The effects of Heisenberg constraint on the classical cross sections in proton hydrogen collision

Iman Ziaeian1,2 and Károly Tokési1,*

1 Institute for Nuclear Research (Atomki), 4026 Debrecen Bern tér 18/c, Hungary
2 Doctoral School of Physics, Faculty of Science and Technology, University of Debrecen, PO Box 400, H-4002, Debrecen, Hungary

E-mail: tokesi@atomki.hu

Received 22 December 2021, revised 31 July 2022
Accepted for publication 24 October 2022
Published 17 November 2022

Abstract
The interaction between a proton and a ground state hydrogen atom is studied using a standard three-body classical trajectory Monte Carlo (CTMC) and a quasi-classical trajectory Monte Carlo (QCTMC) model where the quantum feature of the collision system is mimicked using the model potential in the Hamiltonian as was proposed by Kirschbaum and Wilets (1980 Phys. Rev. A 21 834). The influence of the choice of the model potential parameters ($\alpha$, $\xi$) on the initial radial and momentum distribution of the electron are analyzed and optimized. We found that although these distributions may not be as close to the quantum results as the distribution of standard CTMC results, we can find the combination of the ($\alpha$, $\xi$) where the calculated cross sections are closer to the experimental data and closer to the results obtained quantum mechanically. We show that the choice of $3 < \alpha < 5$ is reasonable. To validate our observation, we present cross sections for ionization, excitation, charge exchange (CX), and state selective CX to the projectile bound state. Calculations are carried out in the projectile energy range between 10 and 1000 keV amu$^{-1}$.

Keywords: quasi classical trajectory Monte Carlo model, ionization, excitation, charge exchange

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

1. Introduction
The proton–hydrogen collision system is the simplest collision system in ion–atom collisions. This fundamental one-electron system has great significance for testing various theoretical descriptions where, luckily, a large number of experimental results are available for various channels like ionization, charge exchange (CX), excitation and state-selective CX cross sections.

We have also used the H$^+$ + H collision system to evaluate the effects of the Heisenberg correction term on cross sections in the a quasi-classical trajectory Monte Carlo (QCTMC) model where the quantum features of the collision system are mimicked using the model potential in the Hamiltonian as was proposed by Kirschbaum and Wilets [1].

We note here that the collision processes between ions and atomic hydrogen also have considerable interest for scientists working on fusion plasma research. Neutral beams of hydrogen atoms can be injected into tokamak plasmas to heat and fuel them [2], and they provide powerful plasma composition diagnostic tools through CX spectroscopy [3]. So the accurate cross sections data are essential.

The proton–hydrogen collision system has been widely studied both theoretically and experimentally for various
collision channels. Theoretically, Cohen calculated cross sections for all possible electronic rearrangements in $H^+ + H$ using a quasiclassical-trajectory Monte Carlo energy-bounded approach (QTMC-EB) [4]. This model is proposed to extend the classical trajectory Monte Carlo (CTMC) model. Avazbaev et al [5] used the semiclassical convergent close-coupling (SC-CCC) approach to study the cross sections for excitation, total and state-selective CX channels for a wide range of the proton impact energies from 1 keV to 1 MeV. The latest research on the subject is the development of the quantum-mechanical convergent-close-coupling [6, 7].

The proton–hydrogen collision was also studied extensively experimentally. The ionization cross sections in $H^+ + H$ collisions were obtained by Shah and Gilbody and Shah et al in 1981 and 1987 [8, 9], where the authors claim that the experimental error on the level of 5% or better. The cross sections for CX between a proton and a hydrogen atom have been measured in the low projectile energies by McClure [10]. The collisional excitation of the proton–hydrogen system has been investigated at intermediate energies applying the optical method by Dettleffsen et al [11]. The state-selective CX is another interesting collision channel that has been considered for many years. The experimental data for cross sections of the state-selective CX into 2s and 2p states of the projectile in $H^+ + H(1s)$ collision published in references [12–16].

The CTMC method was introduced in the early 1960s [17–19]. In this method, classical equations of motions are solved numerically, and the initial conditions are chosen randomly [20–22]. Abrines and Percival [23] applied the CTMC method to calculate the electronic and nuclear motions in $p + H$ collisions. It was quite surprising that the classical description was able to reproduce numerous experimental data. One of the advantages of the CTMC method is that many-body interactions are precisely taken into account during the collisions on a classical level.

The QCTMC method was proposed by Kirschbaum and Wilets in 1980 [1]. According to this model, for multi-electron atoms, a basic requirement for improving the standard CTMC method is that the electrons cannot collapse to the nucleus, and two identical electrons cannot occupy the same energy level. The effective potential was introduced to mimic the Heisenberg uncertainty principle and the Pauli constraint. The effectiveness of the QCTMC is justified in many studies. Zajfman [24] presented the ionization and CX cross sections for bare ions on helium atoms by applying the QCTMC model and obtained an excellent agreement with the experimental data. The ionization and CX in multiply charged ion–helium collisions have also been studied at intermediate energies by McKenzie [25]. Cohen evaluated various collision systems by considering the Heisenberg and Pauli constraints [26–30]. In recent years, the use of this model has been considered. Jorgan et al demonstrated the reliability of this approach for $H + H$ and $H^+ + H^-$ collisions [31]. In addition, the differential cross sections for CX in the collision of protons with He have been evaluated using CTMC and QCTMC methods by Bachi and Ottanto [32].

