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Charge transfer in proton–helium collisions from low to high energy

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Abstract

The cross section for charge transfer in proton–helium collisions has been computed in the energy range from 10 eV/u up to 10 MeV/u. Four different methods (full quantal time-independent and time-dependent methods, molecular and atomic basis set semi-classical approaches) valid in different energy regimes have been used to calculate the partial and total cross section for single-electron capture. The results are compared with previous theoretical calculations and experimental measurements and the different theoretical methods used are shown to be complementary for describing the charge transfer reaction. A fit of the cross section, valid for collision energies from 10 eV/u up to 10 MeV/u is presented based on these results.

Keywords: charge transfer, plasma physics, astrophysics

(Some figures may appear in colour only in the online journal)

1. Introduction

The theoretical study of ion–atom charge transfer reactions over a wide range of collisional energies has an important role to play in the determination of the limits of validity of the different methods used to evaluate charge transfer cross sections. At low and intermediate energy (below 50 keV/u), the determination of the cross section is generally divided into two steps [1]. The first is the accurate calculation, beyond the Born–Oppenheimer approximation, of the potential energy curves (PECs) and their non-adiabatic couplings for the quasi molecular ion formed during the collision, and the second is the quantal or classical nuclear dynamics on the coupled PECs. For elementary reactions such as the electron transfer in p + He collisions, which is the simplest two-electron heteronuclear collisional system and a prototypical system to study ion–atom collisions, the intermediate quasi molecular ion is the cation HeH^+. This ion has been used as a test case for accurate calculations for the ground state [2–4] and excited states [5–7] with a variety of methods. Despite the accuracy obtained for the static parameters, the theoretical data for the resulting cross sections are scattered [8–10], demonstrating, if necessary, the difficulty of many-body dynamical calculations.

At higher energy, the different theoretical approaches based on atomic wavefunctions [11–13] correctly reproduce the shape and magnitude of the total cross section but two issues could be raised: firstly, the results obtained with semi-classical methods based on a molecular description of the collision used at intermediate energies and the semi-classical approaches using atomic basis sets for the high energy range rarely overlap, and secondly, a correct description of specific features present in the experimental differential cross sections, arising from dynamical correlation between electrons, is difficult to achieve [14–16].

From the experimental viewpoint, the same problems arise as there is no single method that can be employed to probe the entire range of energies. In addition, most measurements pertain to the total charge transfer cross section only, and no differentiation between capture in the ground or the excited states is available. In the case of charge transfer in p + He collisions, the experimental data are also scarce at low energy [17–19] and show significant discrepancies.

In this work, we will study the charge transfer reaction corresponding to the capture into H(1s),

$$p + \mathrm{He}(1s^2) \longrightarrow \mathrm{H}(1s) + \mathrm{He}^+(1s) \qquad (1)$$

as well as the total capture cross section,

$$p + \mathrm{He}(1s^2) \longrightarrow \mathrm{H} + \mathrm{He}^+(1s) \quad (2)$$

in which a sum over all final states of H is implicit. The total cross section is dominated by capture into 1s, while $n = 2$ states provide the main contribution from the excited states [9, 10]. These reactions will be examined for collision energies ranging from low (10 eV/u) up to high but non-relativistic (10 MeV/u). While the charge transfer cross section cannot be calculated using a single theoretical method over this broad energy range, we will show that by combining several approaches, each valid in a particular energy regime, it is possible to obtain an accurate cross section for the processes (1) and (2).

In addition to its relative simplicity, the p + He charge transfer reaction is also of major relevance in astrophysics and plasma physics. In order to characterize the alpha particle confinement in tokamak fusion test reactors, the energy distribution of the incident alpha particles is obtained from the energy distribution of the helium atoms escaping from the plasmas [20] and reaction (1) will be responsible for a loss in the helium density. The rate constant for reaction (1) is therefore necessary, and can be derived from the cross section and a specific velocity distribution. However, the data available in the Aladdin database [21] are limited to the high energy ranges (from 80 keV/u to 10 MeV/u), which only allows a limited range of validity in temperature for the rate constant. In addition, the low and intermediate energy range are important for modelling astrophysical processes such as the chemistry of the early universe [22].

