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

Interactions of charged particles and hydrogen atoms

by Iman Ziaeian

Supervisor: Dr. Károly Tőkési

UNIVERSITY OF DEBRECEN

Doctoral School of Physics

Debrecen, 2022

Prepared at

The Institute for Nuclear Research, ATOMKI

Introduction

In recent decades, ITER has been developed to take a significant step in supplying energy cleanly and safely by the implementation of fusion power plants [1]. The temperature and pressure inside the thermonuclear reactor are extremely high. Since the reactor wall directly faces the hot plasma, it requires materials with special properties. Due to the unique thermal properties, beryllium is considered as the first wall of the ITER. Chemical and physical erosion of the first wall releases beryllium atoms and several molecular species, which eventually lead to the presence of fully-stripped beryllium ions in the plasma core.

Therefore the accurate knowledge of the interaction between charged particles and hydrogen atoms is the focus of fusion plasma research, including when energetically neutral hydrogen is injected into plasma for heating and diagnostic purposes. [2]. Significant interactions whose knowledge is essential in fusion research are ionization, electron capture, state-selective electron capture, and excitation. 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 quantum-mechanical molecular orbital close-coupling (QMOCC) [3], the atomic orbital close-coupling (AOCC) [4], the hyper spherical close-coupling (HSCC) models [5], using the solution of the time dependent Schrödinger equation (TDSE) [6], the lattice time dependence Schrödinger equation (LTDSE) [7], the classical over barrier model (COBM) [8], one-electron diatomic molecule (OEDM) [9], and the boundary corrected continuum intermediate state (BCCIS) [10]. However, in many cases, quantum-mechanical calculations are very complicated and unfeasible.

So as an alternative calculation scheme and due to the simplicity of calculations, classical models have been developed. In my research work, I also used classical approaches to calculate the collisional cross sections related to fusion research in various collision channels.

During my PhD studies, I performed my calculations using the standard three-body classical trajectory Monte Carlo (CTMC) and the quasi-classical trajectory Monte Carlo (QCTMC) models. The CTMC method is based on the calculation of a large number of individual particle orbits when the initial atomic states are chosen randomly. The cross sections for a given final channel can be obtained from the results of the trajectory calculations. The QCTMC model was proposed by Kirschbaum and Wilets in 1980 [11]. This model represents one step further towards a better description of the classical atomic collisions. In the QCTMC model, the Heisenberg correction term is added via a model potential to the standard classical Hamiltonian of the collision system to mimic the Heisenberg uncertainty principle. The effective potential enforcing 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.

The Main Objective

The collision processes between ions and atomic hydrogen are interesting in fusion plasma research. However, ionic impurities are one of the main problems in controlled thermonuclear fusion plasmas [2]. Due to the high temperature and density in the core, these impurities are fully ionized. The radiative decay of excited impurity ions can be the source for the energy loss of the plasma and can cool the plasma. These radiative decays can be analyzed by electron capture recombination spectroscopy (CXRS) [4] to diagnose impurities. Therefore, it is essential to know the inelastic interaction such as ionization, electron capture, state-selective electron capture, and excitation between bare ions and hydrogen atoms. Eventually, the collision between bare beryllium and atomic hydrogen is one of the most interesting for fusion research because beryllium as a first wall material of ITER is an important impurity. Therefore, the main objective of my research work is the investigation of collision between Be^{4+} and hydrogen atom using both the CTMC and QCTMC model. The data presented in my PhD thesis is extremely important in nuclear fusion power research.

NEW SCIENTIFIC RESULT

Within the classical trajectory Monte Carlo (CTMC) and Quasi-Classical Monte Carlo (QCTMC) models, I have studied the inelastic collision processes of the proton with ground state hydrogen atom, as well as Be^{4+} with ground-state and excited-state hydrogen atom, respectively. The calculations were carried out in a wide range of impact energies, relevant to the interest of fusion research.

In this research work, a significant improvement was taken into account for the classical treatment of ion-atom collision. The challenging part of the three-body quasi-classical trajectory Monte Carlo model is the finding of a relevant range for two important constants in the Heisenberg constraining function, i.e., α_H and ξ_H. I have achieved this goal by analyzing the radial and momentum distributions of the target electron. I found that my model for Be^{4+} + H(*nl*) and H^+ + H(1s) system remarkably improves the obtained cross sections, especially at lower projectile energies.

