Short thesis for the degree of doctor of philosophy (PhD)

Modelling of atomic processes in fusion plasma

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Background

In the last 20 years, the atomic collision processes played a significant role in magnetic confinement nuclear fusion research [1-4]. In the nuclear fusion research, these processes were classified into four principal areas: 1) the hot central plasma where the fusion reactions are expected to occur; 2) the plasma edge where the plasma interacts with the external environment; 3) plasma heating methods, and 4) the diagnostic technology [1-4]. Recently, there has been a great deal of interest in theoretical studies of inelastic cross-sections of plasma-neutral interactions in which plasma interacts with the external environment. This is due to the fact that plasma-neutral collisions, especially a collision between two hydrogen atoms, have proven to be difficult to investigate experimentally. Even more, they are also hard to investigate by quantum mechanical approaches. Therefore, the classical trajectory Monte Carlo model (CTMC) was used to investigate these collision systems. The use of classical treatments provided several advantages over other models. For instance, the classical approach is a none-perturbed method, and all interactions among the particles can be taken into account. In addition, all possible reaction channels can be calculated simultaneously. Plasma-neutrals collisions are complicated and lots of effort is needed to understand the physics beyond all of these processes such as ionization, excitation, electron capture [5]. For instance, in the intermediate energy regime, where the projectile comes in at a speed (v) comparable to the average speed of the orbital electron ($v \sim v_e$), all inelastic processes are important and influence each other [6]. A poor understanding of one process – ionization – for instance, limits the accuracy of the description of all other processes. As a consequence, a quasi-classical trajectory Monte Carlo (QCTMC) model for hydrogen-hydrogen type four-body collision systems was developed by adding the momentum-dependent potential proposed by Kirschbaum and Wilets to the classical standard Hamiltonian [7]. The QCTMC model is an improved version of the standard CTMC model where the Kirschbaum and Wilets potential ensures mimicking quantum features of the collisions. The QCTMC model has been applied earlier with high success for other collisions systems [8]. The method [9-12] uses momentum-dependent effective potentials in a model Hamiltonian to stabilize the multi-electronic atomic and molecular structures, which otherwise would collapse or autoionize in the pure classical description. The potential enforce this condition via the Heisenberg uncertainty principle $r_i p_i \geq \xi_H \hbar$, where r_i and p_i are relative distance and momentum of an electron to the ionic core (nucleus) and ξ_H is a dimensionless constant. This condition is equivalent to the de Broglie description of the hydrogen atom, the electron treated as a particle on an ellipse with wave-like properties. This leads naturally to the quantization of electron momentum and kinetic energy, and consequently a manifold of allowed energy states for the electron relative to the nucleus [13, 14].

The Main Objective

The optical emission spectroscopy of plasma-edge, especially from limiter and diverter regions, brought evidence of the presence of neutral atoms and molecules such as hydrogen atoms [15]. The hydrogen atoms are generated by ion recombination on the fusion reactor's wall and other plasma-facing components and they can be re-emitted to the plasma. Besides hydrogen atoms, the impurities such as carbon, lithium, oxygen, deuterium, and tritium have existed in the plasma edge area. These impurities, for instance, carbon ions and lithium ions, are originated especially from the limiter and the vacuum vessel wall called a diverter, where carbon composites are used in first wall tiles and the lithium ions are used as a potential solution to solve heat flux to the diverter chamber [16].

The main aim of our works was to study the plasma-neutrals inelastic collisions in limiter and diverter regions. The main objective was to develop an accurate theoretical model for the description of inelastic interactions such as ionization, excitation, de-excitation, and electron capture processes for hydrogen-hydrogen type four-body systems. In addition, based on the newly developed codes, the aim was also to create a database for the total cross-sections as raw data for the beam emission spectroscopy (BES) model, a diagnostic tool for the prospective thermonuclear reactor.

NEW SCIENTIFIC RESULTS

Within the classical trajectory Monte Carlo (CTMC) and quasi-classical Monte Carlo (QCTMC) methods, we have studied the inelastic collision processes of the hydrogen atoms, carbon ions, and lithium ions with ground-state hydrogen target atoms in a wide range of impact energies, relevant to the interest of fusion research.

In this research work, significant progress has been made for the theoretical treatment of atom-atom and ion-atom collision systems. In most of the cases, we obtained a very good agreement between the experiment and our standard CTMC data. In particular, excellent agreement between theory and experiment in intermediate energy regions was achieved. However, at lower projectile energies the agreement between experiment and theory was not as good as at intermediate energies. Therefore, in the second part of this thesis, the results based on the QCTMC model for the four-body collision system were introduced. According to previous expectations, the quasi-classical treatment describes reasonably well the cross-sections for various final channels. Furthermore, we found that the calculations by the QCTMC model significantly improved the obtained cross-sections, especially in the low-energy regions.

