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H^+–He($1s^2$) collisions: CTMC calculations of single ionisation and excitation cross sections

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Abstract

The processes of helium single ionisation and excitation by proton impact are reviewed for the collision energy region relevant to He beam fusion edge plasma diagnostics (proton energy $10 < E < 50$ keV). Classical trajectory Monte Carlo (CTMC) calculations have been performed and compared with the existing data. Obtained results for single ionisation are close to available experimental data, while for excitation they are larger by up to a factor of two. For excitation into high quantum numbers, the n^{-3} scaling law is verified by our CTMC calculations.

Keywords: He ionisation by proton impact; He excitation by proton impact; Fusion plasma diagnostics

1. Introduction

The steepness of density and temperature profiles in the outermost region ("edge") of magnetically confined tokamak fusion plasmas is highly significant for the global plasma confinement. Edge plasma profiles are considerably influenced by absolute concentrations and distributions of strongly radiating excited impurity ions. For systematic optimization of the edge plasma profile, a suitable diagnostic technique is needed which permits sufficiently high spatial (≈cm) and temporal (≤ms) resolutions for measuring the plasma density, temperature and impurity concentrations. It has been proposed to inject a fast (typical injection energies 10–50 keV/amu) neutral helium diagnostic beam into the edge plasma and to observe the resulting characteristic He I line radiation along the He beam path. This He I radiation is produced from collisions between fast He atoms and the different plasma particles (electrons, hydrogen-isotope and impurity ions) [1,2]. From different He I emission line profiles measured along the diagnostic beam a suitable inversion algorithm can reproduce the edge plasma density profile, as shown for the conceptually similar fast Li beam diagnostics [3,4]. In contrast to the latter technique, however, fast He beam diagnostics may also provide the edge plasma temperature profile [1]. Moreover, suitably intense diagnostic He beams can conveniently be produced by "He doping" of standard neutral hydrogen beams for plasma heating [2]. The inversion algorithm contains all atomic data relevant for the collisional reactions with He atoms which give rise to He I line radiation. Therefore, the success of the complete diagnostic method depends critically on the quality (i.e. accuracy) of the atomic data base. As will be shown below, only scarce and probably not very accurate cross sections exist in the literature for excitation and ionisation of He atoms in collisions with hydrogen-isotope ions (protons, deuterons).

Investigation of single ionisation and excitation cross sections from proton collisions with ground state helium atoms also provides a test for the applicability of different theoretical and experimental methods. Experimental single ionisation cross sections are well established for intermediate to high proton collision energies E, typically higher than 20 keV [5,6,15], but they show large discrepancies for collision energies relevant to injection energies of diagnostic helium beams ($10 < E/m < 50$ keV/amu). Inconsistencies of single excitation cross sections have been pointed

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out by Fritsch [7,8] and de Heer et al. [9]. Experimental cross sections for particular electronic transitions obtained by different groups present similar energy dependencies at proton collision energies from 100 to 200 keV, but considerably deviate from each other in absolute magnitude. For proton collision energies of present interest ($E < 50$ keV), a review of the existing database status (see below) revealed a particular lack of reliable He I excitation cross sections.

During the last 15 years, theoretical studies on single ionisation based on both quantum-mechanical and classical methods have been extensively developed. Single electron transitions into excited states have been studied only in the quantum-mechanical framework. Accurate cross sections for both processes have been produced at proton collision energies higher than 100 keV, but still these processes are not satisfactorily described at lower E, especially below 25 keV.

In the present work we have performed classical trajectory Monte Carlo (CTMC) calculations of cross sections for H^+–He collisions for

single ionisation (σ_i)

$$H^+ + He(1s^2) \rightarrow H^+ + He^+ + e^- \quad \text{(I)}$$

and excitation (σ_e)

$$H^+ + He(1s^2) \rightarrow H^+ + He(1s, n) \quad \text{(II)}$$

in the proton impact energy range from 5 up to 200 keV. We note that in our classical calculations the "active" electron is treated as a spinless particle and therefore singlet and triplet states of the He atom cannot be distinguished. This means that in reaction (II) both singlet and triplet transitions with the same principal quantum numbers n are implicitly included. We are particularly interested in single electron transitions into higher principal quantum numbers n with $n = 4$–6, where the classical method is expected to provide reliable results. In order to compare in detail our calculations with data available in the literature, we have collected previously compiled experimental and theoretical data together with recent quantum-mechanical and classical calculations. Cross sections for

