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# INDC International Nuclear Data Committee

## Data for Atomic Processes of Neutral Beams in Fusion Plasma

### Summary Report of the Third Research Coordination Meeting

IAEA Headquarters, Vienna, Austria

24 – 26 November 2021

Prepared by

C. Hill

June 2022

**IAEA Nuclear Data Section**

**Vienna International Centre, A-1400 Vienna, Austria**

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## Abstract

10 experts in the field of atomic collisional physics and neutral beam modelling for magnetic confinement fusion devices, together with IAEA Staff met online from 24 – 26 November 2021 for the Third Research Coordination Meeting of the IAEA Coordinated Research Project (CRP) F43023: *Data for Atomic Processes of Neutral Beams in Fusion Plasma*. They described progress since the previous project meeting in February 2019, discussed open issues and reviewed the coordinated research and code comparison activities conducted as part of the CRP. The proceedings of the meeting are summarized in this report.

June 2022

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# 1. Introduction

The IAEA Coordinated Research Project (CRP) on *Data for Atomic Processes of Neutral Beams in Fusion Plasma* ("Neutral Beams") is intended to provide evaluated and recommended data for the principal atomic processes relevant to heating and diagnostic neutral beams in fusion plasmas. Previous Research Coordination Meetings (RCMs) of this CRP were held in June 2017 and February 2019; this report summarizes the third and final RCM, held in November 2021. This meeting was held online because of the restrictions imposed in response to the COVID pandemic ongoing at the time. Summary reports of these meetings and more information about the background and the objectives of the project can be found on the AMD Unit's website at https://amdis.iaea.org/CRP/neutral-beams.

There were 10 research groups represented in the meeting, from nine Member States of the IAEA. The proceedings of the meeting are summarized in Section 2 and the discussions in Section 3. Work plan reviews from each participating group are provided in Section 4. The list of participants is in Appendix 1 and the meeting agenda is given in Appendix 2. Summary abstracts of presentations are presented in Appendix 3.

## 2. Proceedings

The meeting was opened by the staff of the Atomic and Molecular Data Unit, C. Hill and K. Heinola, and, after a brief introduction from the participants, the CRP goals and meeting objectives were reviewed. Participants presented their research activities during the second period of the CRP in the first half of the meeting, which was followed by discussion sessions focused on the two Code Comparison Workshop activities: *Atomic collision cross section calculations* and *Neutral Beam Modelling*.

The presentation session started with a presentation by A. Kadyrov (Curtin University) on recent progress in applications of the wave-packet convergent close-coupling (WP-CCC) approach to ion-atom collisions relevant to the CRP: this is particularly relevant to the proton-hydrogen system, for which the ionisation cross section is the subject of major uncertainties; Y. Wu (Institute of Applied Physics and Computational Mathematics) then outlined his group's work on ion-atom collisions in the low- to intermediate-energy range and K. Tőkési (Institute for Nuclear Research, Hungarian Academy of Sciences) presented his work on calculations of heavy-particle collisions of hydrogen atoms with H, C and Li ions using the Classical Trajectory Monte Carlo (CTMC) computational technique. After a short break, C. Illescas (Universidad Autónoma de Madrid) presented her group's comparison of the CTMC and (Grid) Time-Dependent Schrödinger Equation (GTDSE) techniques applied to the calculation of state-dependent cross sections for electron capture and H excitation and ionisation within the $Be^{4+}$ + H system. Nicolas Sisourat (Sorbonne Université) then summarised his work with Alain Dubois on recent theoretical developments to their semiclassical non-perturbative approach for one and two-electron collision systems with reference to the calculation of electron capture, excitation and ionization cross sections for collisions of fully stripped hydrogen, helium and lithium ions with atomic hydrogen in the ground state and in excited states up to $n = 3$. Finally, K. Tőkési gave a second presentation on the development of a three-body quasi-classical Monte Carlo model which accounts for the quantum features of collisional processes better than CTMC at modest computational cost.

