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Ionization of Hydrogen Atom by Proton Impact—How Accurate Is the Ionization Cross Section?

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Abstract: For the control of fusion reactors, we need to accurately know all the possible reactions and collisional cross sections. Although large-scale trials have been performed over the last decades to obtain this data, many basic atomic and molecular cross section data are missing and the accuracy of the available cross sections need to be checked. Using the available measured cross sections and theoretical predictions of hydrogen atom ionization by proton impact, critical analysis of the data is presented. Moreover, we also present our recent classical results based on the standard classical trajectory Monte Carlo (CTMC) and quasi-classical trajectory Monte Carlo (C-QCTMC) models. According to our model calculations and comparison with the experimental data, recom-mended cross sections for ionization of hydrogen were presented in a wide range of pro-jectile impact energies. We found that, while in the low energy region, the experimental cross sections are very close to the C-QCTMC results, at higher energies, they are close to the results of our standard CTMC results.

Keywords: proton-atom collision; ionization; classical trajectory Monte Carlo method; collision

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Citation: Tőkési, K.; Alassaf, S. Ionization of Hydrogen Atom by Proton Impact—How Accurate Is the Ionization Cross Section? *Atoms* **2023**, *11*, 122. https://doi.org/10.3390/atoms11090122

Academic Editor: Claudio Mendoza

Received: 6 March 2023
Revised: 29 April 2023
Accepted: 10 May 2023
Published: 15 September 2023

1. Introduction

The currently used energy production methods will not be able to satisfy the energy needs of humanity in the long run. In the absence of a rapid increase in energy storage efficiency, it is becoming increasingly urgent to develop an environmentally friendly and regulated new energy source. One of the best solutions in the future would be the implementation of fusion power plants. It is of cardinal importance to understand the processes that govern the behavior of the plasma that is used in nuclear fusion devices. On a microscopic level, the plasma is governed by the collisions of its composing particles. For the control of a fusion reactor, we need to know accurately, in principle, all possible reactions and collisional cross sections, such as excitation, ionization, recombination, and charge transfer cross sections.

Although the accurate knowledge of the interaction of protons and hydrogen atoms is a crucial point in fusion research, the accuracy of the known cross is not well defined and needs further investigations to clarify and validate the cross section data. In the past, the collision process has been modeled using a wide range of theoretical techniques [1–6], but there have been significant discrepancies between their results. Leung and Kirchner's [7] results validate some of these previous conclusions by calculating the cross sections of hydrogen atoms in their first and second excited states for impact energies ranging from 1 to 300 keV. At the same time, they reveal continuing discrepancies in other models. The scattering of protons by hydrogen atoms has been investigated in several previous theoretical studies [1,8–14]. The cross sections in a collision between charged particles and atomic hydrogen have been studied using various quantum-mechanical models and methods such as applying the convergent close-coupling (CCC) [6] approach, the quantum-mechanical molecular orbital close-coupling (QMOCC) [15], the semiclassical two-center close-coupling method with atomic basis sets [16], the hyper spherical close-coupling (HSCC) models [17], using the solution of the time dependent Schrödinger equation (TDSE) [18], the lattice time dependence Schrödinger equation (LTDSE) [19], the classical over barrier model (COBM) [20], the one-electron diatomic molecule (OEDM) [21], and the boundary corrected continuum intermediate state (BCCIS) [22] models. However, in many cases, quantum-mechanical calculations are very complicated and unfeasible. Therefore, as an alternative calculation scheme and due to the simplicity of calculations, classical models have been developed and used to obtain the corresponding cross sections [23–37].

In this work, we present the total ionization cross sections of a neutral hydrogen atom by protons. The main objectives of the present study are to compare the available cross section data with each other obtained either experimentally or theoretically. Moreover, we also present our recent classical trajectory Monte Carlo (CTMC) and quasi-classical trajectory Monte Carlo (QCTMC) results. Based on our model calculations and comparison with the experimental data, we present our recommended cross sections for the ionization of hydrogen by proton impact for a wide range of impact energies relevant for fusion research. Atomic units are used throughout unless stated otherwise.