Due to the lack of experimental data for Be^{4+} + H(*nl*) system, I compared my results with quantum-mechanical approaches for various channels. I found that my results are very close and are in good agreement with the previously obtained quantum-mechanical results. Also, for H^+ + H(1s) system, I found excellent agreements between my QCTMC (α_H= 3.5, ξ_H = 0.9354) results with previous experimental data as well as quantum-mechanical ones. I also generated a database for state-selective electron capture cross sections in the collision between bare ions and ground state hydrogen atom. I believe that my model, with its simplicity, can be an alternative way to calculate accurate cross sections and maybe can replace the results of the quantum-mechanical models, where the quantum mechanical calculations become complicated.

The summaries of the new results are collected in the form of 6 thesis points as follows:

Thesis point 1

I improved the classical description of the one electron atomic system by including a model potential in the Hamiltonian of the system mimicking quantum features. In this case, I used the fact that, for atoms, a necessary condition for stability is that the electrons are not allowed to collapse to the nucleus.

a) The influence of the choice of the model potential parameters (α,ξ) on the initial radial and momentum distributions of the electron are analyzed and optimized. I found that for ground state hydrogen, the reasonable range of α_H is expected to be $\alpha_H \geq 3.5$ in the QCTMC model.

b) I considered three calculation schemes during the investigation of the effect of the Heisenberg correction term between the bodies. I found that the effects of the correction term between the target electron, target nuclei, and projectile plays an important role in the calculation of cross section for all exit channels.

c) I calculated the cross sections for various exit channels, like excitation, ionization, and electron capture, and compared them with previous quantum-mechanical and experimental results. I obtained excellent agreement between my QCTMC (α_H= 3.5, ξ_H = 0.9354) results and previous ones in H^{+}+H(1s) collision.

Scientific Journal: Journal of Physics B: Atomic, Molecular and Optical Physics

Impact Factor: 2.44, Q2

Status: Submitted (Under review)

Thesis point 2

I performed the calculations for ionization, electron capture, and low-level excitation cross sections in Be^{4+}+H(1s) collision system using the CTMC and QCTMC models. Due to the lack of experimental data, I compared my results with the previous quantum-mechanical approaches. I draw the conclusion that the classical treatment can describe the cross sections reasonably well.

Scientific Journal: Atom

Impact Score: 2.42, Q2

Status: Published

Doi: 10.3390/atoms8020027

Cited by : 4 (Independent: 2)

Thesis point 3

I calculated the electron capture cross sections into $n = 2$, and $nl = 2s, 2p$ states of the projectile in the collision between Be^{4+} and ground state hydrogen atom in wide impact energies range based on CTMC and QCTMC models. I found that the QCTMC method can reasonably describe the state-selective cross sections in a wide projectile energy range. My calculations provide a reliable estimation of fusion related state-selective cross sections, especially in low impact energies.

Scientific Journal: Physics Letters A

Impact Factor: 2.65, Q2

Status: Accepted

Thesis point 4

I presented the electron capture cross sections into $n = 3, 4, 5, 6, 8, 10$ and $nl = 3l, 4l, 5l$ states of the projectile in $Be^{4+} + H(1s)$ using CTMC and QCTMC models. I found that the QCTMC cross sections are higher than the CTMC ones at low energies. Including the potential correction term to mimic the Heisenberg uncertainty principle in the classical

Hamiltonian, I have shown that my QCTMC electron capture cross sections into the projectile states, *n* = 3, 4, 5 and *nl* = 3s, 3p, 3d, 4s, 4p, 5s, 5d, 5f are in excellent agreement with quantum-mechanical results.

Scientific Journal: Scientific Reports

Impact Factor: 4.379, D1

Status: Published

Doi: 10.1038/s41598-021-99759-y

Cited by : 1

Thesis point 5

I performed a three-body classical trajectory Monte Carlo method to calculate the *nl* state-selective electron capture cross sections in Be^{4+}+ H(2*lm*) collisions. I presented the state-selective cross sections for electron capture into Be^{3+}(*nl*) (*nl* = 2s, 2p, 3s, 3p, 3d, 4s, 4p, 4d, 4f) states as a function of impact energy. I compared my results with the theoretical approaches. I found that the CTMC method can able to describe reasonably the cross sections of the electron capture channel from the excited states of the H atom.

Scientific Journal: The European Physical Journal D

Impact Factor: 1.425

Status: Published

Doi: 10.1140/epjd/s10053-021-00127-2

Cited by : 2 (Independent: 1)

Thesis point 6

I presented a state-selective electron capture cross sections database from the ground state hydrogen atom regarding the classical calculations for the first time. A standard three-body classical trajectory Monte Carlo (CTMC) and quasi-classical trajectory Monte Carlo (QCTMC) models were employed for impact energies between 10 and 200 keV/amu relevant to the fusion research. The projectile ions are H^{+}, He^{2+}, Li^{3+}, Be^{4+}, B^{5+}, C^{6+}, N^{7+}, and O^{8+}. The cross sections are tabulated for each value of the final quantum numbers *n*, *l*, *m*.