The second day of the meeting started with the final presentation on collisional calculation methods, given by T. Kirchner (York University) on Basis Generator Method (BGM) calculations for ion-atom collision systems. There followed a discussion session, described in Sections 3.1 and 3.2 below.

The session concerning neutral beam modelling started with a presentation from J. Ko (Korea Institute of Fusion Energy) on beam emission spectra research at the KSTAR facility in Daejeon, Republic of Korea, focused on recent progress made on the polarimetric and spectral Motional Stark Effect (MSE) diagnostic systems on the KSTAR tokamak experiment. O. Marchuk (Forschungszentrum Jülich) then described his own group's use of atomic data for MSE modelling, with reference to the derivation of a general expression for the excitation cross sections in parabolic states within $n = 3$ for an arbitrary orientation between the direction of the motion-induced electric field and the proton-atom collisional axis. G. Pokol (Institute of Nuclear Techniques, Budapest University of Technology and Economics) described upgrades to the RENATE Open Diagnostics neutral beam modelling code, and M. O'Mullane (University of Strathclyde) gave a presentation on the most recent work towards the addition of uncertainties to the ADAS beam model.

| Reactant #1 and energy | Reactant #2 | Excitation probabilities and cross sections (*m*-resolved) | Density matrix elements | Ionization probabilities and cross sections | Charge-exchange probabilities and cross sections | *nl*-resolved excitation probabilities and cross sections |
|---|---|---|---|---|---|---|
| H(1s) + … 10 keV – 1 MeV | $H^+$ | AK, AD | AK, CI | AK, YW, CI, AD | AK, YW, CI, AD | AK, YW, AD |
| | $He^{2+}$ | AK, AD | AK, CI | AK, YW, CI, AD | AK, YW, AD | AK, YW, AD |
| | **$Li^{3+}$, $C^{3+}$, $O^{3+}$** | **TK** | | **TK** | **TK** | **TK** |
| | $Be^{4+}$ | **AD, AK** | CI | CI, **AD, AK** | CI, YW, **AD, AK** | CI, **AD, AK** |
| | $C^{6+}$ | AK | AK, CI | AK, CI | AK, YW, AD-limited | AK |
| | $Ne^{10+}$ | **AK** | CI | CI, **AK** | CI, YW, **AK** | **AK** |
| | H(1s) | (CI), KT, AD, **AK** | (CI) | AK, CI, KT | (CI), KT | (CI), KT |
| | $H_2$ | | | KT | | |
| H(2s, $2p_0$, $2p_1$) + … 10 keV – 1 MeV | $H^+$ | AK, CI, TK, **AD** | AK, (CI), (TK) | AK, (CI), TK, KT | AK, (CI), KT, TK | AK, (CI), KT, TK |
| | $He^{2+}$ | **AD** | | **AD** | **AD** | **AD** |
| | $Be^{4+}$ | **TK, AD** | | (CI), **TK**, **AD** | (CI), **TK**, **AD** | CI **TK**, **AD** |
| | $C^{6+}$ | | | CI, KT | CI, KT | CI, KT |
| | $N^{7+}$ | | | CI | CI | CI |
| | $Ne^{10+}$ | | | KT | KT | KT |
| | H(1s) | | | KT | KT | KT |
| | $H_2$ | | | | | |
| H(n>2) + … | $H^+$ | (CI), AD | (CI) | (CI), KT, **AD** | (CI), KT, **AD** | (CI), KT, **AD** |
| | $He^{2+}$ | AD | | AD | AD | AD |
| | $Be^{4+}$ | | | KT, (AD) | KT, (AD) | KT, (AD) |
| | $C^{6+}$ | | | (CI) | (CI) | (CI) |
| | $Ne^{10+}$ | | | KT | KT | KT |
| | H(1s) | | | KT, (AD) | KT, (AD) | KT, (AD) |
| | $H_2$ | | | | | |
| He ($1s^2$ $^1S$) + … | bare ions, $E_{tot}$ <= 70 keV | AK, (TK), **AD** | | AK, YW, **AD**, TK | AK, YW, **AD**, TK | AK, YW, **AD**, TK |
| He (1s2s $^3S$) + … | bare ions, $E_{tot}$ <= 70 keV | | | YW, (AD) | YW, (AD) | YW, (AD) |
| Li (2s) + … | bare ions, $E_{tot}$ <= 50 keV | **TK, AK** | | KT, YW, (AD), **TK, AK** | KT, YW, (AD), **TK, AK** | KT, YW, (AD), **TK, AK** |
| Na (3s) + … | bare ions, $E_{tot}$ <= 50 keV | (TK), AK | | KT, (AD), (TK), AK | KT, (AD), (TK), AK | KT, (AD), (TK) |