2. Theory

2.1. CTMC Model

In the early 1960s, the classical trajectory Monte Carlo method (CTMC) was established. Using the 3-body approximation, a set of 18 coupled equations of motion need to be solve numerically, with the initial conditions chosen randomly [24–30]. Abrines and Percival calculated the electronic and nuclear motions in H^+ + H collisions using the CTMC method [23]. It was quite surprising that the classical description could reproduce so much experimental data. In general, the CTMC method is a non-perturbative method and the many-bodies interactions, or reaction channels, can be studied simultaneously, which is one of the advantages of the CTMC model. In our standard three-body classical trajectory Monte Carlo model, the three particles are the electron e with mass m_e, the projectile ion P with mass m_P and the target nucleus T with mass m_T. Figure 1 shows the relative position vectors of the three-body collision system. The $\vec{r}_e$, $\vec{r}_P$ and $\vec{r}_T$ represent the position vectors for the electron, projectile ion and target nucleus, respectively (see Figure 1).

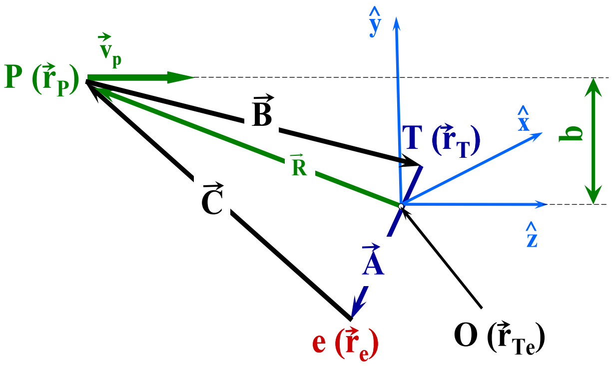

Figure 1. Schematic illustration of the position vectors $\vec{r}_e$, $\vec{r}_P$ and $\vec{r}_T$ in the laboratory frame in three-body approximation. The relative positions are defined as: $\vec{A} = \vec{r}_e - \vec{r}_T$, $\vec{B} = \vec{r}_T - \vec{r}_p$ and $\vec{C} = \vec{r}_p - \vec{r}_e$, in such way that $\vec{A} + \vec{B} + \vec{C} = 0$. R is the relative coordinate of the projectile with respect to the electron-target center of mass.

The Hamiltonian equation for the three particles can be written as:

$$H_0 = T + V_{coul} \tag{1}$$

where

$$T = \frac{\vec{P}_p^{\,2}}{2m_p} + \frac{\vec{P}_e^{\,2}}{2m_e} + \frac{\vec{P}_T^{\,2}}{2m_T}, \tag{2}$$

$$V_{coul} = \frac{Z_p Z_e}{\left|\vec{r}_p - \vec{r}_e\right|} + \frac{Z_e Z_T}{\left|\vec{r}_e - \vec{r}_T\right|} + \frac{Z_p Z_T}{\left|\vec{r}_p - \vec{r}_T\right|}, \tag{3}$$

are the total kinetic energy and the Coulomb potential energy of the interaction system. In addition, $\vec{r}$, $\vec{p}$, Z and m are the position, momentum vector, the charge and the mass of the corresponding particles p; projectile, e; electron, T; target, respectively. The total cross sections can be calculated as follows:

$$\sigma = \frac{2\pi b_{max}}{T_N} \sum_j b_j^{(i)}, \tag{4}$$

and the statistical uncertainty of the cross sections is given by:

$$\Delta\sigma = \sigma \left(\frac{T_N - T_N^{(i)}}{T_N T_N^{(i)}} \right)^{\frac{1}{2}} \tag{5}$$

where T_N is the total number of trajectories calculated for impact parameters less than b_{max}, $T_N^{(i)}$ is the number of trajectories that satisfy the criteria for ionization, and $b_j^{(i)}$ is the actual impact parameter for the trajectory corresponding to the ionization process.

