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1997 J. Phys. B: At. Mol. Opt. Phys. 30 101

(http://iopscience.iop.org/0953-4075/30/1/012)

J. Phys. B: At. Mol. Opt. Phys. **30** (1997) 101–113. Printed in the UK PII: S0953-4075(97)76140-6

Convergent TCAO close-coupling calculations for electron transfer, excitation and ionization in intermediate keV He^{2+}–H collisions

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Received 9 July 1996

Abstract. Our recently developed two-centre atomic orbital (TCAO) close-coupling method is applied to He^{2+}–H(1s) collisions in the impact energy range from 20–400 keV amu^{-1}. Convergent cross sections are obtained for this system by using a large number of bound and pseudostate basis functions on the target and a limited number of bound states on the projectile. Cross sections for electron transfer to 1s, 2ℓ, 3ℓ, 4ℓ and 5ℓ, for excitation to 2ℓ, 3ℓ, 4ℓ and 5ℓ and for ionization are presented and compared with available experimental data and other theoretical calculations. The accuracy of the previous TCAO close-coupling calculations is challenged and the reliability of some experimental data for this system is questioned.

1. Introduction

The one-electron ion–atom collision system He^{2+}–H is the simplest asymmetric system which has been extensively studied theoretically in the past decades (Winter 1988, Fritsch and Lin 1991, Bransden and McDowell 1992). However, most of these investigations are concerned with the electron transfer process at low impact energies (below 20 keV amu^{-1}), where electron transfer is the dominant process and the collision physics can be well understood in terms of quasi-molecular potential curves of $(HeH)^{2+}$. For impact energies above 20 keV amu^{-1}, excitation and ionization processes begin to compete with the electron transfer process, and eventually they become dominant over electron transfer as impact energy goes beyond 70 keV amu^{-1}. Reliable theoretical prediction of the electronic transition cross sections for such processes is not only of fundamental interest, but also of vital importance in diagnostics of high-temperature fusion plasma. Nevertheless, accurate calculations for excitation and ionization cross sections are extremely difficult since there are a virtually infinite number of open channels which are strongly coupled with each other in the considered impact energy range. There exist only a few calculations in the literature, in which excitation and ionization cross sections for this collision system have been evaluated for impact energies above 20 keV amu^{-1}.

The first comprehensive study of the excitation process in He^{2+}–H collisions was performed by Fritsch *et al* (1991), for impact energies from 1–300 keV amu^{-1}, using a two-centre atomic orbital (TCAO) close-coupling method. In their calculations, the basis

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0953-4075/97/010101+13$19.50

set consists of 23 projectile-centred bound/pseudostates and 31 target-centred bound/pseudostates (referred as He23H31 hereafter). The calculated excitation cross sections to 2ℓ and 3ℓ show pronounced structures around 60 keV amu^{-1}. Their predicted structures, interestingly, appeared to have been confirmed experimentally by Hughes *et al* (1994) and Donnelly *et al* (1991) from observing Lyman alpha and Balmer alpha emissions, respectively. However, this kind of structure for excitation to 2ℓ is absent in a smaller size close-coupling calculation by Bransden *et al* (1983), using a single-centred basis set of 19 target-centred bound/pseudostates for impact energies above 75 keV amu^{-1}. Below 75 keV amu^{-1}, their basis set was supplemented by projectile-centred 1s, 2s and 2p states. Later, Errea *et al* (1992) successfully extended their MO approach, modified with a common translational factor for this system, to high impact energies up to 300 keV amu^{-1}. Their evaluated excitation cross sections to $n = 2$ and 3 do not have pronounced structures above 35 keV amu^{-1}. But they did not publish partial excitation cross sections to 2ℓ and 3ℓ. Experimentally, excitation cross sections to np states have been reported by Detleffsen *et al* (1994) using the optical method. Their data do not appear to have any structure, though the data have large error bars. We consider these structures in excitation cross sections around 60 keV amu^{-1} to be difficult to understand. Physically, all structures in the integrated cross sections have to originate from some competing physical mechanisms, such as the minima in the excitation cross sections in H^+–H collision at about 10 keV amu^{-1}, which results from the competition between rotational coupling and radial coupling. As a matter of fact, the physical structures should be independent of the basis set used in calculations. In other words, we believe that the structures in the excitation cross sections to 2ℓ and 3ℓ states above 20 keV amu^{-1} in He^{2+}–H collision remain to be understood both theoretically and experimentally.

There have been a few coupled channel calculations regarding ionization and electron transfer cross sections in He^{2+}–H collision in the intermediate impact energy region. Winter (1988) used a triple-centre expansion to evaluate these two cross sections at impact energies below 50 keV amu^{-1}. His ionization cross sections overestimated the experimental data (Shah *et al* 1988) by about 10–30%. Our own group (Shingal and Lin 1989) performed TCAO close-coupling calculations for this system in the impact energy range from 2–900 keV amu^{-1}, using a basis set of 20 projectile-centred and 22 target-centred bound/pseudostates (He20H22). The calculated ionization cross sections fall below the experimental data (Shah and Gilbody 1981) at higher energies. Recently, Toshima (1994) performed large size TCAO close-coupling calculations for a multiply charged ion colliding with atomic hydrogen in the energy range from 1–400 keV amu^{-1}. For He^{2+}–H collision, he used a basis set consisting of 96 projectile-centred and 100 target-centred bound/pseudostates (He96H100). He only published ionization and charge transfer cross sections, which are in good agreement with the experimental data. However, his ionization cross section seems to vary not very smoothly with energy at higher impact energies.