In section 2, we briefly describe the theoretical methods used to compute the charge transfer cross section in the various energy regimes. The results obtained with each approach are presented in section 3 and compared with previous theoretical calculations and experimental measurements in each energy range. By combining the different approaches, we present a fit for reactions (1) and (2) that reproduces the cross section from 10 eV/u up to 10 MeV/u.

2. Theory

As previously mentioned, a unique theoretical method cannot be used to describe charge transfer over the entire energy range considered in this work. We therefore studied the reactions (1) and (2) using several approaches valid in different energy regimes that are overlapping. These methods can then be combined to obtain the charge transfer cross section over several orders of magnitude in energy.

For energies below 1 keV/u, we computed the cross section using two fully quantal methods. Both approaches are based on the knowledge of the PECs and non-adiabatic couplings for the relevant molecular states of the HeH^+ ion. We included the eight electronic states which correlate asymptotically with either $H^+ + He(1sn\ell\,{}^1L)$ or $H(n\ell) + He^+(1s)$ with $n \leqslant 2$, as well as the corresponding non-adiabatic radial and rotational couplings. Since the entrance channel in (1) and (2) is a singlet state, the triplet states of HeH^+ can be neglected. The molecular data were taken from [6], and details on the *ab initio* calculations can be found in this reference. The first method employed is time-dependent and is based on the propagation of a Gaussian wave packet on the PEC of the initial state. The time-propagation is realized by the split-operator algorithm [23] in the diabatic representation, and the S-matrix elements are calculated with the flux operator method [24] with a complex absorbing potential. This method has been previously described and used to compute charge transfer cross sections in several systems [25–28]. The second method is a time-independent approach which was used to ensure the validity of our results, in particular at low energy. The close-coupled scattering equations are solved in the diabatic representation using the log-derivative method [29, 30] with appropriate asymptotic conditions. This method is particularly helpful at the lowest energies considered here, because the wave packet approach can lead to numerical instabilities.

For energies between 0.5 and 50 keV/u, the cross section was calculated with an eikonal semi-classical approach in the impact parameter approximation [31]. The wavefunction is expanded in a set of molecular wavefunctions and the PECs and non-adiabatic couplings for the molecular electronic states discussed above are used. In the intermediate energy range, electron translation factors (ETFs) can have a significant impact on the cross section. Their effect was included through the approximation of the common translation factor [32], in the form first introduced in [33]. In this approach, the matrix elements of the operators x^2, xz and z^2 in the basis of the electronic wavefunctions are used to correct the radial and rotational non-adiabatic couplings. These matrix elements were calculated with the MOLPRO package [34] using the methodology described in [6].

For collision energies greater than 20 keV/u, we employed the non-relativistic semi-classical approach originally developed by Eichler and Chan [11, 35, 36] to treat the capture of the electron of a hydrogenic target in an arbitrary n, ℓ state by a projectile ion into an arbitrary n', ℓ' state. The method uses hydrogenic atomic wavefunctions and is based on the eikonal approximation. A classical rectilinear trajectory for the projectile with respect to the target nucleus is assumed. It includes the effect of translation factors as well as the eikonal phase factor [11], while multielectron effects are treated by means of an effective nuclear charge. The major advantage of this approach is that it results in an analytical expression for the cross section that can be written as the product of the well-known Oppenheimer–Brinkman–Kramers cross section multiplied by a scaling factor [36]. In consequence, the cross section for capture into the ground state as well as excited states can be readily evaluated. Despite its simplicity, the method has been shown to give accurate result for energies above 20 keV/u [11]. Relativistic effects can be safely neglected at 10 MeV/u [37], although they become important at higher energies.

3. Results and discussion

3.1. Low energy collisions ($E < 1$ keV/u)

The cross sections for the capture reactions (1) and (2) are presented in figure 1 for energies between 15 eV/u and 2 keV/u.