In this work, the interaction between a proton and a ground state hydrogen atom is studied using a standard three-body CTMC and a QCTMC model where the quantum feature of the collision system is mimicking by the potential proposed by Kirschbaum and Wilets [1]. Although our calculation system is one of the simplest systems, we apply the constrained potential in the description of the hydrogen atom. We expect improvements in the cross section calculations compared with the standard CTMC model because with the model potential we include quantum behavior in the classical system. The paper is organized as follows. In section 2, we describe the calculation models. Section 3 presents our results. In section 3.1 we show the distance and momentum dependent behavior of the model potential. We define the initial conditions of $r$ (radial distance between electron and hydrogen) and $p$ (linear momentum of the electron) in the QCTMC in section 3.2. To find the appropriate constants ($\alpha \cdot \xi$) used in Heisenberg potential function, firstly, we study the electron radial and momentum distribution in the QCTMC method in section 3.3. Secondly, we obtain the cross sections for all possible channels, such as target ionization in section 3.5, projectile CX in section 3.6, projectile state-selective CX target in section 3.7, and target excitation in section 3.8 in $p + H$ collisions. Finally, we predict the optimal combination of constants ($\alpha \cdot \xi$) by simultaneously analyzing and comparing the previous theoretical methods and experimental data with our theoretical calculations. The conclusions are summarized in section 4.

2. Theory

2.1. CTMC model

In the present work, we perform our calculations based on the standard three-body CTMC model. The electron $e$ of mass $m_e$, the projectile ion $P$ of mass $m_P$ and the target nucleus $T$ of mass $m_T$ form a three-body approximation. 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](https://example.com/figure1.png)
The Hamiltonian equation for the three particles can be written as:

$$H_0 = T + V_{\text{cont}},$$  \hfill (1)

where

$$T = \frac{\vec{p}_e^2}{2m_e} + \frac{\vec{p}_p^2}{2m_p} + \frac{\vec{p}_T^2}{2m_T},$$  \hfill (2)

$$V_{\text{cont}} = \frac{Z_pZ_e}{|\vec{r}_p - \vec{r}_e|} + \frac{Z_eZ_T}{|\vec{r}_e - \vec{r}_T|} + \frac{Z_pZ_T}{|\vec{r}_p - \vec{r}_T|},$$  \hfill (3)

are total kinetic energy and Coulomb potential of interaction system. Also, $\vec{r}, \vec{p}, Z$ and $m$ are the position, momentum vector, the charge and the mass of the given particles $p$; projectile, $e$; electron, $T$; target, respectively. The equations of motion taking into account the Hamiltonian mechanics is given as follows:

$$\vec{\dot{r}}_e = -\frac{\delta H}{\delta \vec{r}_e} = -\frac{Z_pZ_e}{|\vec{r}_p - \vec{r}_e|^3}(\vec{r}_p - \vec{r}_e) + \frac{Z_eZ_T}{|\vec{r}_e - \vec{r}_T|}|\vec{r}_e - \vec{r}_T|,$$  \hfill (4)

$$\vec{\dot{r}}_T = -\frac{\delta H}{\delta \vec{r}_T} = -\frac{Z_pZ_T}{|\vec{r}_p - \vec{r}_T|}|\vec{r}_p - \vec{r}_T| - \frac{Z_eZ_T}{|\vec{r}_e - \vec{r}_T|}|\vec{r}_e - \vec{r}_T|,$$  \hfill (5)

$$\vec{\dot{r}}_p = -\frac{\delta H_{\text{FMD}}}{\delta \vec{p}_p} = \frac{Z_pZ_e}{|\vec{r}_p - \vec{r}_e|}|\vec{r}_p - \vec{r}_e| + \frac{Z_eZ_T}{|\vec{r}_p - \vec{r}_T|}|\vec{r}_p - \vec{r}_T|,$$  \hfill (6)

The velocities of objects according to Hamiltonian mechanics are obtained as follows:

$$\vec{\dot{r}}_e = \frac{\partial H_{\text{FMD}}}{\partial \vec{p}_e} = N_e\vec{\dot{p}}_e,$$  \hfill (7)

$$\vec{\dot{r}}_T = \frac{\partial H_{\text{FMD}}}{\partial \vec{p}_p} = N_T\vec{\dot{p}}_T,$$  \hfill (8)

$$\vec{\dot{r}}_p = \frac{\partial H_{\text{FMD}}}{\partial \vec{p}_p} = N_p\vec{\dot{p}}_p,$$  \hfill (9)

where we define $N_e = \frac{1}{N}$. These differential equations were integrated with respect to the time by the 4th order Runge–Kutta method with an adaptive step size, starting from a given configuration of the collision for a given set of initial conditions [33]. The center-of-mass of the target atom is the origin of our coordinate system in the laboratory frame, and the velocity vector of the projectile is parallel to the $z$-axis (see figure 1).

The total cross sections are calculated by:

$$\sigma = \frac{2\pi b_{\text{max}}}{T_N} \sum_j b_j^{(i)},$$  \hfill (10)

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

$$\Delta\sigma = \sigma \left( \frac{T_N - T_N^{(0)}}{T_N T_N^{(0)}} \right)^{1/2},$$  \hfill (11)

where $T_N$ is the total number of trajectories calculated for impact parameters less than $b_{\text{max}}$, $T_N^{(0)}$ is the number of trajectories that satisfy the criteria for the corresponding final channels, and $b_j^{(i)}$ is the actual impact parameter for the trajectory corresponding electron capture processes.

In the classical calculations, the classical principal quantum number ($n_c$) and the classical orbital angular momentum ($l_c$) are given by:

$$n_c = Z_eZ_T \left( \frac{\mu_T}{2\mu_e} \right)^{1/2},$$  \hfill (12)

$$l_c = \sqrt{m_e [(x\dot{y} - y\dot{x})^2 + (x\dot{z} - z\dot{x})^2 + (y\dot{z} - z\dot{y})^2]},$$  \hfill (13)

where $\mu_T$ is the reduced mass of the target nucleus and the target electron. $x$, $y$, and $z$ are the Cartesian coordinates of the electron relative to the nucleus and $\dot{x}$, $\dot{y}$, and $\dot{z}$ are the corresponding velocities. The classical values of $n_c$ are ‘quantized’ to a specific $n$ level if they satisfy the relation:

$$[(n - 1)(n - 1/2)]^{1/3} \leq n_c \leq [(n + 1)(n + 1/2)]^{1/3}.$$  \hfill (14)

Since $l_c$ is uniformly distributed for a given $n$ level [34], the quantal statistical weights are reproduced by choosing bin sizes such that

$$l \leq l_{n_c} \leq l + 1,$$  \hfill (15)

where $l$ is the quantum-mechanical orbital angular momentum.