electron transfer ionisation (σ_{ti})

$$H^+ + He(1s^2) \rightarrow H + He^{2+} + e^- \quad \text{(III)}$$

double ionisation (σ_{di})

$$H^+ + He(1s^2) \rightarrow H^+ + He^{2+} + 2e^- \quad \text{(IV)}$$

total free electron production ($\sigma_- = \sigma_i + \sigma_{ti} + 2\sigma_{di}$), and single electron transitions into states with $n = 2, 3$ have also been reviewed. Tables for this collected data can be found on the web site (http://www.iap.tuwien.ac.at/www/atomic/hedatabase/).

2. Computational details

A consistent classical theoretical study of proton collisions with helium atoms requires a four-body formulation, where all particles interact by Coulomb potentials. The two electrons on the helium atom are strongly correlated and both of them have to be taken into account in the collision dynamics. However, even for this simple collision system, theoretical calculations at the collision energies of present interest become extremely difficult whenever both electrons and their Coulomb interaction are explicitly treated, mainly because of the initial conditions determination.

In the present work, a three-body Hamiltonian formulation (3CTMC) has been chosen for a simplified description of the collision dynamics. The three particles considered in this formulation are: (a) the incoming proton, (b) the "active" target electron and (c) the He^+ core.

We have performed two sets of calculations where the electron-He^+ core interaction is described either by a pure Coulomb potential with effective charge $Z_{eff} = 1.6785$ or by the model potential proposed by Reinhold and Falcon [10]. In both cases, the initial configuration of the helium atom ground state has been constructed according to the two-body micro-canonical distribution. The 3CTMC code used in the present work has been made available by the Laboratory of Gas and Plasma Physics at the University of Paris-Sud, where preliminary data have been obtained by Katsonis and Maynard [11]; it has been previously used in order to evaluate atomic data for ion–atom collisions [12]. The model takes into account the dynamics of one active electron of the target. For the helium case, the contribution of the second electron has to be included in the calculations of the reaction cross sections. By assuming that the two electrons are independent (independent electron approximation, IEA), the cross sections for single ionisation σ_i and excitation σ_e are expressed in terms of one-electron probabilities:

$$\sigma_i = 2\sigma_i^c P_e^c = 2\sigma_i^c(1 - P_i^c - P_{ec}^c) \quad (1)$$

$$\sigma_e = 2\sigma_e^c P_{n=1}^c = 2\sigma_e^c \left(1 - P_i^c - P_{ec}^c - \sum_{n>1} P_n^c\right) \quad (2)$$

P_i^c, P_{ec}^c, P_n^c and P_e^c denotes respectively the one-electron probabilities for

- single ionisation (reaction (I)),
- single electron capture,
- single excitation into energy level with principal quantum number n, and
- total single excitation $\left(P_e^c = \sum_{n>1} P_n^c\right)$,

as calculated by the 3CTMC model. σ_i^c and σ_e^c are the corresponding cross sections. Expression (1) remains correct when the "active" electron is ejected but not captured by the projectile and the other electron is not removed from the target. Expression (2) is used when only one electron is excited and the other remains in the ground state. P_n^c is

calculated by classifying the electron trajectories according to the following rule [13]:

$$0.5(E_n + E_{n-1}) \leq E_{cl} \leq 0.5(E_n + E_{n+1}) \quad (3)$$

where E_{cl} is the classical binding energy at the end of each collision event, leading to excitation of the target. All classical binding energies lying within the above interval belong to the energy level E_n. This energy level is defined as the average of the energies of the singlet states, corresponding to the same principal quantum number n. Calculations are performed for one-electron transitions into energy levels with $n = 4$–6, where the 'hydrogenic' approximation is expected to be more appropriate than for lower exited states $n < 4$.

For comparison, we also used the expression proposed in [14], which was derived from the classical phase space density. However, no considerable deviations have been found for excitation into the energy levels considered here. For each collision energy, 8×10^5 trajectories have been numerically integrated; the maximum statistical error is 7% for single ionisation and 20% for the least probable excitation channel considered here ($n = 6$). In the next paragraphs we will compare the present results with collected experimental and theoretical data. The validity of the IEA and the 'hydrogenic' representation of the helium atom are also discussed.