The structures discussed above are not specific only to the He^{2+}–H collision. In fact, they appear in many two-centre atomic orbital (TCAO) close-coupling calculations for other collision systems. Recently, we have investigated this problem for H^+–H collision at impact energies of 5 keV and above (Kuang and Lin (1996a, b), to be referred to as papers A and B, respectively). We have demonstrated that the spurious oscillatory structures in previous large-scale TCAO close-coupling calculations for H^+–H collision are due to the simultaneous use of the short-ranged pseudo-continuum states on both collision centres. It is shown that reliable excitation cross sections can only be obtained with a large number of basis states on the target and a limited number of bound states on the projectile. In other words, structures in the excitation cross sections of H^+–H collision are artificial and

basis dependent. We believe that the same reason should explain the structures seen in the calculations by Fritsch *et al* (1991) for the He^{2+}–H system despite these structures having been 'confirmed' by experiments (Hughes *et al* 1994, Donnelly *et al* 1991). It is the goal of the present paper to examine this problem theoretically and at the same time to provide reliable cross sections for electron transfer to 1s, 2ℓ, 3ℓ, 4ℓ and 5ℓ, for excitation to 2ℓ, 3ℓ, 4ℓ and 5ℓ and for ionization at impact energies of 20–400 keV amu^{-1}.

2. Basis sets and the TCAO close-coupling method

As in paper A, the even-tempered basis set (Reeves 1963) is used in the present study. Each function in such a basis set consists of an exponential multiplied by a solid harmonic, i.e. a spherical harmonic multiplied by r^l. A set of even-tempered basis functions is thus defined as

$$\chi_{klm}(\boldsymbol{r}) = N_l(\zeta_k)\,\mathrm{e}^{-\zeta_k r}\mathcal{Y}_{lm}(\boldsymbol{r}) \qquad \mathcal{Y}_{lm}(\boldsymbol{r}) = r^l Y_{lm}(\hat{\boldsymbol{r}}) \tag{1}$$

where $N_l(\zeta_k)$ is a normalization constant, and the orbital exponents, ζ_k, are taken to form a geometric sequence $\zeta_k = \alpha\beta^k,\ k = 1, 2, \ldots, N$, where the two parameters α and β can be determined by energy minimization. The atomic states used for the TCAO close-coupling method are then expanded in terms of the set of even-tempered basis functions,

$$\phi_{nlm}(\boldsymbol{r}) = \sum_k c_{nk}\,\chi_{klm}(\boldsymbol{r}) = \sum_k c_{nk} N_l(\zeta_k)\,\mathrm{e}^{-\zeta_k r}\mathcal{Y}_{lm}(\boldsymbol{r}) \tag{2}$$

where the linear coefficients c_{nk} can be readily determined by diagonalizing the single-centred atomic Hamiltonian. Use of an even-tempered basis set enables us to evaluate two-centre matrix elements very efficiently.

Within the semiclassical impact parameter approximation, the two-centre atomic orbital close-coupling method is to expand the time-dependent wavefunction $\Psi(\boldsymbol{r}, t)$ in terms of bound atomic orbitals plus continuum states (BBC expansion) with the plane-wave electronic translational factors

$$\Psi(\boldsymbol{r}, t) = \sum_i a_i(t)\phi_i^A(\boldsymbol{r}, t) + \sum_j b_j(t)\phi_j^B(\boldsymbol{r}, t) + \sum_k c_k(t)\phi_k^C(\boldsymbol{r}, t) \tag{3}$$

where we have explicitly distinguished the set of continuum states $\{\phi_k^C(\boldsymbol{r}, t)\}$ from the two sets of bound states $\{\phi_i^A(\boldsymbol{r}, t)\}$ and $\{\phi_j^B(\boldsymbol{r}, t)\}$ on centre A and centre B, respectively. The actual continuum states for the ion–atom collision system need not associate with a specific centre (either target or projectile). It is conceptually clear that there is only one set of continuum states—either centred on the target or on the projectile. The transition amplitudes $\{a_i,\ b_j,\ c_k\}$ are obtained through the standard procedure (Brankin *et al* 1992) by solving the first-order coupled ordinary differential equations with the proper initial condition.

Since we are mainly interested in the excitation and ionization cross sections, the pseudo-states will be placed on the target only, as in paper B. The target-centred basis set consists of 174 atomic states/pseudostates with $\ell \leqslant 5$ as given in paper B. To test convergence of the evaluated cross sections, we have carried out close-coupling calculations with different numbers of projectile-centred states. We started with the single-centred expansion using 174 target-centred bound/pseudostates only. Then we added four projectile-centre states (1s, 2s, $2p_0$ and $2p_1$) into the basis set forming the set He4H174, since these 2ℓ states are resonant charge transfer channels. Finally, we included all bound states (table 1) up to $n = 5$ (total 35) on the projectile centre into the calculation, i.e. the basis set He35H174. The numerical aspects for the present work are the same as in papers A and B, except that