2.2. QCTMC model

In one electron collision systems, the effective potential is introduced to mimic the Heisenberg uncertainty principle. This approach was proposed by Kirschbaum and Wilets [1]. In this case, the Hamiltonian consists of constraining potential, $V_H$, motivated by the Heisenberg principle is added to the pure Coulomb inter-particle potentials describing the atom. Thus

$$H_{\text{FMD}} = H_0 + V_H,$$  \hfill (16)

where $H_0$ is the usual Hamiltonian containing the total kinetic energy of all bodies and Coulomb potential terms between all pairs of electrons and between the nucleus and electrons, respectively. The extra term is

$$V_H = \sum_{a=1}^{N} \sum_{b=1}^{N} \sum_{i=1}^{N} f(r_{ai} \cdot P_{ai}; \xi_H, \alpha_H),$$  \hfill (17)

where $a$ and $b$ denote the nuclei and the $i$ index the electrons. Also, $r_{\alpha\beta} = r_{\alpha} - r_{\beta}$ and relative momenta are:

$$P_{\alpha\beta} = \frac{m_\alpha P_\alpha - m_\beta P_\beta}{m_\alpha + m_\beta}.$$  \hfill (18)

The Heisenberg correction function is defined as [1]:

$$f(r_{\alpha\beta} \cdot P_{\alpha\beta}; \xi, \alpha) = \frac{\xi}{4\alpha r_{\alpha\beta}^2 \mu_{\alpha\beta}} \exp \left\{ \alpha \left[ 1 - \left( \frac{r_{\alpha\beta} P_{\alpha\beta}}{\xi} \right)^2 \right] \right\}.$$  \hfill (19)

In our simulations, the correction term is taken into account between the target electron and both of target nucleus and projectile. This calculation schema is called a target–projectile centered calculation. We note that we also did calculations
using other calculation schemas to determine the influence of correction terms on the cross sections (see section 3.4). These are the following: (1) projectile-centered, when the correction term is taken into account between target electron and projectile, (2) target-centered, when the correction term is taken into account between target electron and the target nucleus. The correction term according to projectile-centered and target centered are expressed as:

\[
f(\vec{r}_p, \vec{r}_{pe}; \varepsilon_H \cdot \alpha_H) = \frac{\xi_H^2}{4\Omega_P^2 \xi_H^2} \exp \left\{ \alpha_H \left[ 1 - \left( \frac{\vec{r}_p \cdot \vec{r}_{pe}}{\varepsilon_H} \right)^4 \right] \right\} \tag{20}
\]

\[
f(\vec{r}_T, \vec{P}_{Te}; \varepsilon_H \cdot \alpha_H) = \frac{\xi_H^2}{4\Omega_P^2 \xi_H^2} \exp \left\{ \alpha_H \left[ 1 - \left( \frac{\vec{r}_p \cdot \vec{P}_{Te}}{\varepsilon_H} \right)^4 \right] \right\} \tag{21}
\]

It is worth noting that the vector direction \(\vec{r}_e\) is from the target to electron and \(\vec{r}_{pe}\) is from the projectile to electron, respectively. The equations of motion taking into account the Hamiltonian mechanics and the Heisenberg correction term is given by:

\[
\dot{\vec{r}}_e = \frac{\delta H}{\delta \vec{r}_e} = -\frac{Z_e Z_p}{|\vec{r}_p - \vec{r}_e|^3}(\vec{r}_p - \vec{r}_e) + \frac{Z_e Z_T}{|\vec{r}_e - \vec{r}_T|^3}(\vec{r}_e - \vec{r}_T)
+ \left( \frac{\xi_H^2}{2\Omega P \mu e|\vec{r}_e - \vec{r}_T|^2} + \frac{\vec{p}_{Te}^2}{\xi_H^2 \mu P} \right) \times e \left[ 1 - \left( \frac{|\vec{r}_p - \vec{r}_{Te}|}{\xi_H} \right)^4 \right] \left(\vec{r}_e - \vec{r}_T\right) C_T \tag{22}
\]

\[
\dot{\vec{r}}_T = -\frac{\delta H}{\delta \vec{r}_T} = -\frac{Z_p Z_e}{|\vec{r}_p - \vec{r}_T|^3}(\vec{r}_p - \vec{r}_T) + \frac{Z_p Z_T}{|\vec{r}_e - \vec{r}_T|^3}(\vec{r}_e - \vec{r}_T)
+ \left( \frac{\xi_T^2}{2\Omega P \mu e|\vec{r}_e - \vec{r}_T|^2} + \frac{\vec{p}_{Pe}^2}{\xi_H^2 \mu Pe} \right) \times e \left[ 1 - \left( \frac{|\vec{r}_p - \vec{r}_{Pe}|}{\xi_H} \right)^4 \right] \left(\vec{r}_e - \vec{r}_T\right) C_P \tag{23}
\]

\[
\dot{\vec{P}}_p = \frac{\delta \mathcal{F}_{\text{FMD}}}{\delta \vec{P}_p} = \frac{Z_p Z_e}{|\vec{r}_p - \vec{r}_e|^3}(\vec{r}_p - \vec{r}_e) + \frac{Z_p Z_T}{|\vec{r}_e - \vec{r}_T|^3}(\vec{r}_p - \vec{r}_T)
+ \left( \frac{\xi_H^2}{2\Omega P \mu e|\vec{r}_e - \vec{r}_T|^2} + \frac{\vec{p}_{Pe}^2}{\xi_H^2 \mu Pe} \right) \times e \left[ 1 - \left( \frac{|\vec{r}_p - \vec{r}_{Pe}|}{\xi_H} \right)^4 \right] \left(\vec{r}_e - \vec{r}_T\right) C_P \tag{24}
\]