In the final session of the meeting, on the third day, the *Atomic Processes of Neutral Beams in Fusion Plasma* Code Comparison Workshop activity was discussed (see Section 3.3, below).

The meeting concluded with some tentative planning for a future, in-person Consultancy Meeting to be held at the IAEA in 2022 and discussion of the CRP final report, which is expected to take the form of a review article on atomic data for neutral beam modelling, to be submitted to a suitable journal (possibly *Nuclear Fusion*).

# 3. Discussions and Conclusions

## 3.1 Status of ion-atom collision data assembled during the CRP

The table above updates that of Section 3.2 (p. 11) of the report of the Second Research Coordination meeting (IAEA publication INDC(NDS)-0780, February 2019). Shaded cells indicate data needs of lower priority. Participants are identified by their initials; where initials are given in parentheses, calculation of these data sets is ongoing. Data sets calculated since the previous meeting are highlighted in bold text.

## 3.2 Code Comparison Workshop on Electron Dynamics of Atomic Collisions

The discussion session concerning the Code Comparison Workshop on Atomic Collisions was chaired by the Workshop coordinator, N. Sisourat. The status of participants' calculations was reviewed and a format and set of metadata for submission of calculated cross sections established. The collisional system, $Be^{4+}$ + H (1s; 2s; $2p_0$; $2p_1$), and energies had previously been agreed. The key processes (ionization, excitation, electron capture) were confirmed, with the initial focus to be on *n*-dependent processes, with *nl*-dependence to follow when available.
A deadline of 5 weeks (before the end of 2021) for submission of these calculated data sets was agreed. After aggregation by N. Sisourat and A. Dubois, they will be reviewed at a subsequent meeting in 2022. Updates to the comparison exercise will be posted on the AMD Unit's website in advance of the CRP final report.

It was emphasised by M. O'Mullane that the data produced by the CRP should be made available to neutral beam modellers, and it was confirmed that the AMD Unit's new CollisionDB database will be available to store all published cross section and rate coefficient data from participants.

The matrix of calculated data (Section 3.1, above) was reviewed and participants requested to complete it with their latest results.

## 3.3 Code Comparison Workshop on Beam Penetration

The discussion session concerning the Code Comparison Workshop on Neutral Beam Penetration and Photoemission modelling was chaired by Gergő Pokol (Wigner Research Centre for Physics, Budapest University of Technology and Economics). Nine constant temperature and density profiles and three variable profiles (ITER scenario, ITER scenario with a scrape-off layer "blob", and Island diverter scenario) were considered, with beams consisting of H, D, T and possibly Li and Na neutrals. Three beam energies, 30, 100 and 1000 keV were adopted for simulation. Further details are available at https://amdis.iaea.org/workshops/neutral-beam-penetration-and-photoemission. The codes compared are RENATE, RENATE-OD, BBNBI, FIDASIM, SOS, CHERAB, and CRM.

Interim results from the exercise have been presented at the 47th European Conference on Plasma Physics [1]; the deadline for the remaining data to be submitted for comparison was set to the end of 2021. Plans for a report of the outcome of the Workshop exercise were explored; this is likely to take the form of a peer-reviewed article in a suitable journal, possibly *Atoms* or *Journal of Physics B*. A report will also been given at the 32nd Symposium on Fusion Technology (SOFT-2022) in September 2022.

