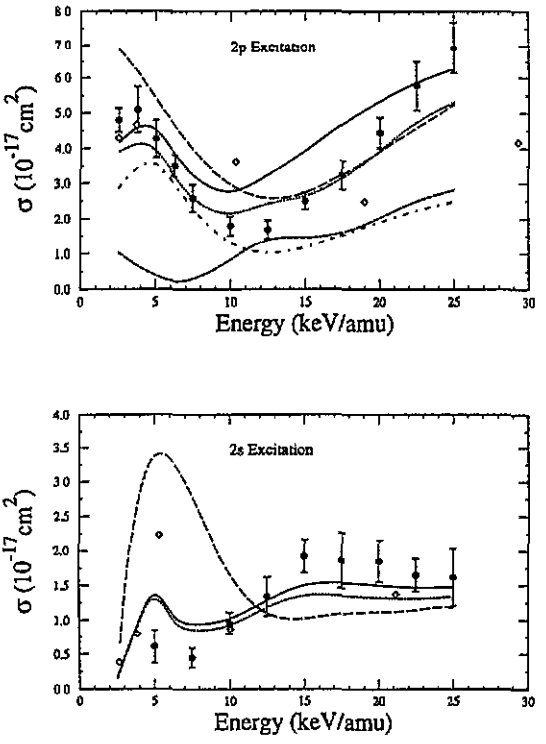

Figure 1. Excitation cross sections to 2p and 2s states in He^+–H collisions. The full curve is our calculated excitation cross sections including cascade contribution from $n = 3$ states, the dotted curve is our calculated 'true' 2p or 2s excitation cross sections. The long dashes are from the pseudo-one-electron model with an asymmetric atomic-orbital basis B1 by Ermolaev *et al* (1994) and the open diamonds are from their two-electron atomic-orbital basis B2. The full circles with error bars are the experimental data from Geddes *et al* (1994). In the upper figure the excitation cross sections to $2p_0$ (short dashes) and to $2p_1$ (dashes–dots) from the present calculation are also shown.

to be significant in view that excitation to $n = 3$ state is already much smaller than excitation to $n = 3$ states. For the same reason as we mentioned in the beginning, both calculations by Ermolaev *et al* (1994) should also be modified with the cascade contributions in order to compare them with the experimental measurements.

For excitation cross sections to the H(2p) states, our calculated results are almost identical to those from the pseudo-one-electron model with asymmetric atomic-orbital basis B1 by Ermolaev *et al* (1994) for the impact energies larger than 12 keV amu^{-1}, while the difference becomes larger at lower energies. This is understandable considering that B1 has only one capture channel (1s') included, which is certainly not enough since the dominant capture channels for the low impact energies are the $n = 2$ states. Note that the dominant capture channels for $He^+ + H$ are different from $H^+ + H$. Besides this defect, the Pauli exclusion principle was not taken into account in the calculation with B1 basis. Since our calculation has taken both facts into account, our calculated results are in best agreement with the experimental data for the entire impact energy region. The largest overall discrepancy with the measurement occurs in the calculations with the two-electron atomic orbital basis B2 by Ermolaev *et al* (1994). This is most likely due to the incompleteness of the basis set B2 used.

To calculate Lyman-alpha emission cross sections, we have to add contribution from excitation to the 3s and 3d states to the 'true' H(2p) excitation cross sections since these states decay to the 2p state. The discrepancy between our calculated results and the experimental data is largest near the minimum at around 10–15 keV amu^{-1} where our calculations show a non-negligible contribution from the cascade effect. As shown in figure 2, our calculated excitation cross sections to the $n = 3$ states in their energy region are in good agreement with the experimental data of Donnelly *et al* (1991). Thus the discrepancy can only be due to the $n = 2$ excitation cross section in this region. In comparison, the results of Errea *et al* (1989) are about a factor of three to four higher than the experimental data for energies above 10 keV amu^{-1}; therefore, their results are not shown in the figure.

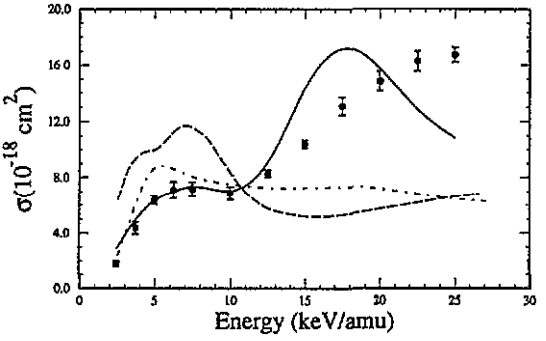

Figure 2. Cross sections for Balmer-alpha emission in He^+–H collisions. The full curve is from the present calculation. The long dashes are from the pseudo-one-electron model with asymmetric atomic-orbital basis B1 by Ermolaev *et al* (1994) and the chain curve is from their two-electron atomic orbital basis B2. The full circles with error bars are the experimental data of Donnelly *et al* (1991).

