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

Modelling of singly charged ion-atom collisions in fusion plasma

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Background

The accurate knowledge of the inelastic electron processes in ion-atom collisions has a significant importance in various scientific fields, such as, particle beam therapy [1,2], modelling and diagnosing fusion plasmas within tokamak reactors, and studying atomic and molecular structures [3].

Among the inelastic electron processes, ionisation is especially important in the study of fusion plasma, particularly in the study of magnetically confined fusion plasma within tokamaks. The distribution and concentration of excited impurity ions in fusion plasma influence the profiles of the plasma edge. In order to provide an accurate evaluation of plasma parameters, a diagnostic approach involving the injection of a high-speed particle beam into the plasma edge is employed, which lead to a high spatiotemporal resolution [4].

The collision of the injected particle beam with plasma components provides an insight into the profiles of the plasma edge by generating emission lines. However, the stability of these confinement systems can be compromised, leading to plasma disruptions characterized by rapid losses of magnetic and thermal energy, i.e., thermal quench [5,6]. Effective disruption mitigation strategies [7,8] are vital for ensuring the safe and dependable operation of fusion reactors.

Disruption mitigation involves various approaches, including the injection of significant gas quantities into the plasma to expedite cooling and quenching. While effective, this process introduces notable impurities into the plasma [9]. Noble gases and various methods [7,8,10–12] have been proposed for disruption mitigation, considering differences in mass, ionization, and reflection coefficients of noble gas particles at the plasma boundary [13].

Gas injection in tokamaks also plays a vital role in plasma diagnostics. Alkali beams, such as lithium and sodium, have proven invaluable for measuring plasma turbulence and electron density profiles, especially within the scrape-off layer and plasma edge [14,15].

Various high-energy beams, including hydrogen isotopes and helium, serve dual purposes in heating fusion plasma and diagnostic processes within tokamak reactors [4,16–18]. Nitrogen seeding is another strategy aimed at cooling the edge plasma within tokamak reactors [19].

In the pursuit of improved magnetic fusion plasma performance and enhanced protection for plasma-facing components, fusion experiments have explored the use of liquid lithium [20]. Lithium's reactivity leads to ionization, resulting in collisions with neutral atoms at the plasma's edge. A significant study by Wolfrum et al. [21] explored sodium as an alternative diagnostic beam to lithium, citing advantages such as a lower emitter temperature and a larger charge exchange cross-section in collisions involving helium and carbon impurities.

To achieve accurate diagnostics and effective regulation of plasma in proximity to tokamak reactor walls, a deep understanding of the cross-sectional properties of collision systems within the edge plasma is imperative. Precise cross-sectional data acquisition is pivotal in simulating and regulating the plasma effectively.

The applied method

During my PhD study, the classical trajectory Monte Carlo model (CTMC) [22,23] was used to investigate collision systems related to fusion plasma. The CTMC method is as a non-perturbed method, enables the consideration of all interactions among particles within the system. Moreover, it allows for the simultaneous calculation of all reaction channels. To analyse collisions effectively, the collision system is reduced to a three-body problem, employing a Garvey-type distance-dependent model potential [24]. This reduction combines the bound electrons and the core of the projectile ion as a single object, a procedure similarly applied to the target atom. In the target, the active electron of the target is considered as one body, while the core and remaining bound electrons form the another. The CTMC method is then apply for the calculations, providing the total cross sections in a wide impact energy range, typically around from tens of keV to tens of MeV. Furthermore, single and double differential cross sections are presented in the specific energy range of 30-60 keV, aligning with the energies relevant to plasma diagnostics in nuclear fusion applications.