There was some discussion about the inclusion in the code comparison exercise of cross section data, particularly for charge-exchange collisions, calculated by different computational methods within the CRP: these data will be ready by mid-2022, and will be discussed at the follow-up consultancy meeting.

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## 4. Work Plan Reviews

### Alain DUBOIS, Laboratoire de Chimie Physique – Matière et Rayonnement (LCPMR), Sorbonne Université

Since the first meeting of our CRP, the activities of the LCPMR group have followed two directions:

### *1. The methodological and numerical development needed to investigate the electronic processes and systems relevant for the CRP*

- We have thus developed a code for solving non-perturbatively the time-dependent Schrödinger equation (within a semiclassical approach and an asymptotic state representation of the electronic wavefunction) for systems and processes involving one and two (or quasi-two) active electrons. This new code is totally independent of our original program (working up to four active electrons) and therefore allows mutual comparisons to track for numerical instabilities and convergence, among other. Its originality lays in the optimal connection with quantum chemistry codes (to generate basis sets of electronic states), in memory saving and in the possibility to use atomic orbitals of high angular momenta.
- These two available codes and approaches, based on L2 Gaussian type orbital representation, are designed to describe efficiently bound-bound transitions (as capture and excitation processes) but are less adapted for single and multiple ionization processes. We have thus developed a general method based of artificial intelligence and machine learning algorithms to be able to discriminate and interpret our results in term of single and double ionization cross sections. This method was illustrated for antiproton-helium collisions at intermediate impact energies [1].

### *2. The calculations of total and partial, integral and differential cross sections for several relevant collision systems*

- Collisions involving excited target/projectile prior to scattering. This domain has not been studied much in the past since (i) it is not related to any actual experimental investigations and (ii) it is complex to tackle in modeling (need of high number of states and angular momenta, …). In that context, we have investigated collisions between H(*nl*) (with $n = 1, 2$ and 3) and fully stripped ions ($H^+$, $He^{2+}$, $Li^{3+}$) using the codes presented above. We have produced tables of cross sections for ionization, capture and excitation, for benchmarking and future comparison with other theoretical investigations [2]. We have used also an approach based on pure classical mechanics (CTMC method) to study $H^+$-H(nl) with n up to 10 to look for scaling laws [3].

- MeV collisions involving $C^{4+}$ excited in the metastable 1s2s $^3S$ state and helium, focusing on the production of autoionizing states after capture. This was done in collaboration with experimentalists from Universities of Heraklion and Ioannina [4].
- Collisions Involving multi-active electron collision systems and processes: among others we mention the study of $N^{5+}$ - $H_2$ collisions [5] and double electron capture in $H^+$ - $H^-$ collisions [6], with Peking Y. Wu's group, and the study of single capture at the level of differential cross sections in $C^{4+}$ - He collisions, with XW. Ma and XL. Zhu's experimentalist team in Lanzhou (P.R. China) [7].

While systems in the last two item are not directly relevant for the objectives of the CRP, their investigations were crucial for the benchmarking of our method and thus allowed us to evaluate the (overall good) accuracy of the data provided for the CRP-relevant systems.

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**Clara ILLESCAS, Department of Chemistry, Universidad Autónoma de Madrid (UAM)**

## *Summary of the research carried out by the UAM Group*

In connection with the IAEA CRP F43023, we have carried out the calculations of cross sections for total ionization and, total, *n*-partial and *n,l*-partial charge exchange and excitation of the target in collisions of neutral H with some fully stripped impurity ions. We have employed two different methods, the Classical Trajectory Monte-Carlo method (CTMC) and the numerical solution of the time-dependent Schrödinger equation (GTDSE). We have focused our attention on collisions of $Be^{4+}$ ions with H(1s), H(2s) and H(2p) targets at energies of 20, 100 and 500 keV/u. We have constructed a hydrogenic initial distribution to describe the H($n$=2) target, which improves the results respect to those of the standard microcanonical CTMC calculations. We have carried out two separate GTDSE calculations, one with the origin

of the electron coordinates placed on the H nucleus which allows us to determine excitation cross sections and, a second one, with the origin placed on $Be^{4+}$ that yields electron capture cross sections.
We have been able to assess uncertainties to the produced data in the case of GTDSE and to assess statistical uncertainties in the CTMC data.