It is interesting to note that the excitation cross section to H(2p) states show a minimum near 10 keV amu^{-1}, or more precisely that the cross section rises below 10 keV amu^{-1}. This phenomenon is quite common, for example, in $H^+ + H$ collisions (Fritsch and Lin 1982) and is a consequence of the effect of rotational coupling for low-energy collisions. To illustrate this point, we show the partial excitation cross sections to $2p_1$ and $2p_0$ substates. Note that the $2p_1$ state is dominant at low energies as the result of the rotational coupling. The preferential population of $2p_1$ substate implies that the Lyman-alpha radiation will be strongly polarized—a result to be confirmed in future experiment. Note that similar polarization has been determined in $H^+ + H$ collisions (Hippler *et al* 1988).

The excitation cross sections to the 2s state are shown in the lower frame of figure 1. In this case, the cascade contribution is from excitation to the 3p state. However, 3p state decays predominantly to 1s, and has only 12% branching ratio for decay to the 2s. The excitation cross section to the 2s is much smaller than the excitation cross section to the 2p; therefore, it is more sensitive to the model used. Due to the same reason mentioned above, the disagreement between the calculations by Ermolaev *et al* (1994) and the measurements is larger, and our results are again in much better agreement with the experimental data of Geddes *et al* (1994). Again, the results from Errea *et al* (1989) differ much more from the experimental data and are not shown in the figure.

3.2. Excitation to n = 3 states

We have also obtained excitation cross sections to the $n = 3$ states, from which cross sections for Balmer-alpha emission can be determined using $\sigma(\mathrm{H}\alpha) = \sigma(3s) + 0.12\sigma(3p) + \sigma(3d)$. The resulting cross sections for Balmer-alpha emission from excited target H results are shown in figure 2 together with the calculations by Ermolaev *et al* (1994) and the experimental data of Donnelly *et al* (1991). Since cross sections for Balmer-alpha emission are even smaller than the 2s excitation cross sections, they are more difficult to evaluate with higher accuracy. The two calculations by Ermolaev *et al* (1994) show larger discrepancy with the measurement than ours. Our results agree with the experimental data quite well except for higher energies where the discrepancy is probably due to the limitation of the basis set since ionization becomes important at higher energies.

3.3. Electron capture cross sections

The close-coupling calculation also gives total electron capture cross sections. In figure 3 we compare the various theoretical results with the experimental data reported in Olson *et al* (1977). The full curve is for the total capture cross sections from the present calculation, including electron capture to the $n = 1$, 2 and 3 states. The chain curve is from the two-electron atomic orbital basis B2 obtained by Ermolaev *et al* (1994), including the same $n = 1$, 2 and 3 states. The dotted curve is from Errea *et al* (1989), including electron capture to the $n = 1$ and 2 only. The measured experimental data certainly include the contributions from electron capture to the higher states, but such contributions are negligible.

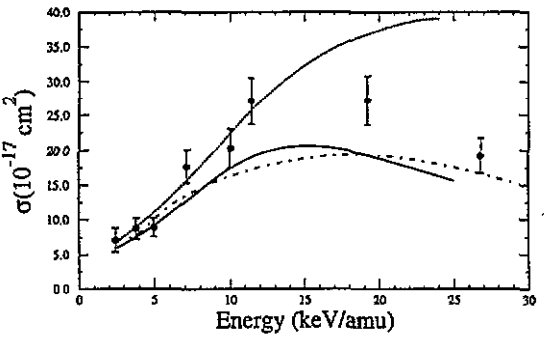

Figure 3. Capture cross sections in He^+–H collisions. The full curve is from the present calculation, the dotted curve is from the calculations by Errea *et al* (1989), and the chain curve is from the two-electron atomic-orbital basis B2 by Ermolaev *et al* (1994). The full circles with error bars are the experimental data from Olson *et al* (1977).

Our calculated total electron capture cross sections are very close to those evaluated by Ermolaev *et al* (1994) and are about 30–50% too low in comparison with the experimental data in the 10–25 keV amu^{-1} energy region. Note that the total electron capture cross section is about five to ten times larger than excitation to the $n = 2$ states, and thus such a large discrepancy between our calculated results and the experimental data given in Oson *et al* (1977) is difficult to understand. There is no other experimental data for electron capture in this energy region. At energies above 100 keV amu^{-1}, there are measurements by Hvelplund and Anderson (1982). They claimed that the data in Olson *et al* are about 50% higher than theirs if one compares the total energy dependence of the two sets of data. Our calculation seems to support this contention.

In view of the fact that the present calculation gives quite reasonable results in comparison with experiments for the weaker excitation channels, the 30–50% discrepancy for the larger total electron capture cross sections with experiment is not acceptable. In our close-coupling calculation, all these cross sections are obtained simultaneously. We thus suspect that the experimental data reported in Olson *et al* are questionable and new measurements are called for. On the other hand, it is desirable that close-coupling calculations based on the two-electron model be carried out to check the results from the present calculation.

4. Conclusions

In conclusion, we have shown that the $He^+ + H$ collision system can be approximated as a one-electron system and the excitation and charge transfer cross sections can be determined using the two-centre atomic orbital expansion method. Our results for the excitation cross sections to the $n = 2$ states and for the Balmer-alpha emission cross sections are in best agreement with the experimental data by Geddes *et al* (1994) and by Donnelly *et al* (1991), respectively. Failure of the other theoretical studies is probably due to the limited basis set used in their calculations. We also showed that total electron capture cross sections reported in Olson *et al* (1977) apear to be too large and new measurements are called for.

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