2.2. QCTMC Model

In 1980s, the quasi-classical trajectory Monte Carlo (QCTMC) method was proposed by Kirschbaum and Wilets [31] as an improved version of the standard CTMC model. The effective potential was introduced to mimic the Heisenberg uncertainty principle and the Pauli Exclusion Principle for multi-electronic systems. The effectiveness of the QCTMC is elaborated in several studies [27–30,32–36]. Despite the fact that our calculation system is the simplest system, we use the Heisenberg correction term in the description of the hydrogen atom. The effective correction potential enforces the Heisenberg uncertainty principle $rp \geq \xi_H \hbar$, where r and p are the distance and momentum of an electron with respect to a nucleus and ξ_H is a constant. It was shown that significant improvement can be reached in the one electron collision systems also if the effective potential is introduced to mimic the Heisenberg uncertainty principle [27–30]. In our case, the Hamiltonian can be written as:

$$H_{FMD} = H_0 + V_H, \tag{6}$$

where H_0 is the standard Hamiltonian (see Equation (1)), containing the total kinetic energy and Coulomb potential energy terms for all bodies. The correction term is defined as:

$$V_H(r_{\lambda\nu} \cdot p_{\lambda\nu}; \xi \cdot \alpha) = \frac{\xi}{4\alpha r_{\lambda\nu}^2 \mu_{\lambda\nu}} exp\left\{ \alpha \left[1 - \left(\frac{r_{\lambda\nu} p_{\lambda\nu}}{\xi} \right)^4 \right] \right\}, \tag{7}$$

where, $r_{\lambda\nu} = r_\nu - r_\lambda$ is the relative distance between the electron and the nucleus (target or projectile) and the corresponding relative momenta are:

$$p_{\lambda\nu} = \frac{m_\lambda p_\nu - m_\nu p_\lambda}{m_\lambda + m_\nu} \tag{8}$$

$\mu_{\lambda\nu}$ is the reduced mass of the particles α and ν. The α and ξ are the Heisenberg adjustable hardness and dimensionless parameters, respectively.

In our work, we applied two versions of the QCTMC model: (1) the target-centered scheme (T-QCTMC) when the correction term is taken into account between the target electron and target nucleus, and (2) the target-projectile centered scheme (C-QCTMC) when the correction term is taken into account between the target electron and both the target nucleus and projectile.

3. Results and Discussion

To study the ionization cross section of the ground state hydrogen atom by proton impact, we employed a 3-body CTMC method and a QCTMC method. We performed the simulations with an ensemble of 5×10^6 primary trajectories for each energy. Our calculation was performed in the energy range between 10 keV and 1000 keV.

Figures 2 and 3 shows the target ionization probabilities as a function of impact parameter for projectile impact energies of 50 and 100 keV, respectively. The energy dependent impact parameter of the ionization probabilities was fitted by a Gaussian function. The peak maxima of the results of the Gaussian fitting are also shown in Figures 2 and 3. We found significant difference in the peak maxima of the ionization probabilities at lower energy. At smaller projectile velocities, due to the longer interaction time when the correction term can influence the motion, not only the ionization probabilities are changing but also the impact parameter picture. The correction shifted the probability distributions to higher b values. The target-centered T-QCTMC when the Heisenberg correction term includes only the electron of the target and the target nuclei shows the largest peak of the ionization probabilities. For higher incident energy, the probability distribution in the peak intensities show similar behavior to that for the lower energies; however, the peak maxima are at almost the same position. The correction term did not influence the impact parameter distributions any more.