Table 1. Even-tempered basis functions used to generate the bound states of He^+ up to $n = 5$. The eigenenergies (au) were obtained from diagonalizing the atomic Hamiltonian. $\alpha = 0.185$, $\beta = 1.342$, $N = 9$ for s, $\alpha = 0.258$, $\beta = 1.224$, $N = 7$ for p, $\alpha = 0.265$, $\beta = 1.255$, $N = 5$ for d, $\alpha = 0.300$, $\beta = 1.220$, $N = 3$ for f, $\alpha = 0.400$, $\beta = 1.000$, $N = 1$ for g.

n	s	p	d	f	g
1	−2.000 00				
2	−0.500 00	−0.500 00			
3	−0.222 22	−0.222 22	−0.222 22		
4	−0.125 00	−0.125 00	−0.125 00	−0.125 00	
5	−0.079 93	−0.080 00	−0.080 00	−0.080 00	−0.080 00

the integration with respect to z $(= vt)$ was carried from $z_i = -400$ to $z_f = 400$ au in all these calculations.

3. Results and discussion

3.1. Excitation cross sections to n = 2, 3, 4 and 5

Excitation cross sections to 2ℓ and 3ℓ from the present close-coupling calculations with basis sets He4H174 and He35H174 are shown in figures 1 and 2. They are compared to the previous close-coupling calculations by Fritsch *et al* (1991), the first Born approximation (Bates and Griffing 1953), as well as the experimental data of Hughes *et al* (1994) and Detleffsen *et al* (1994). The results from Bransden *et al* (1983) are not shown since their calculation is of the same nature as our He4H174 calculation but with fewer target-centre states. It is clear that the excitation cross sections from Fritsch *et al* have pronounced structures around 60 keV amu^{-1}, while the excitation cross sections from the present two calculations are rather smooth over the entire impact energy region.

Surprisingly, experimental measurements for excitation cross sections to 2s and 2p states by Hughes *et al* (1994) from observing Lyman alpha emission seems to support the structures predicted by Fritsch *et al*. Even with an additional estimated uncertainty of ±30% by the original authors (Hughes *et al* 1994), these structures are still quite evident. Intuitively, we expect the excitation cross sections to be quite smooth in this impact energy region since there is no known physical mechanism to account for these structures in the energy range considered. These kinds of structures were not appreciated until recently (Kuang and Lin 1996a, b). In papers A and B, we demonstrated that similar structures in the H^+–H collision result from the simultaneous use of the short-ranged pseudo-continuum states on both collision centres. The basis set used by Fritsch *et al* for the He^{2+}–H collision system did include $n = 2$, 4f and 3ℓ united orbitals ($Z = 3$) on both centres; however, these states become pseudo-continuum states asymptotically. As in the H^+–H collision, we believe that these pseudostates give rise to the structures in the excitation cross sections at higher impact energies. Although these united orbitals on both centres might be used safely for the impact energy below 20 keV amu^{-1}, where ionization and excitation cross sections are small compared to the capture cross section, they cannot be used simultaneously at higher impact energies where cross sections for all three processes are of the same order.

Note that there is some difference in the excitation cross sections evaluated with the two different basis sets He4H174 and He35H174. As expected, electron transfer to the excited states (i.e. $n = 2,\ 3$ and 4) is also important for impact energies below 50 keV amu^{-1},