\[
\dot{\vec{r}}_e = \frac{\delta \mathcal{F}_{\text{FMD}}}{\delta \vec{r}_e} = N_e \vec{P}_e - N_e|\vec{r}_e - \vec{r}_T|^2|\vec{P}_{Te}|^2 \times e \left[ 1 - \left( \frac{|\vec{r}_p - \vec{r}_{Te}|}{\xi_H} \right)^4 \right] \left(\vec{r}_e - \vec{r}_T\right) C_T \tag{25}
\]

\[
\dot{\vec{r}}_T = \frac{\delta \mathcal{F}_{\text{FMD}}}{\delta \vec{r}_T} = N_T \vec{P}_T - N_T|\vec{r}_e - \vec{r}_T|^2|\vec{P}_{Te}|^2 \times e \left[ 1 - \left( \frac{|\vec{r}_p - \vec{r}_{Te}|}{\xi_H} \right)^4 \right] \left(\vec{r}_e - \vec{r}_T\right) C_T \tag{26}
\]

\[
\dot{\vec{P}}_p = \frac{\delta \mathcal{F}_{\text{FMD}}}{\delta \vec{P}_p} = N_p \vec{P}_e - N_p|\vec{r}_e - \vec{r}_T|^2|\vec{P}_{pe}|^2 \times e \left[ 1 - \left( \frac{|\vec{r}_p - \vec{r}_{Pe}|}{\xi_H} \right)^4 \right] \left(\vec{r}_e - \vec{r}_T\right) C_P \tag{27}
\]

For the case of the target-centered schema \(C_T = 1, C_P = 0\), for the case of the projectile-centered schema \(C_T = 0, C_P = 1\) and for the case of the target–projectile centered schema \(C_T = C_P = 1\). We note that by using \(C_T = C_P = 0\) the equation of motions naturally gives back the case of standard three-body equation of motions.

The Heisenberg correlation potential is sensitive to the choice of the two constants \(\alpha\) and \(\xi\). \(\xi_H\) and \(\alpha_H\) are the dimensionless constant and adjustable hardness parameters, respectively, which must be determined. \(\xi_H\) is determined by our requiring \(r_p \cdot \xi = \xi \hbar\) for the ground state of an atom. By considering atomic units \(\hbar = m_e = e = 1\), Hamiltonian of hydrogen atom is defined in a form of

\[
H = \frac{p^2}{2} - \frac{1}{r} + \left( \frac{\xi_H^2}{4\Omega P r^2} \right) \exp \left\{ \alpha_H \left[ 1 - \left( \frac{r}{\xi_H} \right)^4 \right] \right\} \tag{28}
\]

In the ground state or stationary configuration at the lowest energy, \(\frac{\delta H}{\delta r} = 0\) and \(\frac{\delta H}{\delta \psi} = 0\) [1]. This gives
In the case of the hydrogen atom, the binding energy of the electron in the ground state is $-0.5$ a.u. Figure 2 shows the variations of $\xi_H$ according to $\alpha_H$ for ground state hydrogen atom.

3. Results and discussion

To study the collision between $H^+$ and hydrogen atom, we used the standard three-body CTMC and QCTMC methods. We performed a classical simulation with an ensemble of $1 \times 10^6$ primary trajectories for each energy. The calculations are carried out in the projectile energy range between 10 and 1000 keV amu$^{-1}$ when the target hydrogen atom is in the ground state. According to a large number of primary histories, the estimated uncertainties (see equation (11)) of the cross sections are in general around 0.6%.

3.1. Heisenberg constraining potential function dependence on $r$ and $p$

The correction term is a function of the radial ($r$) and linear momentum ($p$) of the target electron (see equation (19)). To define the initial conditions for $r$ and $p$ in the QCTMC model, we changed the initial conditions used in the standard three-body CTMC model. In the first step, we showed the dependence of the Heisenberg correction term on the parameters $r$ and $p$. Figure 3 shows the correction term dependence as a function of $r$ (with some typical constant $p$) and $p$ (with some typical constant $r$), respectively.

Figure 3 shows the exponential dependence of the Heisenberg correction term function as a function of $p$, when $r$ is assumed to be constant, (see figure 3(a)) and as a function of $r$, when $p$ is assumed to be constant (see figure 3(b)). The correction function defined by equation (19) shows a stronger dependence on $r$ than on $p$. Therefore, the Hamiltonian of the system is more sensitive to changes of $r$ than to the changes of $p$. Thereby in the definition of the initial conditions of the QCTMC model we select first the $p$ values and later the corresponding $r$ values satisfying that the total energy of the system is the ground state energy of the hydrogen atom, i.e. $E = 0.5$ a.u.

3.2. Definition of initial conditions of QCTMC model

Finding the pairs of $r_0$ and $p_0$ for the initial condition of the electron is an essential issue in classical calculations. For example, if the potential between hydrogen and electron is net Coulomb potential (without correction term), the initial $r_0$ and $p_0$ values are given as follows:

$$r_0 = \frac{|Z_e Z_T|}{2E_b}$$
$$p_0 = \sqrt{2|E_b|\mu_e}.$$  \hspace{1cm} (32)

where $E_b$ and $\mu_e$ denote the electron binding energy and reduced mass between target and electron, respectively. In the QCTMC model, the Heisenberg correction term is added to the net Coulomb potential which influences the total energy of the target electron and target nucleus. The target electron must be in the ground state energy level and thereby must fulfill relations defined in the equations (34) and (35):

$$\frac{|Z_e Z_T|}{2r} + f_H(r) < 0.5$$  \hspace{1cm} (34)

$$\frac{p^2}{2\mu_T} - \frac{1}{r} + f_H(r) \approx -0.5,$$  \hspace{1cm} (35)

where $f_H(r)$ is the Heisenberg correction term and 0.5 is the binding energy of the electron in ground state hydrogen. Therefore in this case we need an allowed interval in the combination of the initial conditions $(r_0, p_0)$ that provide the ground state energy. Figure 4 shows the allowed interval for $r_0$ and $p_0$ in which satisfy equations (34) and (35) by considering the constants $\alpha_H = 3.5$ and $\xi_H = 0.9354$, respectively.