A computational study of $Be^{4+}$ + H(2s) collisions has been published in Physical Review A [1]. A paper on the calculation of charge-transfer n partial cross sections for collisions of $Be4^{+}$ with H(1s) in a wide energy range (between 1 and 500 keV/u) was previously published in Physical Review A [2]. Collisions of possible interest such proton-Argon collisions where studied in a work published in Journal Physical Chemistry A [3]. Other recently published work includes m- and h-CTMC studies of the $C^{6+}$ + H(1s) and $N^{7+}$ + H(1s) systems [4] and classical and semi-classical studies of $Li^{3+}$ + H(1s) and $Ne^{10+}$ + H(1s) collisions [5].

Our planned future work is to study the inelastic processes of fully stripped low charged ions ($H^{+}$, $He^{2+}$, $Be^{4+}$, $C^{6+}$) in collision with He targets employing semiclassical and classical methods. In the CTMC treatment, our interest is to carry out an explicit two active electrons treatment of the He target in order to describe double electron processes (double ionization, double capture and transfer ionization) and to analyse the relative importance of those respect to the single electron processes at intermediate energies. We are also interested in studying $He^{+}$ + H(1s) collisions. Finally, we are considering to study in deep the benchmark $H^{+}$ + H(1s) collision with the semiclassical GTDSE method. All these planned studies could perfectly be a part of a future collaborative research.

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## Alisher KADYROV, Faculty of Science and Engineering, Curtin University

### *Accurate calculations of state-resolved cross sections for excitation, ionization and charge transfer in collisions of hydrogen isotopes with protons, deuterons, tritons and the main impurity ions in fusion plasma*

We used the two-center wave-packet convergent close-coupling (CCC) approach to calculate cross sections of various ion-atom collisions relevant to fusion plasma. The highly-advanced CCC approach incorporates all underlying processes including excitation and ionization of the atom, electron transfer into bound and continuum states of the ion. As a result the approach is capable of providing the most accurate state-resolved cross sections for all these processes. We have completed practically all the tasks we planned to do within the CRP. During the first year of the CRP we performed highly-accurate calculations of the Balmer-α ($n$=3 to $n$=2) emission when a hydrogen or deuterium beam is injected into the fusion plasma. This required accurate calculations of the cross sections for excitation of 3s, 3p and 3d states of the neutral atom. Almost 90% of the Balmer-α emission comes from 3s and 3d states. In addition, since the plasma contains protons and deuterons, electron transfer to 3s, 3p and 3d states of hydrogen and deuterium atoms will also contribute. There was almost a factor of 2 disagreement between experimental measurements and theoretical calculations for the Balmer-α emission. We resolved this discrepancy by providing highly-accurate data on cross sections of all underlying processes. We provided accurate data for ion scattering on excited states of hydrogen. In particular, we considered further excitation or de-excitation, electron capture and ionisation in proton collisions with H($nlm$), where the principal quantum number $n$ was 2. However, our method can provide cross sections for larger n if required. We provided state-resolved cross sections for excitation, electron transfer and ionization in collisions of various atoms with the main impurity ions in fusion plasma. Specifically, we calculated scattering of protons and $He^{2+}$, $Be^{4+}$, $C^{6+}$ ions with H, and proton scattering on mutielectron He, Li, Na and K targets. Presently, we are doing $Be^{4+}$ ion collisions with H initially in 2s, 2p0 and 2p1 states, $Li^{3+}$ and $Ne^{10+}$ ions collisions with H, and proton collisions with molecular hydrogen including electron capture. Within the framework of the CRP on Data for Atomic Processes of Neutral Beams in Fusion Plasma, so far we have published 17 peer-reviewed papers in high-profile journals. These are listed below in the reverse chronological order.