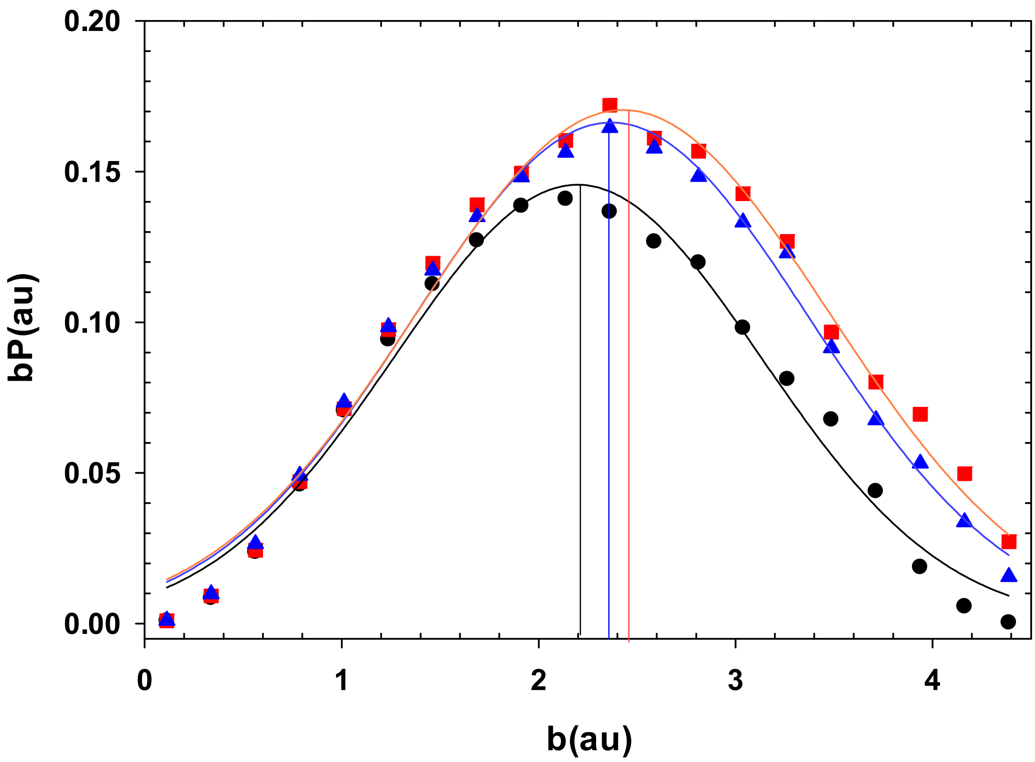

Figure 2. Target ionization probabilities in p + H collisions as a function of impact parameter. Black circles: a CTMC results for 50 keV impact energy. Blue triangles: target and projectile-centered C-QCTMC results for 50 keV impact energy. Red squares: target-centered T-QCTMC for 50 keV impact energy. The lines through the calculated data are the results of the best Gaussian fit to guide the eyes.

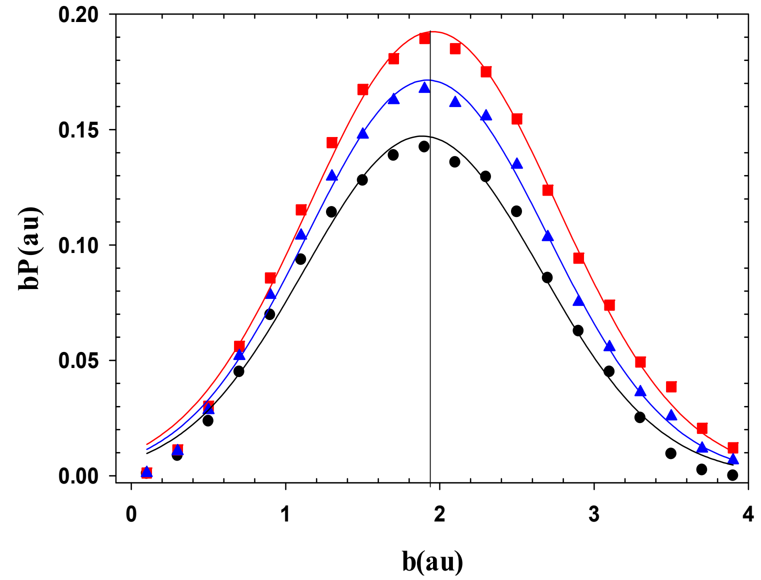

Figure 3. Target ionization probabilities in p + H collisions as a function of impact parameter. Black circles: a CTMC results for 100 keV impact energy. Blue triangles: target and projectile-centered C-QCTMC results for 100 keV impact energy. Red squares: target-centered T-QCTMC for 100 keV impact energy. The lines through the calculated data are the results of the best fit 'Gaussian curve' to guide the eyes.

The corresponding ionization cross sections can be obtained from Figures 2 and 3 by integrating the impact parameter dependent probabilities with respect to the impact parameter.