By fixing the $p$ parameter and finding the root of function $F(r, p)$ (see equation (36)), we specified the new initial conditions in QCTMC model for $r$ parameter in the allowed interval

$$F(r) = \frac{p^2}{2\mu_T} - \frac{1}{r} + f_H(r) + 0.5.$$  \hspace{1cm} (36)

Figure 5 shows the dependence of function $F(r)$ according to $r$. We also consider that the obtained values for $r$ and $p$ in this part must be in the allowed interval (see figure 4). According to figure 5, we found that the initial conditions for the $r$ parameter are around $p = 1$ a.u.

3.3. Radial and momentum distribution

In the QCTMC model, Hamiltonian equations are numerically solved using a fourth-order Runge–Kutta integration method with an adaptive step size. For initialization procedures for the standard microcanonical QCTMC model, we obtained the
radial and momentum distribution of the electron. Figure 6 shows these distributions applying various combinations of $\alpha_H$ and $\xi_H$ in comparison with the corresponding quantum-mechanics results.

According to figure 6, we can see that the radial and momentum distributions are highly influenced by $\alpha_H$ and $\xi_H$. As discussed in section 3.2, we fixed the $p$ and changed the $r$ to find the initial condition in the QCTMC model. Therefore, it is expected that the momentum distribution is not matched to the classical and quantum distributions (see figure 6(b)). Figure 6(a) shows that the standard classical radial distribution is terminated around $r = 2$. Since the Heisenberg constraint is one of the quantum-mechanics concepts we use in the classical simulation, we expect to see the quasi-classical radial distributions in the special quantum zone (beyond $r = 2$). We see this condition for $\alpha_H \gtrsim 3.5$. Therefore the suitable and reasonable range of $\alpha_H$ for the $H^+ + H(1s)$ collision system is expected to be $\alpha_H \gtrsim 3.5$. Furthermore, we note that the distributions are started from non-zero values because due to the Heisenberg constraint, the electron is not allowed to collapse to the nucleus.

To find the adequate combination of $\alpha_H$ and $\xi_H$ for proton and ground state hydrogen collision system in the QCTMC model, we calculated the cross sections of ionization, CX, state-selective CX, and excitation channels as a function of incident energies and compared with the available quantum-mechanics approaches and experimental data.

3.4. Effects of Heisenberg correction term on three different calculation schemes

In the QCTMC model, the effect of Heisenberg correlation potential on the particles in the collision is interesting. Therefore we tested three calculations schemes as described in section 2.2 as follows:

(a) Projectile-centered, where the correction term is considered between target electron and projectile
(b) Target-centered, where the correction term is considered between the target electron the target nucleus
(c) Combined one, i.e., target and projectile centered where the correction term is taken into account between target electron and both the target nucleus and projectile
Figure 6. (a) Radial distribution and (b) momentum distribution. Solid pink line: QCTMC ($\alpha_H = 3, \xi_H = 0.9258$) results, solid red line: QCTMC ($\alpha_H = 3.2, \xi_H = 0.9299$) results, solid green line: QCTMC ($\alpha_H = 3.5, \xi_H = 0.9354$) results, solid black line: QCTMC ($\alpha_H = 4, \xi_H = 0.9428$) results, solid blue line: CTMC results, dashed blue line: quantum-mechanics results.

Figure 7. (a) Ionization and (b) CX cross sections in $H^+ + H(1s)$ collision as a function of impact energy. Solid red line: present CTMC results, solid green line: present target-centered QCTMC results, solid black line: present projectile-centered QCTMC results, solid blue line: present target and projectile centered QCTMC results, dashed line: QTMC-EB [4]. Experimental results are due to: black circles: Shah and Gilbody [8], black triangles: Shah et al [9], blue circles: McClure [10].

Figure 7 shows our CTMC and QCTMC results corresponding to the three calculation schemes of the ionization and total CX cross sections in $H^+ + H(1s)$ collision as a function of the impact energy. We compared our results with the QTMC-EB method and experimental data.

According to figure 7(a), the present CTMC and projectile-centered QCTMC results are almost the same. Furthermore, it can be seen that the target-centered QCTMC results and the target–projectile-centered ones are almost the same. It means that due to the large distance between the electron and the projectile relative to the distance from the electron to the target nucleus, the Heisenberg correction term effect between the electron and the projectile is practically negligible. Therefore, we conclude that the correction term between the target electron and the projectile is ineffective in the ionization channel. According to the previous literature, both CTMC and projectile-centered QCTMC results are in good agreement with the QTMC-EB results of Cohen [4], and the experimental data are shown by Shah and Gilbody [8] at intermediate and high impact energies. Also, the target-centered QCTMC cross sections and target–projectile-centered QCTMC ones are in excellent agreement with the experimental data reported by Shah et al [9] at low impact energies.

On the other hand, according to figure 7(b), the effects of correction term on three different calculation schemes are evidence in the CX channel. The correction term provides the repulsive force between the electron and both target and projectile causes to better transmitting the electron to the projectile states in the CX channel. A better agreement is seen between experimental data and the QCTMC model, where the correction term is taken into account between the target electron and both the target nucleus and projectile at intermediate energies. It is worth noting that we used only the combination scheme as a justifiable cause in our calculations.
3.5. Ionization

Trajectories of particles in collisions are an instructive and exciting way to show the behavior of the projectile, target, and electrons. Figure 8 shows trajectories of the ionization channel (see equation (37)) in the y–z lab frame coordinate system without and with considering the Heisenberg correction term, respectively. The trajectories were obtained at 70 keV amu\(^{-1}\) impact energy. The target electron experiences the attractive Coulomb force from both of target and projectile positive charge. On the other hand, the presence of correction term in the QCTMC model causes continuous changes in the sum of the forces acting on the electron. Therefore it can be seen the distortion in electron trajectory (see figure 8(b)). Also, target repulsion becomes more apparent with the addition of the Heisenberg correction term

\[
H^+ + H(1s) \rightarrow H^+ + H^+ + e^-.
\]  

Figure 9 shows the present CTMC and QCTMC results of ionization cross sections in \(H^+ + H(1s)\) as a function of impact energy. We considered \(\alpha_H = 3, 3.5, 4, 4.5, 5\) with corresponding \(\xi_H\) in the QCTMC model. The Comparison was made with the QTMC-EB method used by Cohen [4], and the experimental data have shown come from Shah and Gilbody [8] and Shah et al [9].