3. Results and discussion

In this section we compare our CTMC calculations with previously compiled experimental and theoretical data for single ionisation and excitation. In order to perform a detailed comparison, we give a brief overview of the status of the existing atomic database for each process separately.

3.1. Single ionisation

3.1.1. Experimental data

Experimental data for ionisation have been discussed in detail by Rudd et al. [5] and by Gilbody [6]. Few experimental methods can provide accurate data for pure single ionisation, especially at low energy collisions (<15 keV). Accurate measurements (within 10%) for individual channels (I), (III) and (IV) have been performed by the Belfast group [15,16] using the crossed beams coincidence counting (CBCC) technique. Experimental studies based on the parallel plate capacitor (PPC) technique provide cross sections for total free electron production (see for example [17]), including contributions from the channels (I), (III), and (IV). Large discrepancies (up to 50%) between different studies involving the above techniques have been found in the literature. Fig. 1 presents compiled data and CTMC calculation results together with detailed measurements for free electron production (σ_-) performed by Rudd et al. [18], in comparison with the pure single ionisation cross sections of Shah et al. [16]. As expected, the former measured cross sections

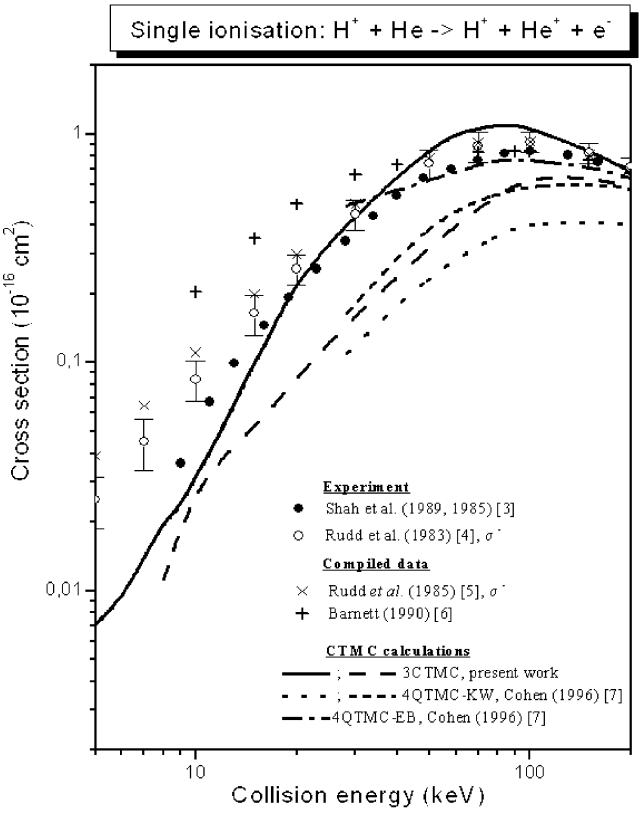

Fig. 1. Single ionisation cross sections as a function of collision energy. Experimental data: full circles, Shah et al. [16]; open circles Rudd et al. [18]. Compiled data: crosses, Rudd et al. [5] and Barnett [20]. CTMC calculations: solid line, present work using Coulomb potential between e^- and He^+ core; dashed line, present work using model potential between e^- and He^+ core; dotted, dashed-dotted and short dashed lines, Cohen [25].

are slightly larger than the latter ones in the energy range from 15 to 200 keV, but they are too large at lower collision energies where transfer and double ionisation are of minor importance compared to pure single ionisation. Coincidence measurements of Afrosimov et al. [19] for pure single ionisation (not shown) deviate considerably from the previous data. The data recommended by Rudd et al. [5] for σ_- are close to the values of Rudd et al. [18], while the data recommended by Barnett [20] for σ_i are considerably larger than the values of Rudd et al. [18] and Shah et al. [16] at proton collision energies $E < 40$ keV.