Figures 4 and 5 shows our present ionization cross sections of the ground state hydrogen atoms as a function of impact energy in comparison with the other theoretical results of Cohen [37], Winter [38], Kolakowska [39], Abdurakhmanov [40,41] and Toshima [42].

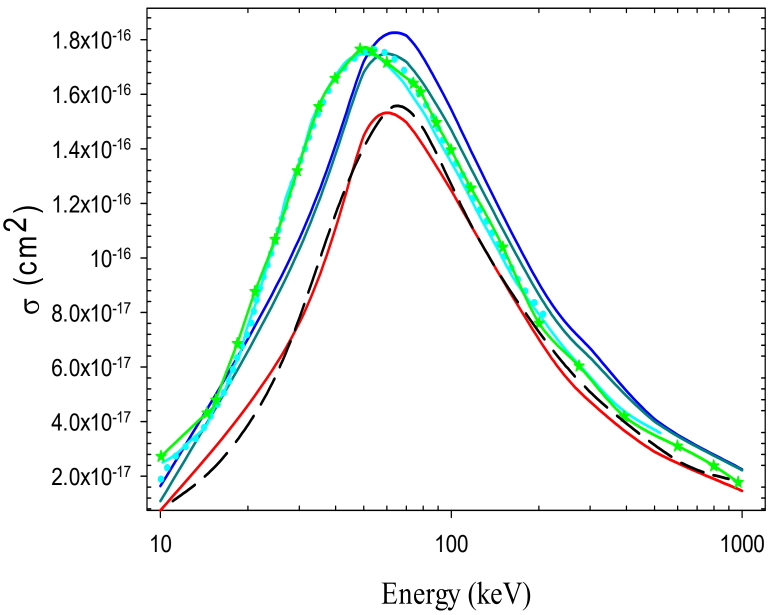

Figure 4. Ionization cross sections in H^+ + H (1s) collision as a function of impact energy. Solid red line: present CTMC results. Blue solid line: present target-centered T-QCTMC results. Dark cyan solid line: present target and projectile centered (fully corrected) C-QCTMC results. Black dashed line: QTMC-EB of Cohen [37]. Cyan solid line: one-center CCC approach of Abdurakhmanov [6]. Cyan dots: two-center CCC approach of Abdurakhmanov [40]. Green stars line: two-center close-coupling calculations of Toshima.