Scientific Journal: Atomic Data and Nuclear Data Tables

Impact Factor: 2.458, Q1

Status: Accepted

Publication related to the thesis

1. **I. Ziaeian** and Károly Tőkési, *Interaction of Be^{4+} and Ground State Hydrogen Atom—Classical Treatment of the Collision,* Atoms, 8 (2020) 27.
   Impact Score: 2.42, Q2

2. **I. Ziaeian** and Károly Tőkési, *State-selective charge exchange cross sections in Be^{4+} - H(2lm) collision based on the classical trajectory Monte Carlo method,* Eur. Phys. J. D. 75 (2021) 1-5.
   Impact Factor: 1.425, Q3

3. **I. Ziaeian** and Károly Tőkési, *State selective classical electron capture cross sections in Be^{4+} + H(1s) collisions with mimicking quantum effect,* Sci. Rep. 11 (2021) 20164.
   Impact Factor: 4.379, D1

4. **I. Ziaeian**, K. Tőkési, *nl-selective classical charge exchange cross sections in Be^{4+} and ground state hydrogen atom collisions,* Accepted in Physics Letters A.
   Impact Factor: 2.65, Q2

5. **I. Ziaeian**, K. Tőkési, *Effects of Heisenberg constraint on the classical cross sections in in proton hydrogen collision,* Submitted to Journal of Physics B: Atomic, Molecular and Optical Physics.
   Impact Factor: 2.44, Q2

6. **I. Ziaeian**, K. Tőkési, *State-selective electron capture cross sections in collision between fully striped ions and ground state hydrogen – classical treatment of the collision,* Accepted in Atomic Data and Nuclear Data Tables.
   Impact Factor: 2.458, Q1

Selected talk

1. **I. Ziaeian**, K.Tőkési. (July 16, 2019) *Classical Simulation of the Collision Between* Be^{+4} *and H*. The 26th International Symposium on Ion-Atom Collisions-virtual format (ISIAC 2019), Sorbonne University, Paris, France.

Seminar talk

1. **I. Ziaeian** and K. Tőkési. (October 14, 2021). *Study the cross sections of the Be4+ and ground state hydrogen collisions in the thermonuclear fusion plasmas using the classical models*. Atomic Energy Research Institute, Centre for Energy Research Eötvös Loránd Research Network, Fusion Plasma Physics Department, Budapest, Hungary.

Conference Publications and Poster

1. **I. Ziaeian**, K.Tőkési, (August 24, 2020) *State-selective Charge Exchange Cross Section in* Be^{+4} *+ H(1s) Collision, Part I*, The 30th Summer school and International Symposium on the Physics of Ionized Gases (SPIG 2020), Sabac, Serbia

2. **I. Ziaeian** and K. Tőkési. (July 16, 2021). *State selective charge exchange cross section in* Be^{4+} *+ H(1s) collisions.* The 27th International Symposium on Ion-Atom Collisions-virtual format (ISIAC 2021), Faculty of Physics, Babes-Bolyai University. Cluj-Napoca, Romania.

3. **I. Ziaeian** and K. Tőkési. (October 5, 2021). *State selective charge exchange cross section in* Be^{4+} *+ H(1s) collisions.* The 2nd Annual virtual meeting on the Molecular Dynamics in the Gas Phase (MD-GAS 2021) – Cost Action CA18212.

References

1. R.A. Pitts, S. Carpentier, F. Escourbiac, T. Hirai, V. Komarov, A.S. Kukushin, S. Lisgo, A. Loarte, M. Merola, R. Mitteau, A.R. Raffray, M. Shimada, and P.C. Stangeby, J. Nucl. Mater. **415** (2011) S957.