3.1.2. Calculated data

Considerable theoretical efforts have been made during the last 15 years in evaluating cross sections for proton collisions with helium atoms. Elaborate quantum-mechanical and classical calculations have been carried out in order to obtain a better physical insight for the collision processes (I), (III), and (IV). Four-body CTMC calculations of Wetmore and Olson [21], where electron-electron correlation was ignored, and of Montemayor and Schiwietz [22], where a radial correlation between the two electrons was considered,

gave improved results for pure single ionisation cross sections at collision energies higher than 100 keV. Still, transfer ionisation is not satisfactorily described. CTMC studies for ionisation processes have also been performed by McDowell and co-workers [23] and by Zaifman and Maor [24]. A considerable improvement has been achieved by Cohen [25] using the so-called quasi-classical trajectory Monte Carlo (QTMC) method, which is emphasizing the stability of the helium atom.

For pure single ionisation (I) Fig. 1 shows our results (full and dashed lines), based on two different types of potentials (see Section 2), and those obtained by Cohen [25]. A better agreement is obtained by our calculations when pure Coulomb interactions are considered. This is explained by the following reasoning: The initial electronic radial distribution according to the model potential presents a cut-off at a distance between the electron and the He^+ core smaller than the one corresponding to the pure Coulomb case [10]. Consequently, the electron is restricted into a smaller collision volume; contributions to ionisation cross sections coming from large impact parameters, which are important at low energies, are therefore suppressed. Our three-body CTMC calculations reproduce quite adequately the form of the experimental single ionisation cross sections; the position of the maximum is situated at 80 keV, being close to the experimental one at 100 keV. At this energy region, our results are about 25% higher than the data of Shah et al. [16]. They are in complete agreement at the energy region around 20 keV, but become smaller (∼30%) at lower energies. We note that at the higher collision energies considered here our results are near those of Schultz and Olson [26] (not shown).

Quantum-mechanical calculations, based on several approximations, have been extensively performed for pure single ionisation cross sections. Fig. 2 compares results obtained by the continuum distorted wave eikonal initial state (CDW-EIS) approximation of Fainstein et al. [27], the close coupling (CC) approach of Slim et al. [28] and Chen and Msezane [29], the two channel plane wave Born approximation (2-CPWBA) of Das and Malik [30], and the multi-electron hidden crossing theory (MEHC) of Krstic et al. [31]. Also included in Fig. 2 are our 3CTMC results for the pure Coulomb case and the experimental data of Shah et al. [16] and Rudd et al. [18]. Calculations of Sahoo et al. [32] using the impact parameter Born approximation (IPBA, not shown) are in agreement with measurements of [18]. The above quantum-mechanical calculations agree with the measurements at different energy regions, reflecting the range of validity of each approximation.

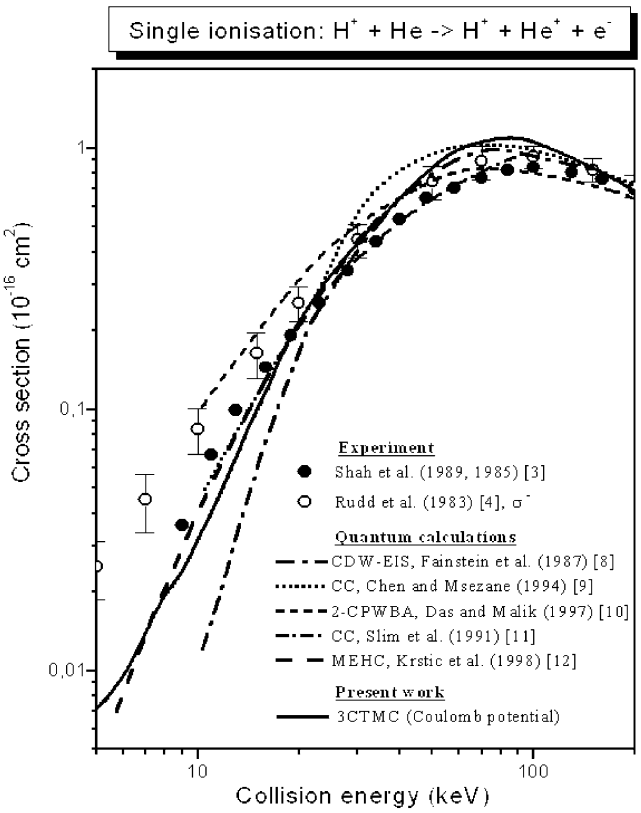

Fig. 2. Single ionisation cross sections as a function of collision energy. Experimental data: as in Fig. 1. Theory: dashed–dotted line, CDW-EIS calculations from Fainstein et al. [27]; short dotted line, CC calculations from Chen and Msezane [29]; short dashed line, 2-CPWBA calculations from Das and Malik [30]; short dashed–dotted line, CC calculations from Slim et al. [28], dashed line MEHC theory from Krstic et al. [31], solid line, 3CTMC calculations, present work.