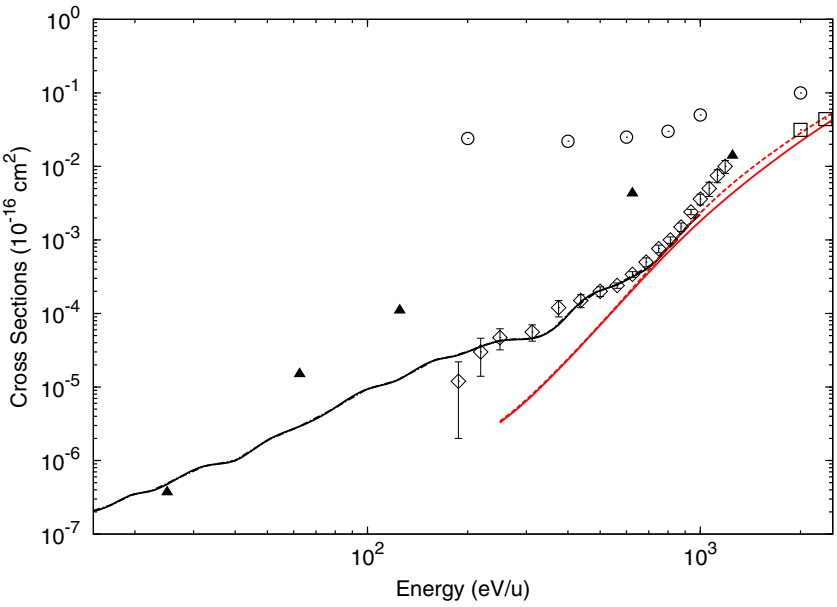

Figure 1. Cross section for reactions (1) and (2) for collision energies between 15 eV/u and 2 keV/u. Theory: black solid line: quantal method, reaction (1); black dashed line: quantal method, reaction (2); red solid line: semi-classical molecular method, reaction (1); red dashed line: semi-classical molecular method, reaction (2); full triangles: Kimura *et al* [38]. Experiments: circles, Stedeford and Hasted [17]; diamonds, Latypov and Shaporenko [18]; squares, Kusakabe *et al* [19].

Below 500 eV/u, the cross sections for both reactions are identical as the contribution from the excited $n = 2$ states is several orders of magnitude smaller than that of the 1s state. The contribution of the excited states increases with increasing energy and becomes significant above 500 eV/u. The capture into the $n = 2$ states accounts for about 30% of the total cross section at 1 keV/u.

As can be seen from figure 1, in the low energy range, the charge transfer cross section increases monotonically with the collision energy. The results obtained with the time-independent and time-dependent quantum approaches showed excellent agreement. We observed that the cross section obtained from the quantal and the semi-classical eikonal methods described in section 2 overlap around 800 eV/u, which is much higher than has been observed in other, heavier systems [27, 39].

Previous theoretical and experimental data are also shown on figure 1. It should be noted that all measurements are for the total capture cross section, which therefore contains a small contribution from the excited states. To the best of our knowledge, there are only two experimental [17, 18] and a single theoretical [38] studies on charge transfer in p + He collisions below 1 keV/u. This might be explained by the fact that since the cross section decreases with decreasing collision energy, its value becomes difficult to evaluate and measure. Measurements were performed in this energy range in the 1950s [17, 40], which show a large discrepancy with our results. The experimental cross section has an almost constant value below 1 keV/u, while we find a cross section decreasing with decreasing energy. This discrepancy with the experimental data has been discussed previously [9] and could reflect the difficulty of measuring this cross section at low energy. At these energies, the collision is governed by the transition between the first two molecular states of HeH^+, which is well described by the Rosen–Zener model [1]. This semi-classical model predicts a cross section decreasing exponentially with the energy, which can be seen in figure 1 (red curve). Below the range of validity of the impact parameter approximation, the cross section continues to decrease with decreasing energy. This is confirmed by another set of experimental data due to Latypov and Shaporenko [18] that produces excellent agreement with our results at low energy. As mentioned above, the reactions (1) and (2) below 1 keV/u have only been the subject of a single theoretical work [38]. Perhaps surprisingly given the simplicity of the system considered, we find discrepancies between our results and those presented in [38]. These calculations were performed by solving the time-independent Schrödinger equation on the PECs corresponding to the two relevant $^1\Sigma^+$ molecular states. Our calculations were performed using both a time-dependent and a time-independent approach, with consistent results, and the origin of the discrepancy is therefore unclear. However, the general behaviour, i.e. a decrease of the cross section with decreasing energy, is the same in both sets of calculations.