2. J. Hackman, and J. Uhlenbusch, J. Nucl. Mater. **128/129** (1984) 418.

3. C. Harel, H. Jouin, and B. Pons, At. Data. Nucl. Data Tables. **68** (1998) 279.

4. W. Fritsch, and C.D. Lin, Phys. Rev. A. **29** (1984) 3039.

5. A.T. Le, M. Hesse, and C.D. lin, J. Phys. B. **36** (2003) 3281.

6. H.J. Lüdde, and R.M. Dreizler, J. Phys. B. **15** (1982) 2713.

7. T. Minami, M.S. Pindzola, T-G Lee, and D.R. Schultz, J. Phys. B: At. Mol. Opt. Phys. **39** (2006) 2877.

8. F. Sattin, Phys. Rev. A**. 62** (2000) 042711.

9. L.F. Errea, C. Harel, H. Jouin, L. Méndez, B. Pons, and A. Riera, J. Phys. B. **31** (1998) 3527

10. M. Das, M. Purkait, and C.R. Mandal, Phys. Rev. A. **57** (1998) 3573.

11. C.L. Kirschbaun, and L. Wilet, Phys. Rev. A. **21** (1980) 834.

UNIVERSITY of DEBRECEN

UNIVERSITY AND NATIONAL LIBRARY
UNIVERSITY OF DEBRECEN
H-4002 Egyetem tér 1, Debrecen
Phone: +3652/410-443, email: publikaciok@lib.unideb.hu

Registry number: DEENK/55/2022.PL
Subject: PhD Publication List

Candidate: Iman Ziaeian
Doctoral School: Doctoral School of Physics
MTMT ID: 10081628

List of publications related to the dissertation

Foreign language scientific articles in international journals (3)

1. **Ziaeian, I.**, Tőkési, K.: State-selective charge exchange cross sections in Be 4+ - H(2lm) collision based on the classical trajectory Monte Carlo method.
   Eur. Phys. J. D. 75 (4), 1-5, 2021. ISSN: 1434-6060.
   DOI: http://dx.doi.org/10.1140/epjd/s10053-021-00127-2
   IF: 1.425 (2020)

2. **Ziaeian, I.**, Tőkési, K.: State selective classical electron capture cross sections in Be4+ ?+?H(1s) collisions with mimicking quantum effect.
   Sci. Rep. 11 (1), 1-9, 2021. EISSN: 2045-2322.
   DOI: http://dx.doi.org/10.1038/s41598-021-99759-y
   IF: 4.379 (2020)

3. **Ziaeian, I.**, Tőkési, K.: Interaction of Be4+ and Ground State Hydrogen Atom-Classical Treatment of the Collision.
   Atoms. 8 (2), 1-11, 2020. EISSN: 2218-2004.
   DOI: http://dx.doi.org/10.3390/atoms8020027

Total IF of journals (all publications): 5,804
Total IF of journals (publications related to the dissertation): 5,804

The Candidate's publication data submitted to the iDEa Tudóstér have been validated by DEENK on the basis of the Journal Citation Report (Impact Factor) database.

24 January, 2022

DEBRECENI EGYETEM
EGYETEMI ÉS NEMZETI KÖNYVTÁR
H-4002 Debrecen, Egyetem tér 1, Pf.: 400
Tel.: 52/410-443, e-mail: publikaciok@lib.unideb.hu

Nyilvántartási szám: DEENK/55/2022.PL
Tárgy: PhD Publikációs Lista

Jelölt: Ziaeian, Iman
Doktori Iskola: Fizikai Tudományok Doktori Iskola
MTMT azonosító: 10081628

A PhD értekezés alapjául szolgáló közlemények

Idegen nyelvű tudományos közlemények külföldi folyóiratban (3)

1. **Ziaeian, I.**, Tőkési, K.: State-selective charge exchange cross sections in Be 4+ - H(2lm) collision based on the classical trajectory Monte Carlo method.
   Eur. Phys. J. D. 75 (4), 1-5, 2021. ISSN: 1434-6060.
   DOI: http://dx.doi.org/10.1140/epjd/s10053-021-00127-2
   IF: 1.425 (2020)

2. **Ziaeian, I.**, Tőkési, K.: State selective classical electron capture cross sections in Be4+ ?+?H(1s) collisions with mimicking quantum effect.
   Sci. Rep. 11 (1), 1-9, 2021. EISSN: 2045-2322.
   DOI: http://dx.doi.org/10.1038/s41598-021-99759-y
   IF: 4.379 (2020)

3. **Ziaeian, I.**, Tőkési, K.: Interaction of Be4+ and Ground State Hydrogen Atom-Classical Treatment of the Collision.
   Atoms. 8 (2), 1-11, 2020. EISSN: 2218-2004.
   DOI: http://dx.doi.org/10.3390/atoms8020027

A közlő folyóiratok összesített impakt faktora: 5,804
A közlő folyóiratok összesített impakt faktora (az értekezés alapjául szolgáló közleményekre): 5,804

A DEENK a Jelölt által az iDEa Tudóstérbe feltöltött adatok bibliográfiai és tudománymetriai ellenőrzését a tudományos adatbázisok és a Journal Citation Reports Impact Factor lista alapján elvégezte.

Debrecen, 2022.01.24.