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## Tom KIRCHNER, Department of Physics and Astronomy, York University

### *Basis Generator Method Calculations for Ion-Atom Collision Systems of Relevance to Neutral Beams in Fusion Plasma: Summary of Activities in Connection with CRP*

The Basis Generator Method (BGM) has been developed over many years as a tool for the solution of time-dependent quantum problems in terms of a dynamically adapted basis set expansion. The bulk of BGM applications deal with ion-atom and ion-molecule collision problems within the semiclassical approximation. For the activities in connection with the

Coordinated Research Project (CRP) on Data for Atomic Processes of Neutral Beams in Fusion Plasma its two-centre implementation (TC-BGM) in which bound projectile states are included explicitly in addition to bound target states and BGM pseudostates, has been used. More specifically, the following problems have been addressed over the course of the CRP:

- We have carried out TC-BGM calculations for proton-hydrogen collisions for 1s, 2s, and 2p initial states in the one to few-hundred keV impact energy range. The calculations required larger basis sets than used previously and, accordingly, took substantial computing time. Convergence has been tested carefully. The work has been published in Ref. [1].
- We have studied low-impact-energy collisions of multiply-charged bare ions ($C^{6+}$ and $O^{8+}$) with atomic hydrogen. In addition, we have considered krypton target atoms. Krypton and hydrogen have very similar (first) ionization potentials, which suggests that low-energy capture collisions of highly-charged ions might be comparable for both targets. Our TC-BGM calculations demonstrate that this is in general not the case and that there can be substantial differences in state-selective capture from hydrogen versus krypton. The main objective of the work was to compare calculated Lyman-line emission counts for both targets with measurements for krypton. It has been published in Ref. [2].
- A similar study with an emphasis on radiative emissions was carried out for slow $Ne^{8+}$ impact on helium atoms and hydrogen molecules and has been published in Ref. [3]. Similar to the calculations of Refs. [1,2] relatively large basis sets were necessary to calculate electron capture into high-lying projectile states, and reasonable convergence was achieved.
- Collisions of $Be^{4+}$ ions with atomic hydrogen in ground and excited initial states have been considered. We have focused on the collision energies of 20, 100, and 500 keV/amu, as agreed upon with the other participants of the CRP, and have calculated target excitation, electron capture, and total ionization cross sections. Reasonably well-converged results have been obtained for H(1s) and H(2s) initial states, but not for H(2p). For the latter we have found that bound projectile states of principal quantum number $n>10$ would be necessary in the expansion. While this is not a problem per se, very large bound-state basis sets lead to conflicts with BGM pseudostates in that numerical linear dependences occur, resulting in singular overlap matrices. These problems may be overcome and are a potential topic of future work.
- Collisions of bare and partially-stripped triply charged ions ($Li^{3+}$, $C^{3+}$, $O^{3+}$) with ground-state hydrogen have been considered. We have looked at collision energies from 1 to 100 keV/amu and have compared our calculations with previous work where available. For the $C^{3+}$ and $O^{3+}$ cases effective potentials to represent the interaction of the initial hydrogen electron with the projectile ion were adopted. For $C^{3+}$ we have checked that our cross-section results do not change dramatically if different potential variants are used. Moreover, our calculations do not indicate that the projectile electrons play an active role in the collision dynamics. The calculations have been completed and the work has been submitted for publication [4].