3.2. Intermediate energy collision (1 keV/u < E <100 keV/u)

The 1s and total charge transfer cross sections are presented in figure 2 for energies between 1 and 100 keV/u. The cross section continues to increase with the energy and reaches a maximum at around 20 keV/u, and decreases at higher energy. The cross sections obtained with the semi-classical molecular and atomic methods overlap at around 70 keV/u in the case of capture into the 1s state, while for the total capture process (2) the overlap occurs around 50 keV/u. The contribution of the $n = 2$ states to the total cross section varies between 5% and 25% depending on the collision energy, as was already demonstrated experimentally [41–44] and theoretically

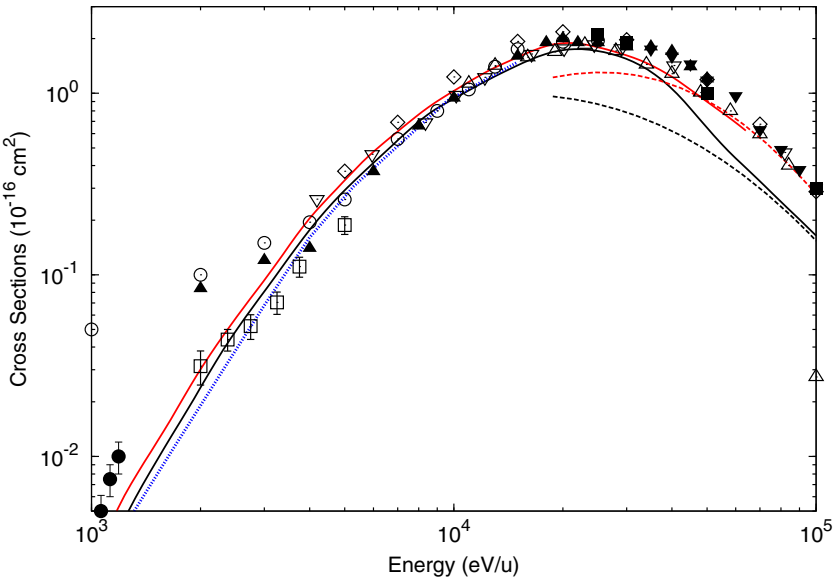

Figure 2. Cross section for reactions (1) and (2) for collision energies between 1 and 100 keV/u. Theory: black solid line, eikonal molecular method, reaction (1); red solid line, eikonal molecular method, reaction (2); black dashed line, eikonal atomic method, reaction (1); red dashed line, eikonal atomic method, reaction (2); dashed–dotted line: Kimura and Lin [9]. Experiments: circles, Stedeford and Hasted [17]; full circles, Latypov and Shaporenko [18]; squares, Kusakabe *et al* [19]; full triangles, Williams and Dunbar [50]; inverted triangles, Stier and Barnett [51]; diamonds, Rudd *et al* [52]; full squares, Martin *et al* [53]; triangles, Shah *et al* [54], full inverted triangles: Allison [40].

[45–47]. The $n = 3$ states have been shown in previous works to contribute to a few percent at most [47–49] so that we believe that the total cross section presented here is accurate.

In the intermediate energy regime, charge transfer in p + He collisions has been the subject of a large number of theoretical studies [8, 10, 45, 46, 48, 49, 55–58], motivated by the abundant experimental data accumulated over the years. Most of these theoretical works are based on the semi-classical impact parameter method and an expansion of the electronic wave function in atomic or molecular orbitals or on improved versions of these theories [9, 47] and include the effect of ETFs.