It can be seen that the CTMC results are in good agreement with QTMC-EB results and experimental data of Shah and Gilbody [8] at intermediate and high energies. The Heisenberg correction term exerts a repulsive force on the electron. Due to the small distance between the electron and the target nucleus, the repulsive force between the electron and the target nucleus is much larger than the repulsive force between the electron and the projectile. Therefore, the ionization cross sections in the QCTMC model are higher than the CTMC ones in the whole range of impact energy. According to figure 9, the QCTMC \((\alpha_H = 3, \xi_H = 0.9258)\) and QCTMC \((\alpha_H = 3.5, \xi_H = 0.9354)\) results match the experimental data of Shah et al [9] at low energies. Also, the QCTMC \((\alpha_H = 3, \xi_H = 0.9258)\) results are in good agreement with the experimental data of Shah and Gilbody [8] at high energies. However, one can see the close agreement between the QCTMC \((\alpha_H = 3.5, \xi_H = 0.9354)\) results and the experimental results due to Shah and Gilbody [8] at high energies.

3.6. Charge exchange

For the illustration of the CX channel (see equation (38)), figure 10 represents the trajectories in the x–z projectile frame for electron, target, and projectile without and with considering the Heisenberg correction term. The presence of the Heisenberg repulsive force (as described in section 3.5) causes
Figure 10. CX trajectories in the $x$–$z$ projectile frame (a) without considering the correction term, (b) with considering the correction term at the typical 70 keV amu$^{-1}$ impact energy. Solid red line: electron trajectory, solid blue line: target trajectory.

Figure 11. Total CX cross sections in H$^+$ + H(1s) collision as a function of the impact energy. Solid red line: present CTMC results, solid blue line: present QCTMC ($\alpha_H = 3$, $\xi_H = 0.9258$) results, dash blue line: present QCTMC ($\alpha_H = 4$, $\xi_H = 0.9428$) results, dotted blue line: present QCTMC ($\alpha_H = 4.5$, $\xi_H = 0.9486$) results, dash-dot–dot blue line: present QCTMC ($\alpha_H = 5$, $\xi_H = 0.9534$) results, dashed black line: present QCTMC ($\alpha_H = 5$, $\xi_H = 0.9534$) results, circles: experimental results are due to McClure [10].

By considering the correction term to mimic the Heisenberg constrain, the repulsive force reduces the effects of the attractive Coulomb force between the electron and target nuclei. Therefore, the tendency of the electron to be placed at the states of the projectile increases. According to figure 11, the QCTMC model increases the CX cross sections compared with CTMC and QTMC-EB methods at low and intermediate impact energies. The QCTMC ($\alpha_H = 5$, $\xi_H = 0.9535$) results are very close to the experimental data.

3.7. State selective CX

We calculated the CTMC and QCTMC results of CX cross sections into 2s and 2p states of the projectile bound state (see equation (39)). The calculations were obtained in the QCTMC model according to $\alpha_H = 3, 3.5, 4, 4.5$ with $\xi_H$ correspondence, respectively (see figures 12 and 13).

The comparison was made with the SC-CCC method used by Avazbaev et al [5], and the experimental data are due to Bayfield [12], Morgan et al [13], Hill et al [14], Ryding et al [15], kondow et al [16] and Stebbings et al [35].

According to figure 12, the QCTMC model improves the results at low energies significantly. At the low energies, the QCTMC ($\alpha_H = 3$, $\xi_H = 0.9258$) and QCTMC ($\alpha_H = 4$, $\xi_H = 0.9428$) results agree with the experimental data of Morgan et al [13]. Also, between impact energies 100–1000 keV, the QCTMC ($\alpha_H = 3$, $\xi_H = 0.9258$) and QCTMC ($\alpha_H = 3.5$, $\xi_H = 0.9354$) results match the SC-CCC [5] method.

Figure 13 shows that the QCTMC ($\alpha_H = 3$, $\xi_H = 0.9258$) and QCTMC ($\alpha_H = 3.5$, $\xi_H = 0.9354$) results are close to the experimental data at low energies. Also, good agreement is seen with the SC-CCC theoretical method [5] at high energies.

Figures 12 and 13 show that, the QCTMC cross sections are higher compared to CTMC ones at lower incident energies. This difference gradually decreases for higher energies. To explain this behavior physically, we focus on two factors: (1) force between the electron and the hydrogen nucleus, (2) interaction time. Heisenberg correction term creates a repulsive force in the opposite direction to the Coulomb force in the QCTMC model. Therefore, the attraction force between the electron target and the target nucleus decreases and the
Figure 12. CX cross sections into 2s state of the projectile in $H^+ + H(1s)$ collision as a function of the impact energy. Solid red line: present CTMC results, solid blue line: (a) present QCTMC ($\alpha_H = 3$, $\xi_H = 0.9258$) results, (b) present QCTMC ($\alpha_H = 3.5$, $\xi_H = 0.9354$) results, (c) present QCTMC ($\alpha_H = 4$, $\xi_H = 0.9428$) results, (d) present QCTMC ($\alpha_H = 4.5$, $\xi_H = 0.9486$) results, dash line: SC-CCC results of Avazbaev et al [5]. Experimental results are due to: red circles: Bayfield [12], black squares: Ryding et al [15], black triangles: Morgan et al [13], crosses: Hill et al [14].