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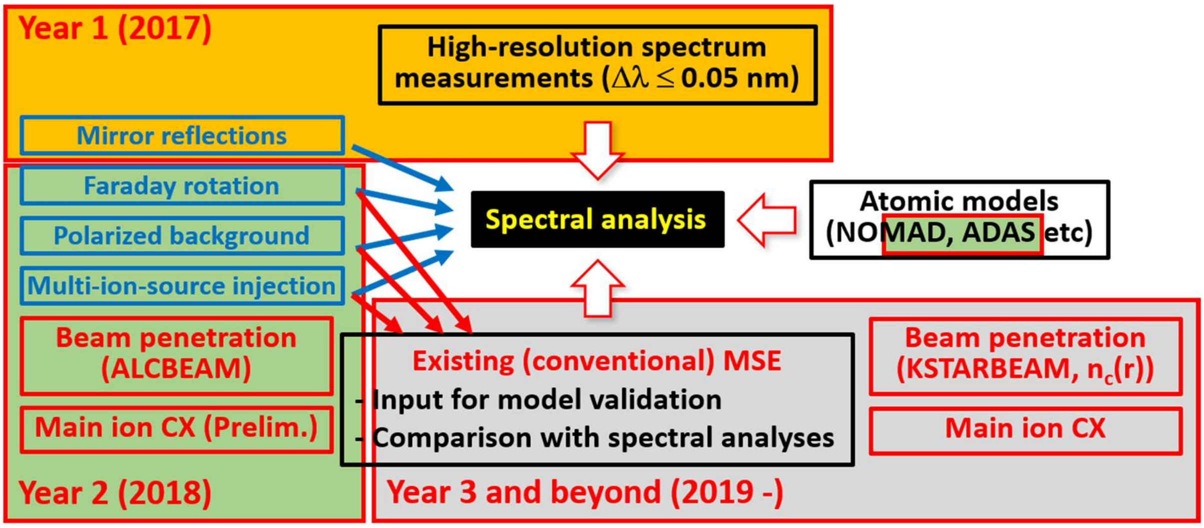
## Jinseok KO, Korea Institute of Fusion Energy (KFE)

### *Summary of the research (2019-2021)*

Several progresses have been made for both polarimetric and spectral motional Stark effect (MSE) diagnostic systems in KSTAR associated with the experimental validation of atomic data for MSE diagnostics. The scope of the research is two-fold: (1) High-precision measurements of beam-emission spectra from KSTAR discharges; and (2) Development of a spectra analysis tool with a modulated interface for atomic data. The strategic work breakdown structure for this scope is given in the diagram below along with some specific work items. Brief summaries on individual work items relevant to the Year 3 (2019 – 2021) are given in the following paragraphs.




**Polarized background light:** The origin and characteristics of polarized background light have been identified. Correlation between the intensity of polarized light from the background signal and the plasma density clearly indicates that some particular channels have a strong dependence of polarized background light on the plasma density. Investigation of the light-of-sight dump on the vacuum vessel wall reveals these channels suffer from strong reflections due to the particular structure at their locations. We've introduced a 25-channel polychrometer-type MSE system that is capable of measuring background part of the polarized light such that the polarized background can be subtracted simultaneously. The cross-check between the existing conventional (single-detector-type) MSE and the polychrometer MSE has been performed by interleaving the fibers to both systems.

**Faraday rotation:** A new effective Faraday-rotation effect calibration technique applicable to superconducting tokamaks has been developed [Ko et al., Rev. Sci. Instrum. 92, 033513 (2021)]. The approach includes the torus pressure scan with a fixed vacuum field to take the secondary neutral beam effect into account. In this way, for a particular pitch angle at a particular location, the MSE can obtain a series of measurements at different torus pressure, from which a polarization angle at 'zero' pressure is extrapolated. A separate experiment where the plasma boundary is jogged in confirms that the measured pitch angle with the Faraday calibration removes residual systematic offsets that exist without the Faraday correction. The calibration also implies that the Faraday effect is dominant in the KSTAR environment.

**Multiple ion source injection:** A systematic methodology has been devised to evaluate the effect of multi-ion-source neutral beam injection on polarimetric MSE measurements [Lee et al., Fusion Eng. Des. 173, 112870 (2021)]. The developed model involves the optimization process of multiple Stokes vectors based on the measured intensities with and without the addition of the second beam source. It is noted that the spectral analysis for two-ion-source beam injection was treated in the last meeting (2019), so this new model will be used in spectral and polarimetric MSE comparison with two-ion-source injection conditions.