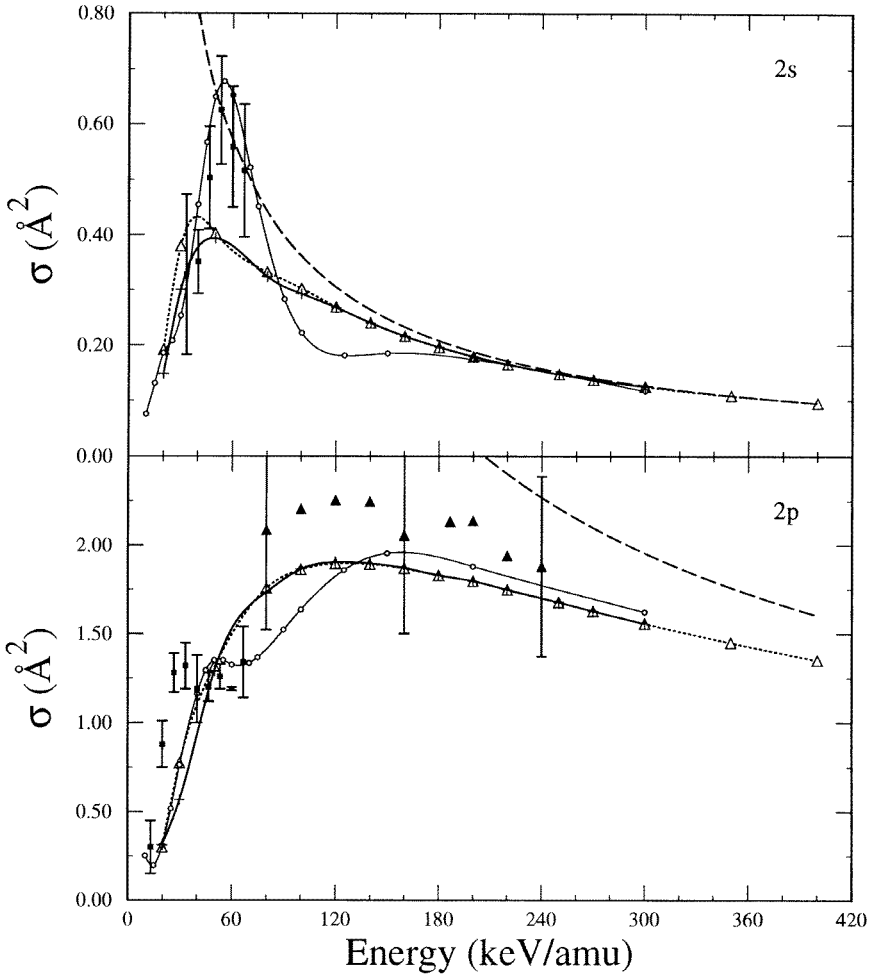

Figure 1. Excitation cross sections to 2s and 2p. Curves are obtained with a cubic spline interpolation through the calculated points (symbols); △, present He4H174; +, present He35H174; ○ , Fritsch *et al* (1991); — — —, first Born; ▲, experiment by Detleffsen *et al* (1994); ■, experiment by Hughes *et al* (1994).

however, these states are absent in the He4H174 set. Therefore we expect that the evaluated excitation cross sections to 2ℓ, 3ℓ and above with the He4H174 set to be less accurate than those obtained with He35H174 in this energy range. This is clear by inspecting the total excitation cross sections to $n = 2$, 3, 4 and 5 in figure 3. It is shown that the evaluated excitation cross section to $n = 5$ with He4H174 fails to converge at impact energies below 50 keV amu^{-1}. Above 120 keV amu^{-1}, the two calculations are coincident with each other. Nevertheless, there exists a subtle difference between the two calculations in the impact energies from 50–120 keV amu^{-1}, which is likely to be caused by the weak linear dependence between the highly excited states on the projectile centre and the basis states on the target centre. Note that the calculated excitation cross sections to the highly excited states ($n = 4$ and 5) are expected to be less accurate than those to the lower excited states ($n = 2$ and 3).

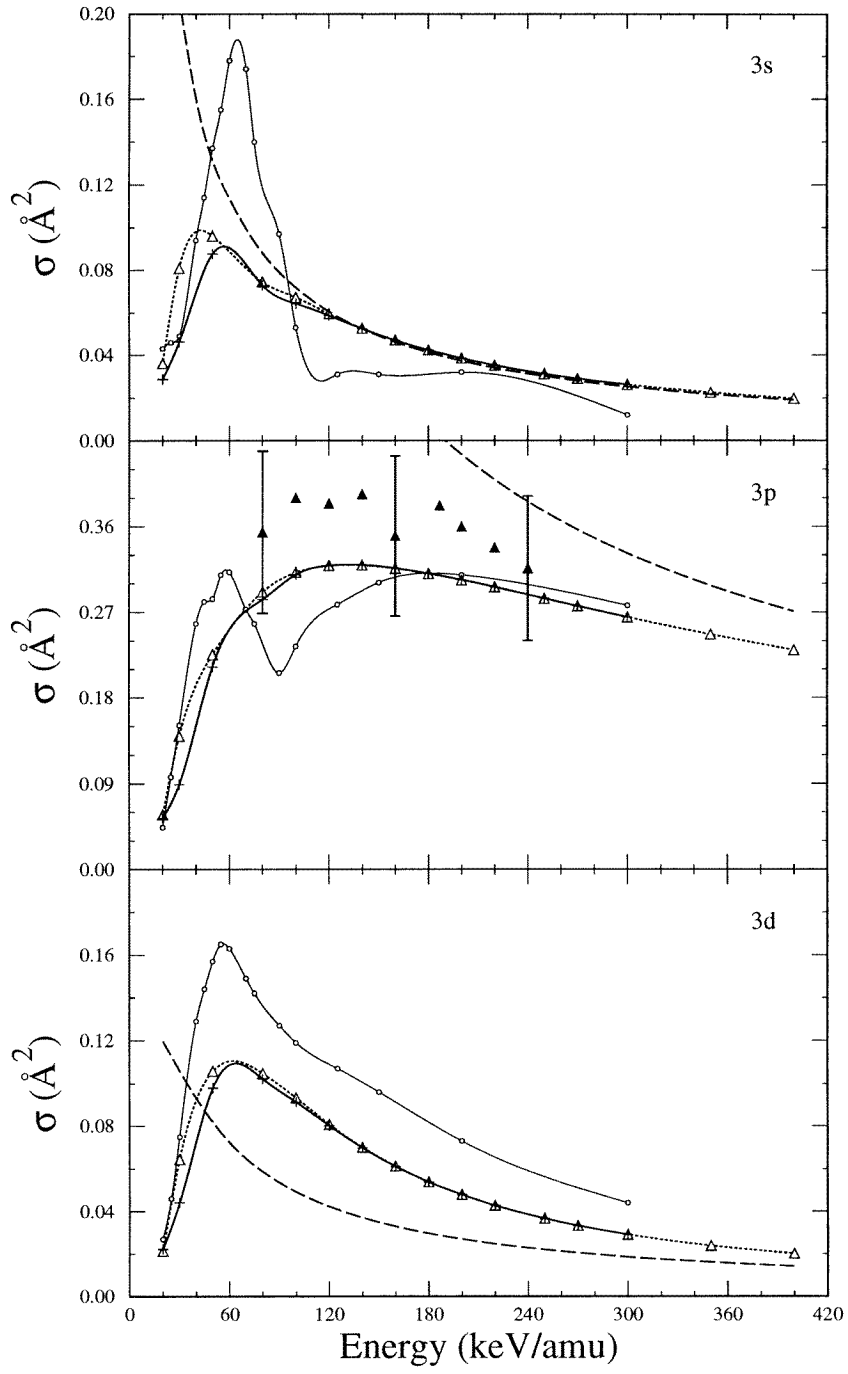

Figure 2. Excitation cross sections to 3s, 3p and 3d. The same notation is used as in figure 1.