My results support the idea that the included quantum correction terms are advantageous in terms of cross-section calculations. It is significant to emphases the role of the Heisenberg correction term is to give more accurate data at low-intermediate energy regions. This may lead to further development and improvement by including more terms approaching the ideal model for a full description of inelastic collision processes.

I have summarized the new results presented in this thesis in the form of 5 thesis points:

Thesis point 1

I prepared and carried out CTMC (Classical Trajectory Monte Carlo) calculations for H(1s)+H(1s) system by testing the previously available results. I calculated the ionization and excitation probabilities as a function of the projectile impact energy and determined the impact parameter dependent probabilities. I presented total cross-section data for ionization and excitation. I found excellent agreement with the previous data, especially in high-energy regions.

P[1, 2]: Tow papers published in a refereed scientific journal and support this dissertation.
P[1]:Impact Score: 2.41, Q2
P[2]: Impact Factor: 1.917, Q2

Thesis point 2

I implemented the Kirschbaum and Wilets model potential into our previously developed standard four-body classical trajectory Monte Carlo model.

a) *I analyzed and optimized the influence of the choice of the model potential parameters (α, ξ) on the initial radial and momentum distribution of the electron.*

b) *I tested and verified the results of our four-body QCTM code partly in comparison with available experimental and theoretical data and partly in comparison with our 3-body QCTMC results with our reduced four-body QCTMC results. The so-called reduced four-body QCTMC model is when the corresponding two-body interactions are switched off mimicking the 3-body collisions.*

c) *I carried out a large number of trajectory calculations based on the QCTMC model for hydrogen-hydrogen collision system in the projectile impact energy range between 5.0 keV-100 keV relevant to nuclear fusion research interest. I presented total cross-section data for ionization. I found excellent agreement between our data and the previous experimental data.*

P[3]: One paper published in a refereed scientific journal and support this dissertation.
P[3]: Impact Factor: 3.676, Q1

Thesis point 3

I performed CTMC and QCTMC calculations to simulate the collision of a hydrogen atom with C^{5+} ion.

a) *I provided baseline data of ionization and electron capture cross-sections in collision between C^{5+} ion with hydrogen atom for the nuclear fusion reactor, which affect the beam penetration efficiency as well as heating efficiency in thermonuclear reactor like tokamak. The calculated cross-sections based on the four-body CTMC model were compared with the available three-body data.*

b) *The four-body model displayed enhanced cross sections at lower projectile energies compared with the three-body results. For understanding of the enhanced cross sections at lower energies* *we performed a so called reduced four-body CTMC and QCTMC calculations when the electron-electron interaction was switched off. I found that for the case of the reduced calculations the enhancement in the cross sections disappeared, emphases the importance of electron-electron repulsion.*

P[4]: One paper published in a refereed scientific journal and support this dissertation.
P[4]: Impact Factor: 3.179, D1

Thesis point 4

I calculated the ionization and capture cross-sections in a collision between Li^{2+} and Li^{3+} ions with ground-state hydrogen atoms using both the CTMC and QCTMC model. I presented total cross sections and also the angular and energy differential cross-sections. My results showed a good agreement with the results of previous publications.

P[5]: One paper published in a refereed scientific journal and support this dissertation.
P[5]: Impact Factor: 2.654, Q2

Thesis point 5

I calculated the ionization, excitation, and de-excitation cross-sections database in a collision between two hydrogen atoms (H(nl)+H(1s)) when the target is in the ground state. The CTMC and the QCTMC simulation methods were employed for impact energy between 50keV to 50MeV, relevant to fusion and astrophysics laboratory research interest. All these cross-sections were tabulated for $H_P(1s, 2s, 2p, 3s, 3p, 3d, 4s, 4p)$ *projectile state.*

P[6]: One Paper published in a refereed scientific journal and support this dissertation.
P[6]: Impact Factor: 2.623, Q1

Publication related to the thesis

P[1]. **S. J. A. Atawneh**, Ö. Asztalos, B. Szondy, G.I. Pokol, and K. Tőkési. Ionization Cross Sections in the Collision between Two Ground State Hydrogen Atoms at Low Energies. Atoms **8** (2020.) 31.
Impact Score: 2.41, Q2.