3.2. Excitation

3.2.1. Experimental data

Experimental studies for one-electron excitation transitions in H^++He collisions have been performed in the 1960s and 1970s, based mainly on optical techniques. Fritsch [7,8] and de Heer et al. [9] pointed out an inconsistency in the experimental data for single excitation into n^1L states, for n = 3, 4, 5 and L = S, P, D. Absolute cross sections for the same transitions measured by different groups [33–39] show the same energy dependence in the overlapping region around 150 keV, but they considerably differ in magnitude. According to Fritsch [7,8] and to de Heer et al. [9], a consistent set of excitation cross sections for each individual transition can be obtained by using as a guide the corresponding experimental data at high energies (E > 500 keV), which either directly or after renormalization agree with the results of the Born approximation [40]. For high impact energy the data of Hasselkamp et al. [38] and Hippler and Schartner [39] can be considered as reliable because they converge there to the ones calculated with the Born approximation, while for energies around 150 keV the data of van den Bos et al. [36] are close to the former average cross sections, particularly for transitions into singlet states with n = 4.

3.2.2. Calculated data

Quantum-mechanical calculations of excitation cross sections have been performed in the late 1960s and early 1970s [41–47]. However, calculations from different investigators

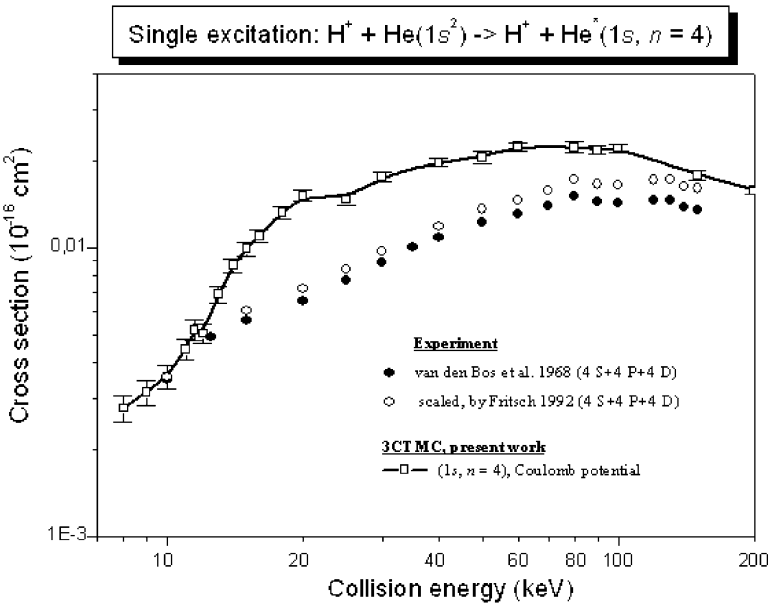

Fig. 3. Excitation cross sections for energy levels with $n = 4$, as a function of collision energy. Experimental data: full circles, van den Bos et al. [36]; open circles, scaled data by Fritsch [8]. 3CTMC calculations: open squares connected by solid line, present work.

frequently deviate from each other especially below 100 keV. Recent calculations based on the symmetric–eikonal (SE) model [48–50] give improved results for transitions into states ($n\ ^1$L), where $n = 2, 3, 4, 5$ and L = S, P, D at collision energies around 100 keV, and they converge to the results of the Born approximation at high E. For collision energies lower than 100 keV the calculations of Rodriguez et al. [50], where both electrons are explicitly treated are somehow in better agreement with the scaled experimental data. However, these calculations do not predict the oscillatory feature of the low energy cross sections observed experimentally [33,36].