3.2. Balmer alpha emission cross section and Balmer H_α polarization fraction

The total cross sections for Balmer alpha emission from direct target excitation can be readily derived from the present calculations. Our results are presented in figure 4 and

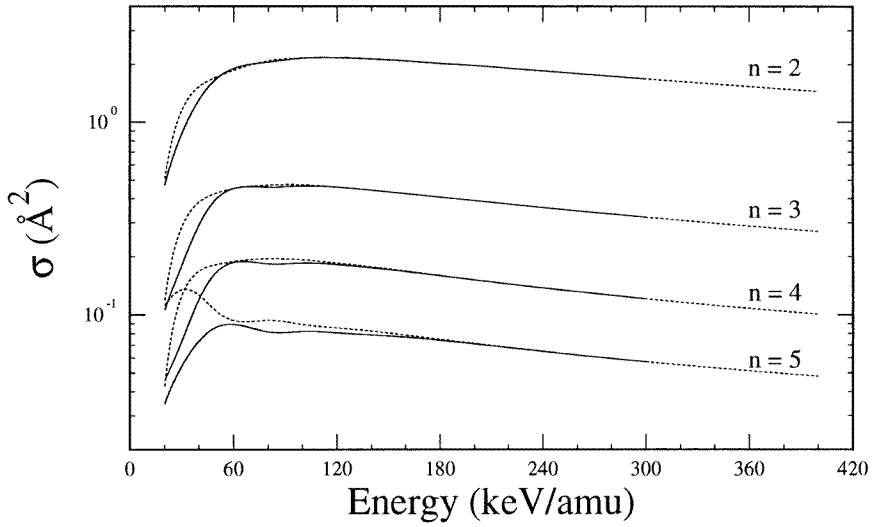

Figure 3. Total excitation cross sections to $n = 2$, 3, 4 and 5 from the present calculations. ——, present He35H174; ····· curve, present He4H174.

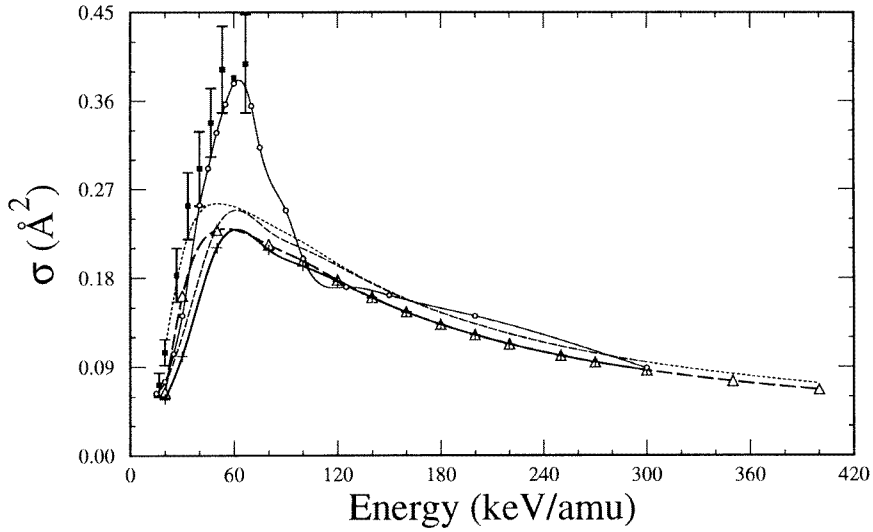

Figure 4. Cross sections for Balmer alpha emission from direct target excitation. ——, present He35H174; – – –, cascade correction included from present He35H174; △, present He4H174; ·····, cascade correction included from present He4H174; ○, Fritsch *et al* (1991); ■, experiment by Donnelly *et al* (1991).

compared to the previous calculation by Fritsch *et al* (1991) as well as with the experiment of Donnelly *et al* (1991). Note the good agreement between the calculation of Fritsch *et al* (1991) and the experimental data. The results from the present He4H174 and He35H174 calculations agree with each other very well but they do not agree with the experiment. Since we have calculated the excitation cross sections to 4ℓ and 5ℓ directly, we have also determined the cascade correction from these levels, but the effect is small.

The discrepancy between the present calculations and the experimental data of Donnelly and co-workers is particularly interesting. Near the peak, the experimental data are about a factor of two higher than what we consider for the converged results. While one may want to doubt the theoretical calculations, we want to point out a similar discrepancy also exists for the H^+–H system. There the Balmer alpha emission cross section for the excitation process obtained by Donnelly *et al* (1991) are about a factor of two larger than all existing theoretical calculations (refer to paper B and references therein). The discrepancy found here for the He^{2+}–H system, together with the existing discrepancy for the H^+–H system, points out the need for further experiments for the excitation cross sections for both systems in the energy range indicated.