As can be seen in figure 2, we find excellent agreement between our results and the accurate atomic-orbital–molecular-orbital matching method calculations of Kimura and Lin [9] for the capture into H(1s). The agreement is only qualitative with previous calculations by other groups [8, 10, 57] that appear to be overestimating the total cross section compared to the experimental data.

For intermediate collision energies, the total charge transfer cross section has been measured by several groups over the past 50 years [17, 19, 40, 50–54, 59]. Below 3 keV/u, we find a discrepancy between our calculations and the measurements from [17, 50]. However, the agreement with the recent experiment by Kusakabe *et al* [19] performed for collision energies between 1.6 and 4 keV corroborates the present calculations.

For collision energies above 3 keV/u, the various experimental results for the total cross section are consistent with one another, although there is still an uncertainty on the absolute value of the cross section. We find a good agreement with our calculations performed with the semi-classical eikonal method. However, for collision energies between 30 and 70 keV/u, we observe that our calculations seem to underestimate the measured total cross section obtained by some groups [50, 51]. This is particularly perplexing as this is precisely the range of energy in which the results obtained with the two semi-classical theoretical methods used in this work overlap. It should still be noted that there are some discrepancies between the various experimental results at those energies.

3.3. High energy collision ($E > 100$ keV/u)

There exists a significant body of work on p + He collisions at high collision energy. The total charge transfer cross section has been the subject of extensive experimental studies in this energy regime [40, 51–54, 60–66]. From a theoretical point of view, ion–atom collisions involving two electrons have been used as prototypical systems to investigate various approaches to describe single-electron capture, usually based on the Born distorted wave (BDW) method or the continuum distorted wave (CDW) method in the framework of three-body [13, 14, 67] or four-body formalisms [12, 68, 69]. Most of these works are also motivated by the description of features in the differential cross section [13, 68, 70] that have been observed in recent experiments on charge transfer and transfer ionization processes [71–73]. In particular, the Thomas classical double scattering process [1] leads to a peak in the differential cross section at small scattering angles [15, 74, 75] that is very sensitive to the theoretical method.

The charge transfer cross sections for reactions (1) and (2) in the high energy regime and up to 10 MeV/u are presented in figure 3 together with experimental data points. The method used in this energy range relies on an effective nuclear charge for He. The best agreement with the measurements was obtained for an effective charge $Z_{\text{eff}} = 1.60$, slightly smaller than the value of 1.6875 obtained from the variational method. The total cross section was obtained by summing