The Main Objective

The main objective of my PhD work is to present a classical treatment of inelastic single electron processes in collision systems related to fusion plasma and other applications. The main focus lies in collision systems involving singly charged ion projectiles (proton, lithium, and sodium ions) and atomic targets (nitrogen and noble gases: helium, neon, argon, krypton, and xenon). The collision system is reduced to a three-body problem and the equations of motion are solved based on the classical trajectories Monte Carlo method [25]. A specific emphasis is on advancing the understanding of ion-atom collisions within the context of modelling and diagnostics of fusion plasma. By delving into the details of these collision processes, we seek to contribute valuable insights that can enhance the accuracy and effectiveness of fusion plasma diagnostics.

NEW SCIENTIFIC RESULTS

Within the classical trajectory Monte Carlo (CTMC), by employing the Garvey-type distance-dependent potential, we have studied the inelastic collision processes of the following systems: collision of singly charged lithium (Li^+) with atomic helium and nitrogen, singly charged sodium (Na^+) with atomic nitrogen, singly charged sodium (Na^+) with atomic noble gases (Ne, Ar, Kr and Xe), and protons with atomic noble gases (Ne, Ar, Kr and Xe) in wide range of impact energies which are relevant to the interest of fusion research.

These investigations have achieved substantial advancements in the theoretical examination of ion-atom collision systems. For systems that have experimental and/or theoretical results available, our CTMC results showed in most of the cases very good agreement with the previous data. We found very good agreement at intermediate energies, and a relatively good agreement at higher energies. However, at lower impact energies (below 10 keV) the agreement between experiment and theory was not good due the limitations of the CTMC method.

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

Thesis point 1

My research involved CTMC calculations to explore $Li^{+} - He$ *and* $Li^{+} - N$ *collision systems. I calculated the ionization and electron capture total cross sections as a function of the impact energy in the range (20 keV-100 MeV) and determined the impact parameter dependent probabilities. I found excellent agreement with the previous experimental and theoretical data.*

P[1]: One paper published in a refereed scientific journal and support this dissertation.
P[1]: Impact Score: 2.53, Q1.
P[5]: Proceeding paper

Thesis point 2

I employed CTMC calculations for $Na^{+} - N$ *collision system. I calculated the ionization total cross sections as a function of the projectile energy in the range (10 keV-10 MeV). Moreover, I calculated the ionisation differential cross sections for impact energies of 30, 40, 50 and 60 keV as a function of the scattering angle and the energy of the ionised electrons. I found that the majority of electrons are ejected at lower angles followed by backscattered electrons. Moreover, I have shown that the majority of these electrons acquire kinetic energies of 20 eV and below.*

P[2]: One Paper published in a refereed scientific journal and support this dissertation.
P[2]: Impact Score: 4.6, D1.
P[5]: Proceeding paper

Thesis point 3

Utilizing CTMC calculations, I examined collision of singly charged sodium ion (Na^+) with atomic noble gases (Ne, Ar, Kr and Xe). I calculated the ionization and electron capture total cross sections as a function of the projectile energy in the energy range between 10 keV and 50 MeV. Moreover, I calculated the ionisation differential cross sections for impact energy of 60 keV as a function of the scattering angle and the energy of the ionised electron. I found that electrons with energies below 10 eV are dominant in the forward scattering. Moreover, for 12 eV electrons, the DDCSs of backscattering and scattering at 90° show relatively identical results. I found that the backscattering DDCS was greater than the scattering DDCS at 90° for both Ne(2p) and Ar(3p) at electron energies larger than 12 eV. Furthermore, I found that the backscattering DDCS for Kr(4p) and Xe(5p) was greater than at scattering of 90° with energies larger than 50 eV.

P[3]: One paper submitted to Scientific reports and support this dissertation.
P[3]: Impact Score: 4.6, D1.

Thesis point 4

Conducting CTMC calculations, I investigated the collision of protons with atomic noble gases (Ne, Ar, Kr and Xe). I calculated the ionization and electron capture total cross sections as a function of the projectile energy in the energy range between 0.2 keV and 50 MeV. Moreover, I calculated the ionisation differential cross sections for impact energy of 35 keV as a function of the scattering angle and the energy of the ionised electron. I found excellent agreement with the previous experimental and theoretical data.