We have also determined Balmer H_α polarization fractions from the present asymmetric close-coupling calculations, which are shown in figure 5. Our two calculations agree with each other for the impact energies above 80 keV amu^{-1}. Both predict the smooth dependence of the polarization fraction with impact energy. Note that there is a slight difference between the two calculations at impact energies below 80 keV amu^{-1}, which may result from the weak linear dependence of the basis set as mentioned above. Since the polarization fraction depends on the excitation cross sections to individual m sublevels, the experimental measurement provides a critical test of various theoretical studies. Recently, Werner and Schartner (1996) measured Balmer H_α polarization fractions of the impact-induced radiation of atomic hydrogen by protons and singly charged helium ions from 40 keV to 1 MeV. They found that the polarization fractions vary smoothly with impact energy in these systems, while all the symmetric close-coupling calculations predicted pronounced structures. We demonstrated in papers A and B that these predicted structures, from the symmetric close-coupling calculations in the p–H system, are basis dependent and therefore artificial. It is desirable to have the Balmer H_α polarization fraction measured for the He^{2+}–H collision system to compare with our prediction here.

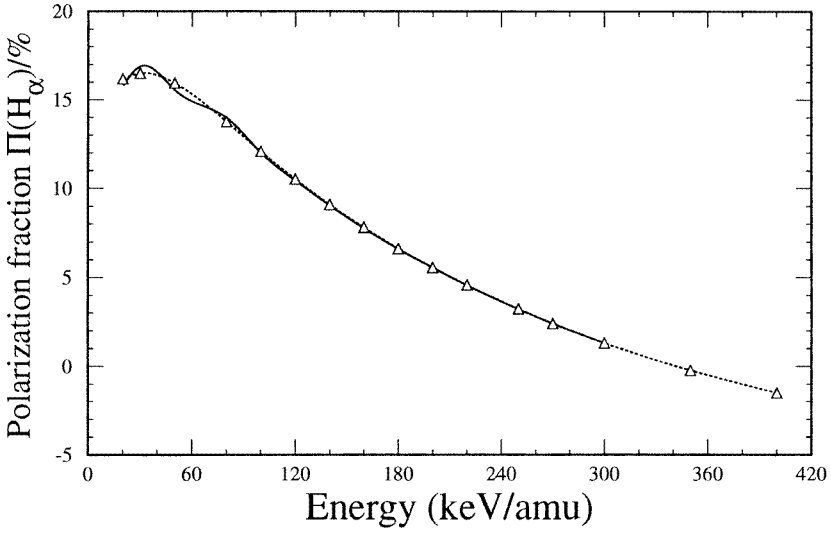

Figure 5. Polarization fraction of Balmer H_α induced by He^{2+} impact. ——, present He35H174; · · · · · ·, present He4H174.

3.3. Ionization cross section

There are a number of high-energy theoretical calculations for the ionization cross section in He^{2+}–H collision in the considered impact energy range. All of these high-energy theories, including the CDW-EIS theory of Crothers and McCann (1983) fail to reproduce the experimental data at impact energies below 100 keV amu^{-1}. The total ionization cross can also be obtained from close-coupling calculations as long as there are enough pseudostates to represent the continuum states. Since our basis sets (He4H174 and He35H174) have a large number of pseudostates, we can readily extract the total ionization cross sections with these two basis sets. The calculated ionization cross sections are shown in figure 6, together with the symmetric TCAO close-coupling calculation by Toshima (1994) with a basis set of He96H100 and the first Born approximation (Bates and Griffing 1953), as well as the experimental data by Shah and Gilbody (1981) and Shah *et al* (1988). Our previous calculation (Shingal and Lin 1989) was not shown since its accuracy is limited by the small number of the basis functions used.

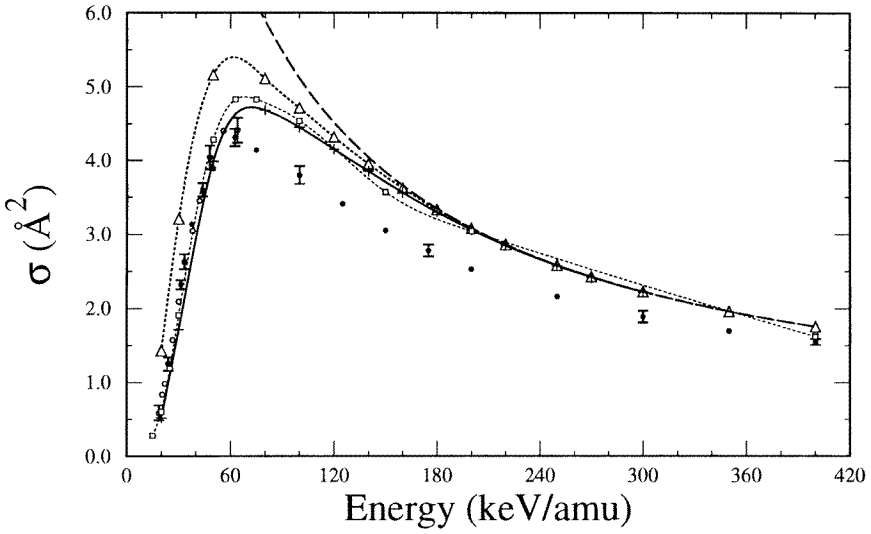

Figure 6. Ionization cross sections. Curves are obtained with interpolation; ——, present He35H174; △, present He4H174; — — —, First Born; □, Toshima (1994); ●, experimental data by Shah and Gilbody (1981); ○, experimental data by Shah *et al* (1988).