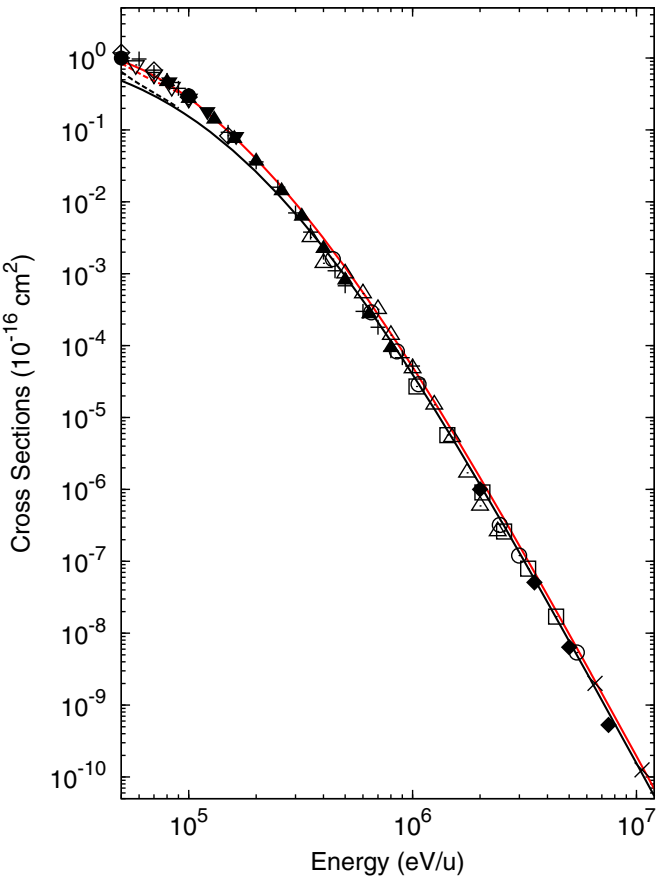

Figure 3. Cross section for reactions (1) and (2) for collision energies between 50 keV/u and 10 MeV/u. Theory: black dashed line, eikonal molecular method, reaction (1); red dashed line, eikonal molecular method, reaction (2); black solid line, eikonal atomic method, reaction (1); red solid line, eikonal atomic method, reaction (2). Experiments: crosses, Berkner *et al* [60]; squares, Schryber [61]; full diamonds, Schwab *et al* [62]; full triangles, Shah and Gilbody [63]; inverted triangles, Shah *et al* [54]; triangles, Williams [64]; full inverted triangles, Stier and Barnett [51]; circles, Welsh *et al* [65]; diamonds, Rudd *et al* [52]; full circles, Martin *et al* [53]; plus signs, Allison [40].

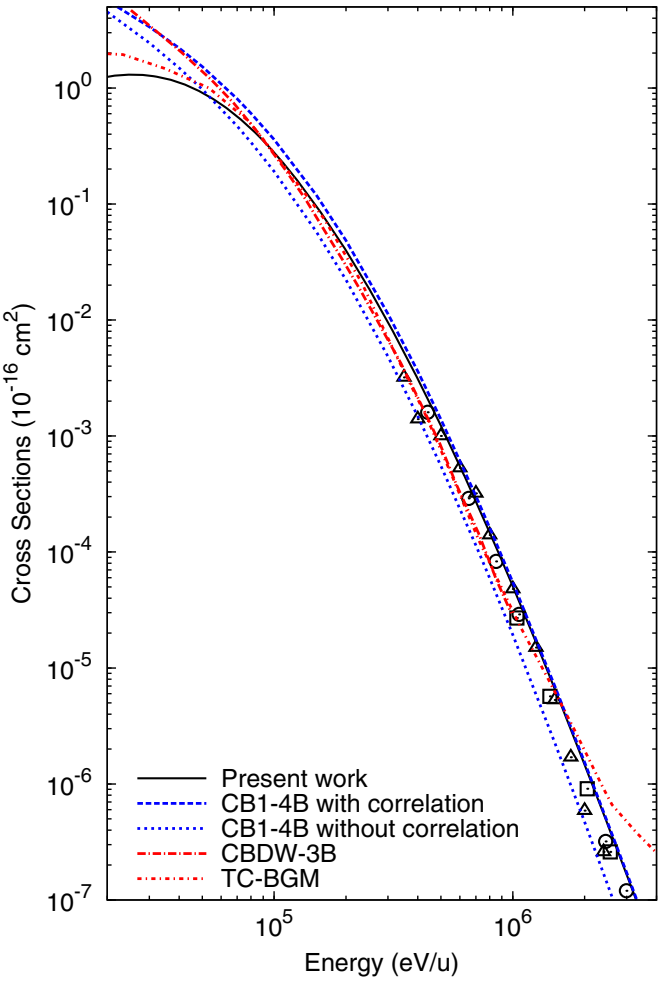

Figure 4. Total charge transfer cross section in p + He collisions compared with selected theoretical and experimental works for collision energies between 20 keV/u and 4 MeV/u. Theory: CB1-4B, Mancev and Milojevic [79]; CBDW-3B (with $Z_{\text{eff}} = 1.33$), Ghanbari-Adivi [14]; TC-BGM method, Zapukhlyak *et al* [70]. Experiments: squares, Schryber [61]; circles, Welsh *et al* [65]; triangles, Williams [64].