P[4]: One Paper published in a refereed scientific journal and support this dissertation.
P[4]: Impact Factor: 1.8, Q2.

Thesis point 5

I employed CTMC calculations to determine the contribution of the inner sub-shells to the total cross section, additionally, to determine the contribution of nuclear-nuclear potential on the collision dynamics. The calculations were performed for the following collision systems: collision of singly charged lithium (Li^+) with atomic helium and nitrogen, singly charged sodium (Na^+) with atomic nitrogen, singly charged sodium (Na^+) with atomic noble gases (Ne, Ar, Kr and Xe), and protons with atomic noble gases (Ne, Ar, Kr and Xe). I found that the inner shells contribution is insignificant at low impact energies (hundreds of keV and less), however, their contribution increases with increasing impact energies. Moreover, I also have shown that nuclear-nuclear potential has no significant effect on the collision dynamics.

P[1,2,3,4]: Three Paper published in a refereed scientific journal and support this dissertation. One paper submitted to Scientific papers and support this dissertation.
P[1]: Impact Score: 2.53, Q1.
P[2,3]: Impact Score: 4.6, D1.
P[4]: Impact Score: 1.8, Q2.

Publication related to the thesis

P[1]. **M. Al-Ajaleen**, A Taoutioui and K. Tőkési. Charge transfer and ionization cross-sections in collisions of singly charged lithium ions with helium and nitrogen atoms. *Plasma Physics and Controlled Fusion* **65** (2023) 065002. **DOI** 10.1088/1361-6587/acc6ed
Impact Score: 2.53, Q1.

P[2]. **M. Al-Ajaleen** and K. Tőkési. Total and differential ionization cross sections in collision between nitrogen atom and singly charged sodium ion. *Scientific Reports* **13** (2023) 14080. **DOI** 10.1038/s41598-023-41134-0
Impact Factor: 4.6, D1.

P[3]. **M. Al-Ajaleen** and K. Tőkési. Total and Differential Cross Sections of Collision of Singly Charged Sodium Ions with Noble Gases, (under review by *Scientific Reports*).
Impact Factor: 4.6, D1.

P[4]. **M. Al-Ajaleen** and K. Tőkési. Interaction of Protons with noble Gas Atoms: Total and Differential Ionization Cross Section. *Atoms* **12** (2024), 28. DOI 10.3390/atoms12050028
Impact Factor: 1.8, Q2.

P[5]. **M. Al-Ajaleen**, A. Taoutioui and K. Tőkési, *Ionization and electron capture processes induced in collisions between singly charged ions and nitrogen atom*, Proceeding of 48th EPS Conference on Plasma Physics, 2022. P1b.405, 1-5.

List of Conference Publications and Posters

1. **M. S. Al-Ajaleen** and Károly Tőkési, *Interaction of electrons and positrons with protons aligned in one-dimension line*. The 27th International Symposium on ion-atom collisions-virtual format (ISIAC 2021), July 16, 2021, Cluj-Napoca, Romania. **Poster**.
2. **M. Al-Ajaleen** and Károly Tőkési, *Interaction of electrons and positrons with two-dimensional proton lattice*. The 32nd International Conference on Photonic, Electronic and Atomic Collisions- virtual format (ViCPEAC 2021), July 20, 2021, Ottawa, Canada. **Poster**.
3. **M. Al-Ajaleen** and Károly Tőkési, *Interaction of electrons and positrons with two-dimensional proton lattice*. Virtual Meeting on the Molecular Dynamics in the GAS phase (MD-GAS 2021) - COST Action (CA18212): 2nd General Meeting, October 4, 2021. **Short Presentations**.
4. **M. Al-Ajaleen**, A. Taoutioui and K. Tőkési, *Ionization and charge exchange cross sections induced in collisions between singly charged ions and He(1s) and N(2p) atoms*, International Conference on Many Particle Spectroscopy of Atoms, Molecules, Clusters and Surfaces (MPS-2022), June 15-17, 2022, Turku, Finland. **Poster**.
5. **M. Al-Ajaleen**, A. Taoutioui and K. Tőkési, *Ionization and electron capture processes induced in collisions between singly charged ions and nitrogen atom*, 48th EPS Conference on Plasma Physics, June 27, 2022, Amsterdam (online), Netherlands. **Poster**.
6. **M. Al-Ajaleen**, A. Taoutioui and K. Tőkési, *Ionization and charge exchange cross sections in collisions between singly charged ions and ground-state atomic nitrogen*, 14th European Conference on Atoms Molecules and Photons (ECAMP14), June 27- July 1, 2022, 2022, Vilnius, Lithuania. **Poster**.
7. **M. Al-Ajaleen**, A. Taoutioui and K. Tőkési, *Ionization and electron capture processes induced in collisions between Li and He(1s) and N(2p) atoms*, 32nd Symposium on Fusion Technology (SOFT), September 18, 2022, Dubrovnik, Croatia. **Poster**.