Our ionization cross sections from both basis sets vary with impact energy smoothly over the entire impact energy region. However, the evaluated ionization cross section with the basis set He4H174 appears to be too large at the low-energy side, due to a lack of highly excited states (i.e. $n = 3$ and 4) in the basis set, as we mentioned previously. The present calculation with the basis set He35H174 agrees very well with the experimental data (Shah *et al* 1988) at impact energies below 60 keV amu^{-1}. Above this energy, our calculation smoothly converges to the first Born approximation and somehow lies above the experimental data by about 20%. The present calculation with the basis set He35H174 is in good accord with the symmetric TCAO close-coupling calculation by Toshima over the entire energy range. Nevertheless, his result is not as smooth as ours which is likely to be due to the simultaneous use of projectile-centred pseudostates and target-centred pseudostates.

In view of the fact that both Toshima's and our close-coupling calculations appear

to have converged, it is difficult to understand the difference between the experimental data and the close-coupling calculations, which is about 20% for impact energies above 60 keV amu^{-1}. This is also true for H^+–H collision, where the close-coupling calculations (see paper B) predict a larger ionization cross section than the experimental value. Although the CDW-EIS theory of Crothers and McCann (1983) does agree with the experimental data by Shah and Gilbody (1981) at the high-energy side, further high-precision measurements for ionization cross sections in both He^{2+}–H and H^+–H collisions are called for in order to resolve this discrepancy.

3.4. Electron capture cross sections

According to our previous study (see paper A), the basis sets (He4H174 and He35H174) are not suitable for obtaining accurate individual electron capture cross sections, especially capture to the weak highly excited states since all the pseudostates are placed on the target centre. The electron capture cross sections to highly excited states with such basis sets will have some small oscillatory structures versus impact energy. However, we do expect electron capture cross sections to the dominant channels to be more stable; therefore, the

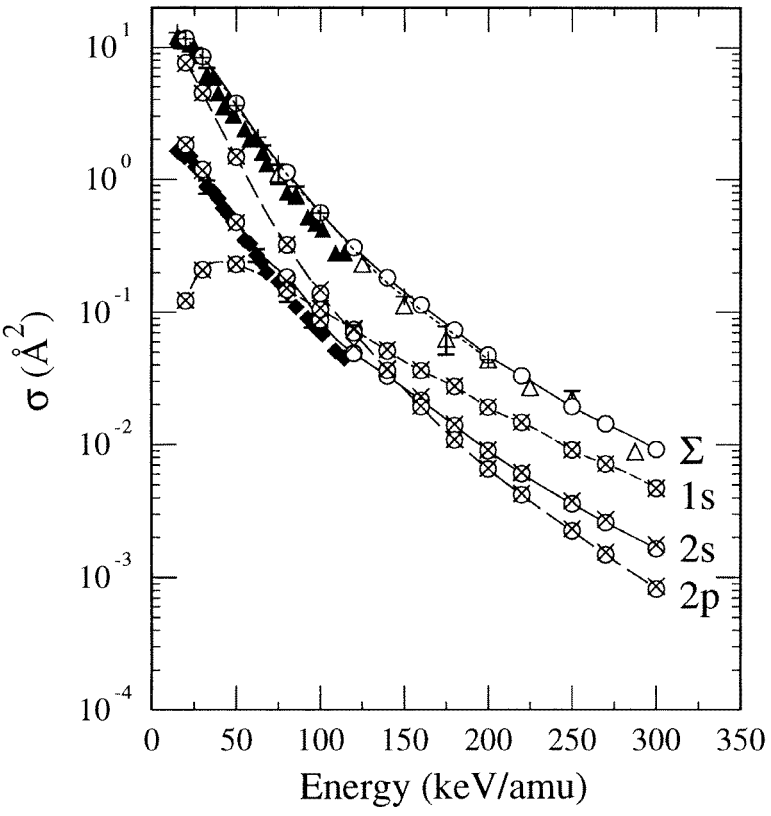

Figure 7. Electron capture cross sections. Theory: ○, present He35H174; ×, present He4H174; +, Toshima (1994). Note that the total capture cross sections (Σ) are obtained by summing over the capture cross sections to $n = 1$, 2, 3, 4 and 5 from the present He35H174. Experiment (total): ▲, Shah and Gilbody (1978); △, Hvelplund and Anderson (1982). Experiment (2s): ♦, Shah and Gilbody (1978).

total electron capture cross section will also be quite stable against the basis set used. It is useful to compare the total electron capture cross section calculated with the present close-coupling calculations with the experimental data (Shah and Gilbody 1978, Hvelplund and Anderson 1982) as well as with other theoretical results (Toshima 1994). Note that the total electron capture cross section can only be obtained with the basis set He35H174. Plotted in figure 7 is not only the total capture cross section but also electron capture cross sections to 1s, 2s and 2p. The evaluated total electron capture cross section with the basis set He35H174 agrees very well with the experimental data and with Toshima's calculation.

For electron capture cross sections to 1s, 2s and 2p, we have also plotted the results calculated from the basis set He4H174. Interestingly, calculations with the basis sets He4H174 and He35H174 are almost coincident with each other. A slight difference is observed in capture cross section to 2s in the impact energy region 80–120 keV amu^{-1}. Nevertheless, the calculated capture cross section to 2s is still in good agreement with the experimental data (Shah and Gilbody 1978). To calculate the smooth capture cross sections to the highly excited states ($n \geqslant 3$), we would have to switch the pseudostates to the projectile centre. This goes beyond the scope of the present paper.