the contributions of all H($n\ell$) levels, and we observe a close correspondence with the experimental data. It is important to note that most of the other theoretical approaches allow the computation of the cross section for the capture in 1s only, which is subsequently scaled by a factor 1.202 to account for the capture in the excited states following an approach first introduced by Oppenheimer [76]. This scaling provides a good approximation to the total charge transfer cross section, but relies on the assumptions that the capture occurs exclusively in the s states and that the contribution of the excited states is independent of the collision energy. Furthermore, it was derived for one-electron systems. In table 1, we present the high-energy cross sections for capture into 1s as well as the contribution of all s states and the total charge transfer cross section summed over all $n\ell$ states. At the highest energies (from 2 to 10 MeV), we observe that only the s states contribute to the capture and that the ratio of the total cross section to the 1s cross section is independent of the energy, as predicted by the Oppenheimer scaling rule. However, the scaling factor has a value of 1.25, close to but larger than the value of 1.202 mentioned above. A similar value was obtained recently with the CB1-4B method [77]. However, at energies below 2 MeV the ratio increases to reach a value of 1.90 at 50 keV. Moreover, as the energy decreases we observe that the contribution of the

Table 1. Cross sections (in 10^{-16} cm^2) for single-electron capture in p + He collisions calculated with the eikonal atomic method. Brackets denote powers of 10. Columns 1–3 contain the cross sections for capture into 1s, all s states, and the total cross section. The last two columns contain the ratio of the cross sections for capture into s states to the capture into 1s, and the ratio of the total cross section to the 1s cross section.

E (keV)	1s	s states	Total	Ratio ns/1s	Ratio tot/1s
50	3.58[−01]	3.96[−01]	6.81[−01]	1.11	1.90
100	9.35[−02]	1.09[−01]	1.60[−01]	1.17	1.71
200	1.28[−02]	1.53[−02]	1.86[−02]	1.19	1.45
500	3.55[−04]	4.30[−04]	4.59[−04]	1.21	1.29
1 000	1.32[−05]	1.62[−05]	1.67[−05]	1.23	1.26
2 000	3.54[−07]	4.38[−07]	4.44[−07]	1.24	1.25
5 000	2.22[−09]	2.77[−09]	2.78[−09]	1.25	1.25
10 000	4.31[−11]	5.40[−11]	5.41[−11]	1.25	1.25

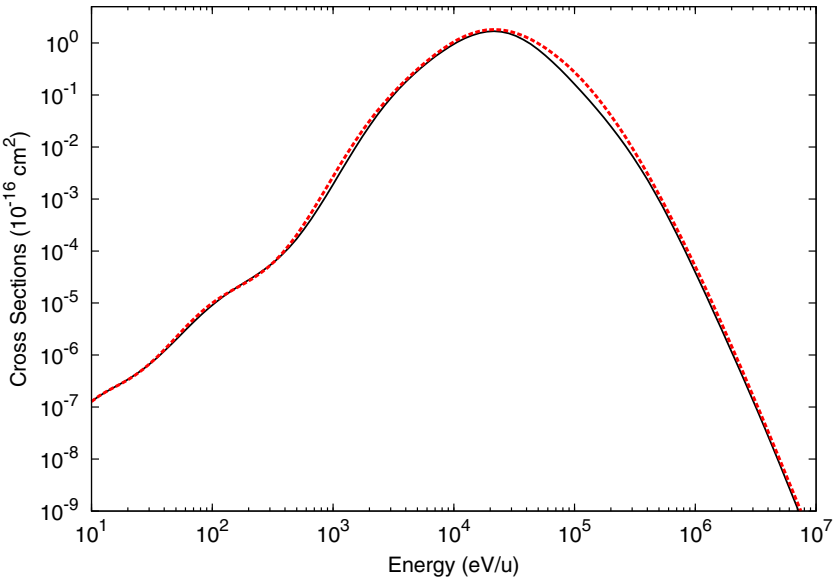

Figure 5. Fit of the cross section for reactions (1) (solid line) and (2) (dashed line) for collision energies between 10 eV/u and 10 MeV/u obtained from a combination of the methods described in section 2.

excited s states gradually diminishes while the contribution of the excited states with $\ell > 0$ increases. Therefore, care must be taken when using the Oppenheimer scaling law, as has been previously noted in $H^+ + H$ collisions [78].