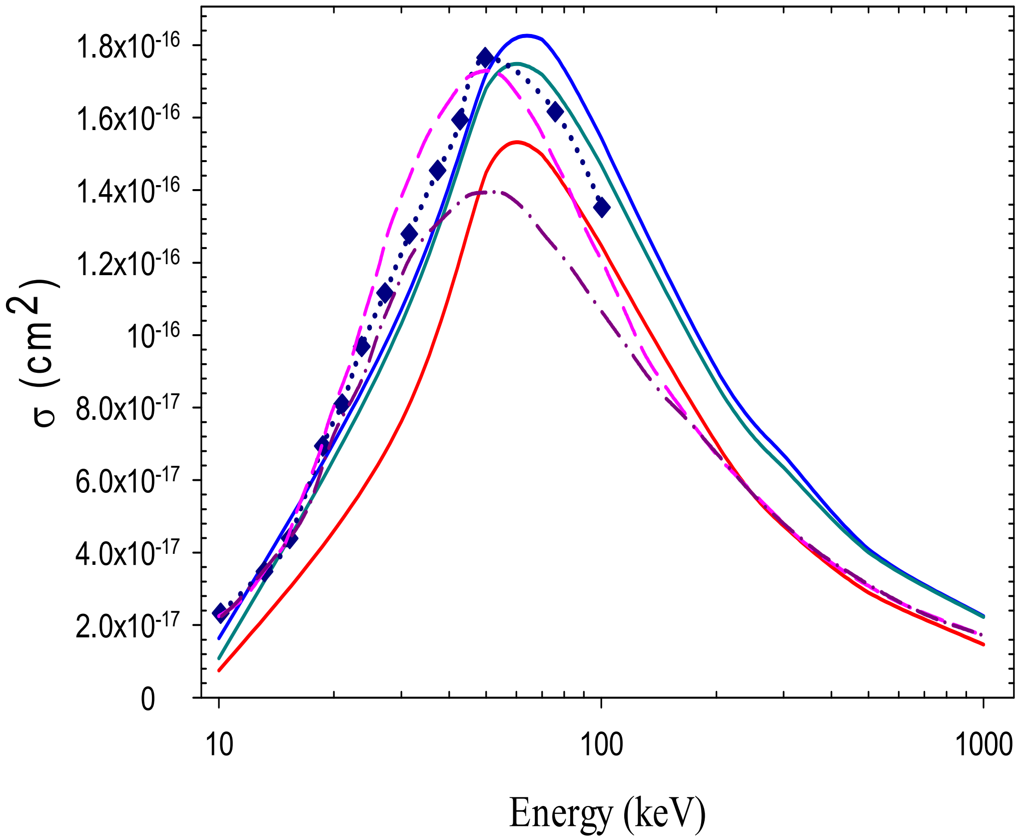

Figure 5. Ionization cross sections in H^+ + H (1s) collision as a function of impact energy. Solid red line: present CTMC results. Blue solid line: present target-centered T-QCTMC results. Dark cyan solid line: present target and projectile centered (fully corrected) C-QCTMC results. Dark blue diamond-dots: Coupled-Sturmian approach of Winter [38]. Dark pink dashed dots line: lattice time dependent Schrödinger equation (TDSE) method of Kolakowska [39]. Pink dashed dots line: QM-CCC results of Abdurakhmanov [41].

Kolakowska used a three-dimensional lattice solution of the time-dependent Schrödinger equation for low quantum states ($n < 3$) combined with classical trajectory Monte Carlo results for high quantum states ($n > 4$) to predict total electron loss and total charge-transfer cross sections for proton collisions with atomic hydrogen at intermediate energies [31]. Kolakowska's calculation shows an excellent agreement with the previous experimental data, particularly at intermediate energy regimes (see Figure 5). Abdurakhmanov and Toshima used the one and two-center close-coupling equations which were built from only target-centered pseudo states. In the one and two-center approaches, they found that the CCC calculations at lower energy regimes are far from experimental data (see Figure 4) [6,40]. This is maybe due to the fact that at these energies, the total electron-loss and electron-capture cross sections are comparable and an order of magnitude larger than the ionization cross section, which is defined as the difference between the two. On the other hand, the one and two-center CCC calculation overestimates all experimental data at the intermediate energy regime. This is due to the fact that the basis set of CCC approaches does not contain abundantly high-lying continuum states that are required for momentum matching [42]. In the present calculations, the results of the standard CTMC underestimate the previous theoretical and experimental data, particularly at low energy regimes most likely because in this energy range, the quantum effects maybe play more roles, but it has excellent agreement with QTMC-BE calculation of Cohen (see Figure 4). Meanwhile, the target-centered T-QCTMC and target and projectile-centered C-QCTMC calculations "i.e., fully corrected version of the CTMC model" exhibit nearly identical behavior at low energies. The target-centered and fully corrected "QCTMC" produces higher cross sections than standard CTMC data and agrees well with the previous theoretical and experimental data (see Figures 4–6), particularly at low energy regimes, demonstrating the impact of the Heisenberg correction as a non-classical potential to represent a quantum effect in order to overcome the theoretical deficiency in the CTMC model in the low energy regime. As a consequence, the target centered and fully corrected QCTMC calculations slightly overestimate all results in intermediate to high energy regimes.