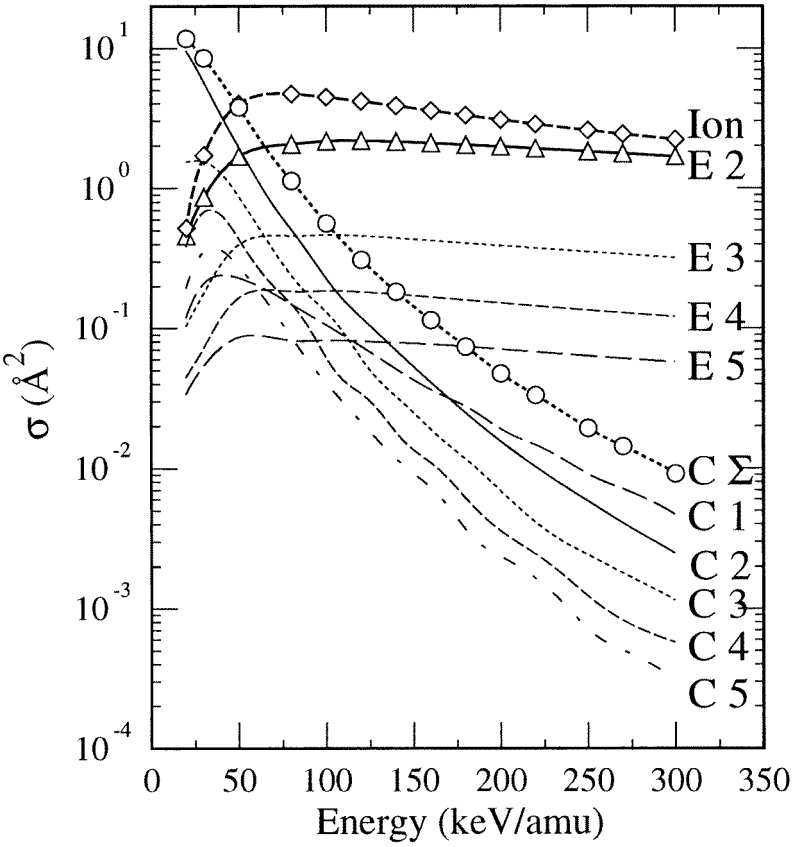

Figure 8. Cross sections for capture, excitation and ionization for He^{2+}–H collision. Ei, excitation to $n = i$; Ci, capture to $n = i$.

3.5. Overall picture of capture, excitation and ionization for He^{2+}–H collision

To complete our careful study of the He^{2+}–H collision system, we have plotted electron transfer, excitation and ionization cross sections obtained with the basis set He35H174 in figure 8. We can clearly see the major features related to this collision system from the figure. As we mentioned previously, electron capture cross sections to the highly excited states ($n = 3$, 4 and 5) are not very smooth; however, they all have the correct magnitude. Moreover, the total capture cross section is pretty smooth over the entire impact energy range. For impact energies below 50 keV amu^{-1}, electron transfer is predominant over ionization and excitation. Above this energy, ionization and excitation to $n = 2$ become dominant. Note that ionization cross sections are always larger than excitation cross section in this energy range (20–400 keV amu^{-1}). Therefore, the correct description for the excitation process requires the proper handling of the ionization channels. In other words, it is not possible to get accurate excitation cross sections without enough pseudo-continuum states incorporated in the close-coupling expansion. Since electron capture cross sections drop quickly with increasing impact energy, we expect that a single-centred expansion would be sufficient at impact energies above 150 keV amu^{-1}.

4. Summary and conclusions

In this paper we have carried out a detailed study of He^{2+}–H collisions in the intermediate 20–400 keV amu^{-1} energy region using the two-centre atomic orbital close-coupling method. We have further confirmed our previous investigation that reliable excitation and ionization cross sections can be calculated with the asymmetric TCAO close-coupling method with a large number of basis states on the target and a limited number of bound states on the projectile. The transition cross sections thus obtained show a smooth dependence on collision energy for impact energies above 20 keV amu^{-1}. Caution must be taken as more projectile-centred states are added to the TCAO close-coupling expansion. However, a certain number of projectile-centre states are necessary in order to extract reliable excitation and ionization cross sections at low energies (below 50 keV amu^{-1}). We believe that the results obtained here are converged at the few per cent level (all the data reported here are available upon request via e-mail).

The total electron transfer cross section obtained here agrees very well with the experimental data as well as other theoretical calculations. However, there exist obvious disagreements between the present calculations and the published experimental data by Donnelly *et al* (1991) and Hughes *et al* (1994) for the excitation cross sections. Based on the present study, the predicted structures in the excitation cross sections to 2ℓ and 3ℓ by Fritsch *et al* (1991) are believed to be artificial and basis dependent. New experiments are called for to resolve this discrepancy.

Acknowledgments

This work was supported in part by the US Department of Energy, Office of Energy Research, Office of Basic Energy Sciences, Division of Chemical Sciences. JYK is partially supported by NSF under grant no DMR-9413513 and CDL is also supported in part by the National Science Council, Taiwan under NSC85-2811-M009-004.

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