3.8. Excitation

To better understand the excitation channel (see equation (40)) without and with considering the Heisenberg correction term, we have shown the electron, projectile, and target trajectories in the x-z lab frame coordinate system in figure 14. The trajectories were obtained at 70 keV amu$^{-1}$ impact energy. The effect of the correction term (as described in section 3.5) adds a repulsive force into the classical calculations. Competition between attractive Coulomb force and repulsive Heisenberg force distorts the trajectory of the electron in the excitation channel

$$H^+ + H(1s) \rightarrow H^+ + H(n, l)^*.$$ (40)

In the following, we show cross sections for $H^+$ induced $1s \rightarrow 2p$ transition in atomic hydrogen by using CTMC and QCTMC methods for $\alpha_H = 3$, 3.5, 4, 4.5, 5 with $\xi_H$ correspondence, respectively (see figure 15). In addition, we compared our results with the experimental data are shown by Morgan et al [13], Detleffsen et al [11], and kondow et al [16]. Also, the comparison is made with the SC-CCC method as a benchmark used by Avazbaev et al [5]. The SC-CCC method based on the impact parameter description is one semiclassical method in which the projectile motion with respect to the target is considered classically by linear trajectories. This classical treatment is valid when the associated de Broglie wavelength, $\lambda_{proj} = \frac{2\pi}{\alpha_0}$, is smaller than the radius of the atomic target ($a_0 = 1$ a.u. for $H(1s)$). According to the relation, $\lambda_{proj} \ll 1$, the SC-CCC method is valid at intermediate and high impact energies for comparison with CTMC and QCTMC models. The main difference between our classical models and the SC-CCC model is based on the treatment of the electronic motion which is described quantum mechanically in SC-CCC and classically in CTMC and QCTMC models.

According to figure 15, we realized that the QCTMC cross sections are higher than CTMC ones at the whole range of impact energies. This behavior can be understood by focusing on the force between the electron and hydrogen nucleus.
Figure 13. CX cross sections into the 2p state of the projectile in H\(^+\) + H(1s) collision as a function of the impact energy. Solid red line: present CTMC results, solid blue line: (a) present QCTMC (\(\alpha_H = 3, \xi_H = 0.9258\)) results, (b) present QCTMC (\(\alpha_H = 3.5, \xi_H = 0.9354\)) results, (c) present QCTMC (\(\alpha_H = 4, \xi_H = 0.9428\)) results, (d) present QCTMC (\(\alpha_H = 4.5, \xi_H = 0.9486\)) results, dashed line: SC-CCC [5]. Experimental results are due to; red circles: Kondow [16], black triangles: Morgan et al [13], crosses: Stebbings et al [35].

Figure 14. Excitation trajectories in the x–z lab frame (a) without considering the correction term, (b) with considering the correction term at the typical 70 keV amu\(^{-1}\) impact energy. Solid red line: electron trajectory, solid green line: projectile trajectory, solid blue line: target trajectory.

Heisenberg correction term generates a repulsive force in the opposite direction to the attractive Coulomb force leads to increasing the probability of electron transferring to the higher level of energy in the excitation channel. One can see that the QCTMC (\(\alpha_H = 3, \xi_H = 0.9258\)) and QCTMC (\(\alpha_H = 3.5, \xi_H = 0.9354\)) results at intermediate and high impact energies are in
good agreement with experimental data and SC-CCC results of Avazbaev et al [5]. The similarity of the QCTMC results at \((\alpha_{\text{H}} = 3, \xi_{\text{H}} = 0.9258)\) and \((\alpha_{\text{H}} = 3.5, \xi_{\text{H}} = 0.9354)\) with the experimental data and with the semiclassical close-coupling approach are very appropriate.

As seen in figures 9, 11–13 and 15, we conclude that the results by considering the QCTMC method significantly improve the cross sections as a function of the impact energies. We also observed the effects of \(\alpha_{\text{H}}\) and \(\xi_{\text{H}}\) on the displacement of cross sections for proton and ground state hydrogen collision systems. Since one combination of \(\alpha_{\text{H}}\) and \(\xi_{\text{H}}\) in Heisenberg potential function should be chosen for collision systems, by investigating the electron radial and momentum distribution and analyzing the experimental data for various final channels, we found that the constants \(\alpha_{\text{H}} = 3.5\) and \(\xi_{\text{H}} = 0.9354\) in the QCTMC model are reasonable in \(\text{H}^+ + \text{H}(1s)\) collisions.

4. Conclusions

We have shown an intensive study of the interaction between a proton and a ground state hydrogen atom. Calculations were performed employing a standard three-body CTMC and a QCTMC models where the Heisenberg correction term is added to the Hamiltonian of the collision system to mimic the Heisenberg uncertainty principle. The projectile energy range was between 10 and 1000 keVamu\(^{-1}\). To increase the accuracy of the calculations, we considered one million trajectories for each impact parameter. Firstly, the initial conditions for distance \((r)\) and linear momentum \((p)\) of the target electron were obtained for the QCTMC model. Secondly, we presented ionization and total CX cross sections in three calculation schemes in \(\text{H}^+ + \text{H}(1s)\) collision. These were the followings: (1) projectile-centered, when the correction term is taken into account between target electron and projectile, (2) target-centered, when the correction term is taken into account between target electron and target nucleus, (3) combined one, i.e., when the correction term is taken into account between the target electron and both the target nucleus and projectile. Our QCTMC results in different schemes were compared with the results of the three-body CTMC model. We found that the effect of the correction term between the target electron and projectile is not noticeable in the ionization channel. However, the correction term between the particles plays an important role in calculations in the CX channel.