P[2]. **S. J. A. Atawneh** and K. Tőkési. Excitation cross sections in a collision between two ground-state hydrogen atoms. Journal of Physics B: Atomic, Molecular and Optical Physics. **54** (2021) 065202.
Impact Factor: 1.917, Q2.

P[3]. **S. J. A. Atawneh** and K. Tőkési. Ionization cross sections in collisions between two hydrogen atoms by a quasi-classical trajectory Monte Carlo model, (To be submitted).
Impact Factor: 3.676, Q1.

P[4]. **S. J. A. Atawneh** and K. Tőkési. Target electron removal in C^{5+} + H collision. Nuclear Fusion, **62** (2021) 026009.
Impact Factor: 3.179, D1.

P[5]. **S. J. A. Atawneh** and K. Tőkési. Ionization Cross Section in Li^{q+} + H Collision. (To be published in Physics letters A).
Impact Factor: 2.654, Q2.

P[6]. **S. J. A. Atawneh** and K. Tőkési. Projectile Ionization, Excitation and De-excitation Cross Section Database in Collision between two Hydrogen Atoms in the Impact Energy between Range between 5.0 keV - 5.0 MeV -part I, Target is in Ground State.
Impact Factor: 2.623, Q1.

List of conference publications and posters

1. **S. J. A. Atawneh** and K. Tőkési. Collision between Two Hydrogen atoms . 30th Summer School and International Symposium on the Physics of Ionized Gases, SPIG2020, 24th-28th of August 2020, Serbia.

2**. S. J. A. Atawneh** and K. Tőkési. Analytical Formulism for the Output Factor Calculation of Small Radiation Beams. 30th Summer School and International Symposium on the Physics of Ionized Gases, SPIG2020, 24th – 28th of August 2020, Serbia.

3. **S. J. A. Atawneh** and K. Tőkési. Interaction of C^{5+} ions with hydrogen atoms. 27th International Symposium on Ion-Atom Collisions (ISIAC), 14th-16th of July 2021, Romania.

4. **S. J. A. Atawneh** and K. Tőkési. Collision between Two-Hydrogen atoms. 32nd International Conference on Photonic Electronic, and Atomic Collisions, 20th-23th of July 2021 – in virtual format (ViCPEAC 2021), Ottawa, Canada.

5. **S. J. A. Atawneh** and K. Tőkési. Interaction of Li^{q+} ions (q= +3, +2) with hydrogen atoms. M D-GAS COST Action (CA18212): 2nd General Meeting, 4th-8th of October 2021.

Seminar talk

1. **S. J. A. Atawneh** and K. Tőkési. Atomic Cross Section for Plasma-wall and Plasma-Edge Interaction Modelling in Controlled Fusion Reactor, Fusion Plasma Physics Department, 12th of October 2021, Budapest, Hungary.

Other publication not related to the thesis

1. **S. J. A. Atawneh** and K. Tőkési. Prompt Lead Exposure of Aqueous Environment Biomonitored by Photosynthetic Bacteria.24th International Symposium on Analytical and Environmental Problems, October 8th-9th October 2018, Szeged, Hungary. (**Short talk)**

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16. Al Atawneh, S.J. and K. Tokesi, *Target electron removal in C5+ + H collision.* Nuclear Fusion, 2021.

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List of publications related to the dissertation

Foreign language scientific articles in international journals (3)

1. **Al Atawneh, S. J.**, Tőkési, K.: Target electron removal in C5+ + H collision.
   Nucl. Fusion. 62 (2), 1-7, 2022. ISSN: 0029-5515.
   DOI: http://dx.doi.org/10.1088/1741-4326/ac3ac5
   IF: 3.179 (2020)
2. **Al Atawneh, S. J.**, Tőkési, K.: Excitation cross sections in a collision between two ground-state hydrogen atoms.
   J. Phys. B-At. Mol. Opt. Phys. 54 (6), 1-8, 2021. ISSN: 0953-4075.
   DOI: http://dx.doi.org/10.1088/1361-6455/abece3
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3. **Al Atawneh, S. J.**, Asztalos, Ö., Szondy, B., Pokol, G. I., Tőkési, K.: Ionization Cross Sections in the Collision between Two Ground State Hydrogen Atoms at Low Energies.
   Atoms. 8 (2), 1-8, 2020. EISSN: 2218-2004.
   DOI: http://dx.doi.org/10.3390/atoms8020031

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1. **Al Atawneh, S. J.**, Tőkési, K.: Target electron removal in C5+ + H collision.
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