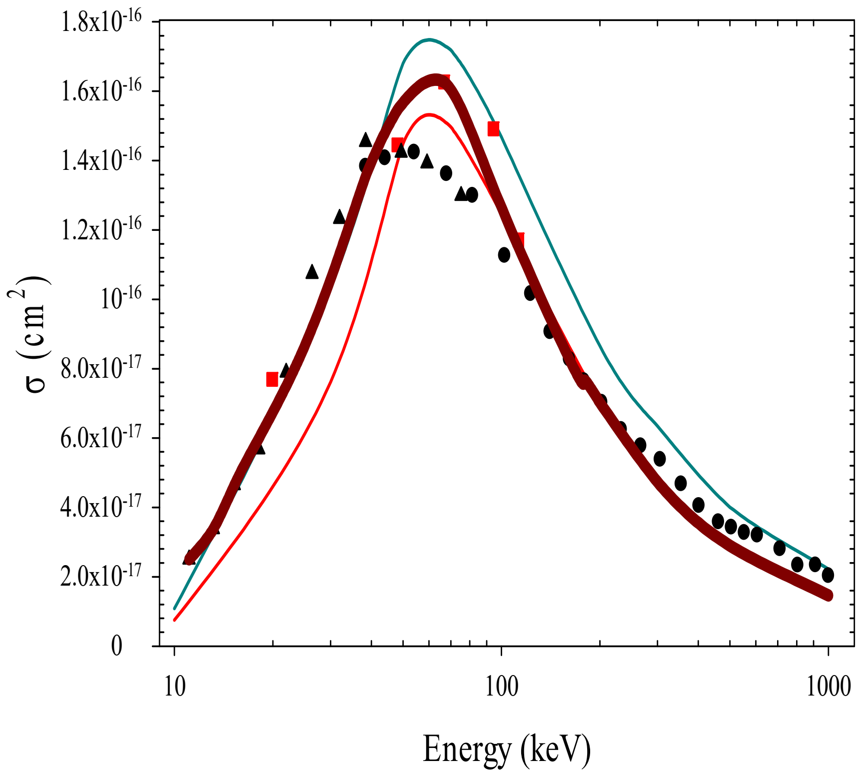

Figure 6. Ionization cross sections in H+ + H (1s) collision as a function of impact energy. Solid red line: present CTMC results. Dark cyan solid line: present target and projectile centered (fully corrected) C-QCTMC results. Dark solid red line: the recommended cross sections based on the comparison with experimental data [42]. Black circles: experimental data of Shah and Gilbody [43]. Black triangles: experimental data of Shah et al. [44], Red squares: experimental data of Kerby et al. [45].

The comparison with experimental results, on the other hand, had the greatest impact on determining the accuracy of our classical and quasi-classical cross section calculations.

Figure 6 shows the ionization cross sections of the ground state hydrogen atoms as a function of impact energy in comparison with the available experimental data of Shah and Gilbody [43], Shah et al. [44], and Kerby et al. [45]. At high energies, above 100 keV, the classical calculation (CTMC) agrees very well with the experimental data of Shah and Gilbody [43]. Meanwhile, at low energy regimes, the QCTMC cross sections are more accurate and agree well with the results of Shah et al. [44]. Figure 6 shows also our recommended cross sections based on our classical simulations.

4. Conclusions

Using the available measured cross sections and theoretical predictions of hydrogen atom ionization by proton impact, the critical analysis of the data was presented. We also presented our recent classical results based on the classical trajectory and quasi-classical trajectory Monte Carlo models. The calculations were performed in the projectile energy range between 10 keV and 1000 keV. It was found that the standard CTMC exhibited a good agreement with the previous experimental data in intermediate to high energy regimes. Moreover, the target-centered T-QCTMC and fully corrected C-QCTMC model showed a higher cross section than standard CTMC results and agreed well with the previous theoretical and experimental data at a low energy regime. We found that the QCTMC model improved the cross section results, especially at low energy regimes. According to our model calculations and comparison with the experimental data, recommended cross sections for ionization of hydrogen were presented in a wide range of projectile impact energies. We found that, while in the low energy region, the experimental cross sections are very close to the C-QCTMC results, at higher energies, they are close to the results of our standard CTMC results.

Author Contributions: Both authors discussed the results and contributed to the final manuscript. S.A. collected the literature data and wrote the manuscript. K.T. developed the CTMC code, performed numerical simulations and supervised the project. All authors have read and agreed to the published version of the manuscript.

Funding: This work has been carried out within the framework of the EUROfusion Consortium, funded by the European Union via the Euratom research and training program (Grant Agreement No. 101052200—EUROfusion). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Commission. Neither the European Union nor the European Commission can be held responsible for them.

Data Availability Statement: The datasets generated during and/or analyzed during the current study are available from the corresponding authors on reasonable request.

Conflicts of Interest: The authors declare no conflict of interest.

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