The oscillatory character of the cross sections is also supported by the close coupling atomic orbital (CCAO) calculations of Fritsch [7,8] for excitation into the 2^1S, 3^1S, 2^1P, 3^1P and 3^1D states, which are in excellent agreement (except for the 2^1S state) with the scaled experimental data at collision energies between 5 and 30 keV.

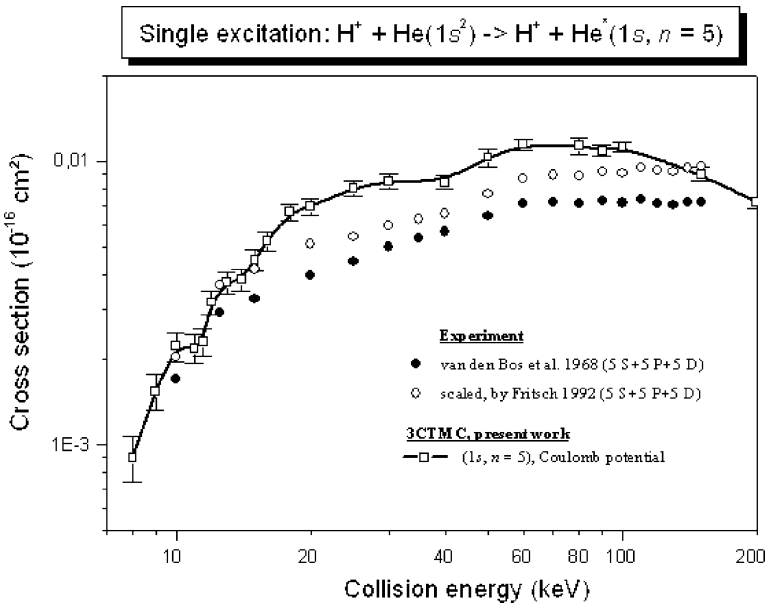

Fig. 4. Excitation cross sections for energy levels with $n = 5$, as a function of collision energy. Symbols as in Fig. 3.

Although several CTMC models have been used for evaluating ionisation and single electron capture channels, none of them have been applied to the study of helium excitation by proton impact until now. Therefore, in the present work total excitation cross sections into energy levels with $n = 4$–6, covering the energy region from 8 to 200 keV have been calculated according to the 3CTMC model described in Section 1. Calculations were performed for the case where the interactions between the three particles are of pure Coulomb type. Results obtained with a model potential between the "active" electron and the He^+ core (not shown) are considerably lower than the experimental data, as was the case for single ionisation. Figs. 3 and 4 show our results for excitation into energy levels with $n = 4$ and 5, together with the sum of the experimental values of van den Bos et al. [36] for transitions into 4^1S, 4^1P and 4^1D, and 5^1S, 5^1P and 5^1D states, respectively. Also included are the scaled data by Fritsch [8]. Note that the oscillatory structure observed in each individual channel (S, P and D) is suppressed when we add the corresponding cross sections. For excitation into energy levels with $n = 4$ our results are larger by up to a factor of two at 20 keV, but converge to the scaled data in the upper and lower collision energy limits considered here. This discrepancy can be attributed to the fact that the single

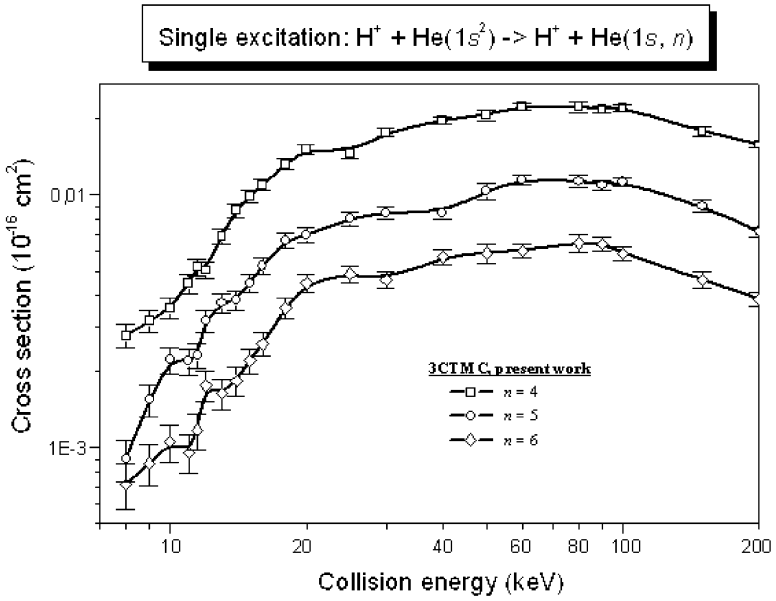

Fig. 5. Excitation cross sections for energy levels with $n = 4$–6 obtained by the 3CTMC model as a function of collision energy.