In figure 4, we compare our results for the total charge transfer cross section to previous theoretical studies. We observe a good agreement between the various methods at high energy. However, at energies below 100 keV/u, the approaches based on the three- or four-body CDW and BDW theories overestimate significantly the cross sections, which means that there is no overlap with results in the intermediate energy range. The two-centre basis generator method used by Zapukhlyak *et al* [70] presents the correct behaviour, but fails for energies above 2 MeV/u. Some works have focused on the role of electronic correlation in p + He collisions, in particular on the differential cross section [79]. However, when compared to other monoelectronic approaches for the total charge transfer cross section, no significant effect could be noticed due to the inclusion of such correlation effects. We therefore believe that the methods used in the present work, which give a correct behaviour both below 100 keV/u and above 2 MeV/u, are accurate enough for the computation of the charge transfer cross section.

Finally, we should note that in a recent paper, Kim *et al* [15] were able to experimentally determine the contributions of the ground and excited states of both the projectile and the target, the latter being essentially due to the Thomas scattering. They showed that at energies between 630 and 1200 keV/u, the capture into 1s represents between 75% and 77% of the total cross section, while we find values between 77% and 79% at the same energies.

3.4. Fit of the cross section

Based on the previous discussion of our results and the complementarity of the different methods, we present a recommended cross section for the reactions (1) and (2) obtained from a least-square fit of the data in figure 5. We selected the data obtained with the quantal methods in the range from 10 to 700 eV/u, with the eikonal molecular method in the range from 0.7 to 60 keV/u, and with the eikonal atomic method in the range from 60 keV/u to 10 MeV/u. Due to the wide range of collision energies considered in the present work, the large variation of the cross section over this range, as well as the structures present in the cross section in the low-energy regime (see figure 1), an accurate fit of the cross section is difficult to achieve with few parameters. We opted for a Fourier expansion in logarithmic scale,

$$\log(\sigma) = a_0 + \sum_{n=1}^{7} (a_n \cos[nw \log(E)] + b_n \sin[nw \log(E)]) \tag{3}$$

where E is in units of eV/u and the cross section is in units of 10^{-16} cm^2. The coefficients for the expansion (3) are presented in table 2 for reactions (1) and (2). The resulting fit reproduces the cross sections with an uncertainty of less than 25% between

Table 2. Cross section fit coefficients for equation (3).

Coefficient	Process (1)	Process (2)
a_0	−5.167	−4.887
a_1	−5.200	−5.060
a_2	−0.326 5	−0.760 7
a_3	−0.378 6	−0.605 3
a_4	−0.043 99	−0.255 0
a_5	−0.053 18	−0.174 3
a_6	−0.069 57	−0.142 7
a_7	0.010 72	−0.019 07
b_1	0.113 1	−0.725 4
b_2	1.279	1.029
b_3	0.486 7	0.300 3
b_4	0.194 4	0.106 2
b_5	0.130 5	0.091 36
b_6	0.035 01	−0.011 04
b_7	−0.045 30	−0.048 71
w	0.780 0	0.812 7

100 and 400 eV/u, where the structures in the cross section are difficult to reproduce, and of less than 5% over the rest of the energy range for both reactions.

4. Conclusions

Nowadays, the state of the art in the calculation of the charge transfer cross section in ion–atom collisions has reached a degree of accuracy such that the theory can adequately support or complement the experimental data. However, if the cross section for these reactions must be obtained over a wide range of energy, i.e. from a few eV/u to a few MeV/u, different approaches must be used. The number of works trying to collect all information on a wide range of energy for a specific reaction is still sparse [39, 80–82], and these works have illustrated the difficulty to obtain matching results in the collision energy regimes where the different theoretical methods overlap. Moreover, even for the simplest systems, discrepancies with the previous experimental and theoretical studies can appear. The present work points to the same conclusion. Four different methods (full quantal time-independent and time-dependent methods, molecular and atomic basis set semi-classical approaches) have been used in this work, and care has been taken to obtain a smooth description of the cross section from 10 eV/u to 10 MeV/u. This allowed us to construct a fit of the cross section to an analytical expression that can be used conveniently in the modelling of astrophysical and laboratory plasmas.

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