Finally, we obtained the relevant range for two important constants in the Heisenberg constraining function, i.e., \(\alpha_{\text{H}}\) and \(\xi_{\text{H}}\), by analyzing the radial and momentum distributions of the target electron. By comparing the present radial distribution with the quantum-mechanics ones, we found that the reasonable range of \(\alpha_{\text{H}}\) for ground state hydrogen as a target is expected to be \(\alpha_{\text{H}} \geq 3.5\) [36]. To select the most reasonable parameters we performed test calculations to obtain excitation, ionization and CX cross sections for various \((\alpha_{\text{H}}, \xi_{\text{H}})\) combinations. We take the advance in the parameter selection that according to figure 4. We have a little freedom in the selection of \((\alpha_{\text{H}}, \xi_{\text{H}})\) for the correction potential. We used this option to obtain the reasonable parameters based on the comparison of calculated cross sections with experimental and theoretical data. We note, however, that the obtained parameters are used for all reaction channels (like excitation, ionization and CX). The combination of \((\alpha_{\text{H}}, \xi_{\text{H}})\) may element dependent. We found that according to the comparison of our calculated cross sections with the previous experimental and theoretical data, for hydrogen target the \(\alpha_{\text{H}} = 3.5\), and \(\xi_{\text{H}} = 0.9354\) combination provide good numbers for all possible reaction channels. We note, that naturally, these parameters are not universal, for other elements the optimization procedure must be repeated. The parameters we obtained is valid strictly for hydrogen target.

Generally, the CTMC model is a well-known classical treatment for modeling atomic collisions to calculate various cross sections. But due to the lack of quantum features in the standard and original model, the CTMC model is not able to describe accurately the cross sections mostly at lower impact energies when the quantum mechanical character of the collision may dominant. The reason for this is that at lower projectile energies the interaction time is longer in the collision region, therefore the Coulomb interaction between the target electron and projectile should be more significant than at higher energies. Thus, a quantum mechanical description is required to calculate accurate cross sections. In the QCTMC description of the scattering problem, a model potential is introduced to mimic some quantum features of the collision.

Accurate cross section calculations between low charged fully stripped ions (such as \(\text{H}^+\)) with ground state hydrogen is very essential in fusion research. On the other hand, treating atomic collisions with quantum mechanics approaches in many aspects are very complicated or unfeasible. Therefore, the QCTMC model with its simplicity, may have an alternative
of the quantum-mechanical models providing the same results with relatively low computation efforts.

Acknowledgments

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

All data that support the findings of this study are included within the article (and any supplementary files).

ORCID iDs

Iman Ziaeian © https://orcid.org/0000-0002-0269-1429
Károly Tökési © https://orcid.org/0000-0001-8772-8472

References

[1] Kirschbaum C L and Wilets L 1980 Phys. Rev. A 21 834
[2] Anderson H, von Hellermann M G, Hoekstra R, Horton L D, Howman A C, Konig R W T, Martin R, Olson R E and Summers H P 2000 Plasma Phys. Control. Fusion 42 781
[3] Isler R C 1994 Plasma Phys. Control. Fusion 36 171
[4] Cohen J S 1996 Phys. Rev. A 54 573
[5] Avazbaev S K, Kadyrov A S, Abdurakhmanov I B, Fursa D V and Bray I 2016 Phys. Rev. A 93 022710
[6] Abdurakhmanov I B, Kadyrov A S, Avazbaev I and Bray I 2016 J. Phys. B: At. Mol. Opt. Phys. 49 115203
[7] Antonio N W, Plowman C T, Abdurakhmanov I B, Bray I and Kadyrov A S 2021 J. Phys. B: At. Mol. Opt. Phys. 54 175201
[8] Shah M B and Gilbody H B 1981 J. Phys. B: At. Mol. Phys. 14 2361
[9] Shah M B, Elliott D S and Gilbody H B 1987 J. Phys. B: At. Mol. Phys. 20 2481
[10] McClure G W 1966 Phys. Rev. 148 47
[11] Deleijfsen D, Anton M, Werner A and Schartner K H 1994 J. Phys. B: At. Mol. Opt. Phys. 27 4195
[12] Bayfield J E 1969 Phys. Rev. 185 105
[13] Morgan T J, Geddes J and Gilbody H B 1973 J. Phys. B: At. Mol. Phys. 6 2118
[14] Hill J, Geddes J and Gilbody H B 1979 J. Phys. B: At. Mol. Phys. 12 L341
[15] Ryding G, Wittkower A B and Gilbody H B 1966 Proc. Phys. Soc. 89 547
[16] Kondow T, Girnius R J, Chong Y P and Fite W L 1974 Phys. Rev. A 10 1167
[17] Bunker D L 1962 Nature 194 1277
[18] Blais N C and Bunker D L 1962 J. Chem. Phys. 37 2713
[19] Karplus M and Raff L 1964 Theoretical Investigations of reactive collisions in molecular beams: K + CH3I J. Chem. Phys. 41 1267
[20] Olson R E and Salop A 1977 Phys. Rev. A 16 531
[21] Tökési K and Hock K G 1994 Nucl. Instrum. Methods Phys. Res. B 86 201
[22] Ziaeian I and Tökési K 2020 Atoms 8 27
[23] Abrines R and Percival I C 1966 Proc. Phys. Soc. 88 861
[24] Zajfman D and Maor D 1986 Phys. Rev. Lett. 56 320
[25] McKenzie M L and Olson R E 1987 Phys. Rev. A 35 2863
[26] Cohen J S 1995 Phys. Rev. A 51 266
[27] Cohen J S 1997 Phys. Rev. A 56 3583
[28] Cohen J S 1998 Phys. Rev. A 57 4964
[29] Cohen J S 2000 Phys. Rev. A 62 022512
[30] Wilet L and Cohen J S 1998 Contemp. Phys. 39 163
[31] Jorge A, Illescas C, Méndez L and Pons B 2016 Phys. Rev. A 94 022710
[32] Bachi N and Otranto S 2019 Eur. Phys. J. D 73 4
[33] Tökési K and Kóvér A 2000 J. Phys. B 33 3067
[34] Becker R L and MacKellar A 1984 J. Phys. B: At. Mol. Phys. 17 3923
[35] Stebbings R F, Young R A, Oxley C L and Ehrhardt H 1965 Phys. Rev. A 138 1312
[36] Ziaeian I and Tökési K 2021 Sci. Rep. 11 20164