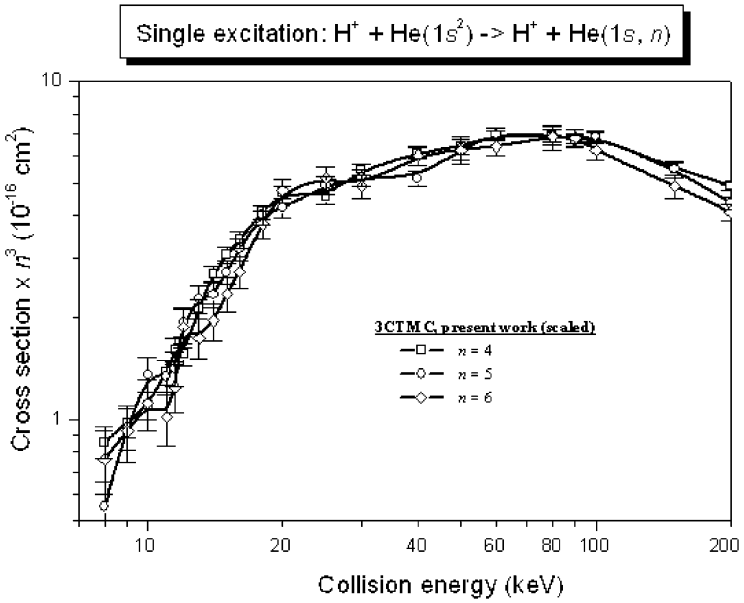

Fig. 6. Scaled excitation cross sections for energy levels with $n = 4$–6 obtained by the 3CTMC model as a function of collision energy.

excitation process, where correlation effects between the two electrons are important, cannot be properly described by a simple 'hydrogenic' representation of the helium atom within the independent electron approximation. However, a better agreement is obtained for excitation into energy levels with $n = 5$, supporting the fact that classical calculations are expected to become more realistic for higher quantum numbers. As mentioned in chapter 1, our classical calculations of the excitation cross sections implicitly include contributions from both singlet and triplet states. Therefore, it is not surprising that our results for transitions into energy levels with $n = 4$ and 5 are larger than the corresponding sum of the scaled data for singlet transitions, particularly at collision energies around 20 keV. In Fig. 5 we display our results for transitions into states with principal quantum numbers $n = 4$–6. As expected, excitation cross sections decrease for transitions into higher energy levels. Moreover, the cross sections follow a n^{-3} dependence, particularly at high energies, as also shown in scaled form in Fig. 6.

4. Summary and conclusions

In the present work, the status of the atomic database for single ionisation and excitation cross sections for proton collisions with neutral helium atoms was reviewed for proton impact energies relevant for He beam diagnostics (10–50 keV). We have mainly focused on the compilation of quantum-mechanical and classical calculations performed during the last ten years. In order to support this evaluation, we also have performed CTMC calculations within the independent- electron approximation, especially at the low collision energies considered here. A fairly good agreement between our calculations for single ionisation and corresponding experimental data has been obtained at proton collision energies from 10 up to 200 keV. Moreover, our CTMC calculations are in fair agreement with quantum-mechanical calculations at different collision energy regions. On the other hand, the single electron transitions into excited He I states cannot be properly described by a three-body classical formulation within the independent electron approximation, as shown by our calculations for transitions into energy levels with $n = 4$, 5. However, for transition into $n = 5$ states, we obtained a satisfactory agreement with scaled data by Fritsch [8]. This result supports the expectation that classical calculations involving the hydrogenic approximation become more realistic for transitions into levels with higher principal quantum numbers.

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