Other Publication Not related to the thesis.

1. **Musab S. Al-Ajaleen** and K. Tőkési. Interaction of Electrons and Positrons with Protons Aligned in One-Dimension Line. *Atoms* **11** (2023) 46. DOI 10.3390/atoms11030046
Impact Factor: 1.8, Q2.

2. **M. Al-Ajaleen** and K. Tőkési. Interaction of electrons and positrons with two-dimensional artificially generated proton lattice and with carbon lattice. *Physica Scripta* **98** (2023) 075404. DOI 10.1088/1402-4896/acd969
Impact Factor: 3.081, Q2.

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List of publications related to the dissertation

<ins>Foreign language scientific articles in international journals</ins> (3)

1. **Al-Ajaleen, M. S. A.**, Tőkési, K.: Interaction of Protons with Noble-Gas Atoms: Total and Differential Cross Sections.
   Atoms. 12 (5), 1-18, 2024. EISSN: 2218-2004.
   DOI: http://dx.doi.org/10.3390/atoms12050028
   IF: 1.8 (2022)

2. **Al-Ajaleen, M. S. A.**, Taoutioui, A., Tőkési, K.: Charge transfer and ionization cross-sections in collisions of singly charged lithium ions with helium and nitrogen atoms.
   Plasma Phys. Control. Fusion. 65 (6), 1-8, 2023. ISSN: 0741-3335.
   DOI: http://dx.doi.org/10.1088/1361-6587/acc6ed
   IF: 2.2 (2022)

3. **Al-Ajaleen, M. S. A.**, Tőkési, K.: Total and differential ionization cross sections in collision between nitrogen atom and singly charged sodium ion.
   Sci. Rep. 13 (1), 1-9, 2023. EISSN: 2045-2322.
   DOI: http://dx.doi.org/10.1038/s41598-023-41134-0
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<ins>Foreign language conference proceedings</ins> (1)

4. **Al-Ajaleen, M. S. A.**, Taoutioui, A., Tőkési, K.: Ionization and electron capture processes induced in collisions between singly charged ions and nitrogen atom.
   In: 48th EPS Conference on Plasma Physics, EPS 2022. / Klinger T, European Physical Society, [Mulhouse], P1b405, 2022. ISBN: 9791096389162

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List of other publications

Foreign language scientific articles in international journals (2)

5. **Al-Ajaleen, M. S. A.**, Tőkési, K.: Interaction of Electrons and Positrons with Protons Aligned in One-Dimension Line.
   Atoms. -. 11 (3), 1-10, 2023. EISSN: 2218-2004.
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   IF: 1.8 (2022)

6. **Al-Ajaleen, M. S. A.**, Tőkési, K.: Interaction of electrons and positrons with two-dimensional artificially generated proton lattice and with carbon lattice.
   Phys. Scr. 98 (7), 1-11, 2023. ISSN: 0031-8949.
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