**Comparison between spectral and polarimetric MSE:** The spectral MSE approach under development has been tested with a wide range of plasma densities and its sensitivity has been compared with that of the polarimetric MSE. The MSE spectra were taken during the 2020 KSTAR campaign under the joint experiment proposal by J Ko and O Marchuk to investigate the deviation of statistical populations in MSE atomic levels with a certain range of plasma density (2 to $3.5 \times 10^{19}$ $m^{-3}$). A spectral fit on the MSE emission has been done to infer vertical fields at several locations. Reasonable agreement in the inferred vertical fields from the spectral and polarimetric analyses has been observed; With slight offsets, the vertical fields from the spectral analysis exhibit similar sensitivity as those from polarimetric MSE over two different vertical field profiles.

**Main-ion charge exchange:** It was reported in the last meeting in 2019 that there was an observation of main-ion charge exchange components around the thermal Balmer alpha region which qualitatively broaden during high confinement regimes. Since then, a multi-Gaussian spectral fit has been done for this region in addition to the MSE fits and evaluated the ion temperatures which are well correlated with the L and H modes.

**Beam penetration code:** The KSTAR version of the beam penetration code (originally, ALCBEAM, introduced in the last meeting in 2019) has been developed (KSTARBEAM) and used to evaluate impurity carbon ($C^{6+}$) density profiles. The beam stopping information is used to calculate the carbon density associated with the effective charge exchange emission rates from ADAS. The carbon density profiles obtained from this analysis confirm that the impurity accumulation during the edge-localized-mode (ELM) free phase while electrons are pumped out, which is consistent with the general observations during the ELM suppression induced by the resonant magnetic perturbation.

## *Challenges*

Acquiring spectral data from the neutral beam penetrating through neutral gas under magnetic fields (beam-into-gas experiments) is important for studying the differences in collisional l-mixing of the beam atoms traveling through a $D_2$ gas versus a plasma and the comparison with the cross section data for H* + $H_2$ collisions. However, the run time for the beam-into-gas experiment is very limited because the tokamak experimental campaign is usually packed with higher-priority 'plasma' experiments. We are considering to utilize pre-campaign commissioning period to perform the beam-into-gas spectrum measurements.

## *Future plans and scopes*

**Measurements of MSE spectra at higher densities and in helium plasmas:** KSTAR recently developed stable plasma control with the plasma current of a mega-ampere or more. This will help expanding the operation plasma density ranges. Also, the slit size of the MSE spectrometer will be further reduced for better spectral resolution. A new joint experiment proposal will be prepared for the 2022 KSTAR campaign for this (J. Ko and O. Marchuk). The result will be added to a database that includes results from JET, Alcator C-Mod etc. Since there is no experimental data of MSE intensities in helium plasmas and therefore, no predictions and studies available for initial ITER plasmas, we will try the MSE spectrum measurements in helium plasmas. The fit procedure needs to be improved further like stabilization (or automation) in establishing initial fit parameters. The number of MSE sightlines for spectrum measurements will be increased (maximum 7 or so). The sensitivity comparison study in the vertical field or pitch angle between spectral and polarimetric MSE approaches will be extended to various advanced operation regimes such as internal transport barrier (ITB) plasmas.

**Main-ion charge exchange:** Direct inference of ion characteristics through main-ion charge exchange signal analyses will be further applied to recent and upcoming high-Ti (> 10 keV) KSTAR discharges. The result will be cross-checked with those from other (impurity-base) Ti diagnostics such as charge exchange recombination spectroscopy and X-ray imaging crystal spectroscopy. The spectral fit will be more refined to include cross-section distortion, halo, and beam-off background components.

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**Oleksandr MARCHUK, Forschungszentrum Jülich (FZJ)**

## *Atomic data in the active beam spectroscopy of fusion plasmas*

The atomic data used in the neutral beam drive spectroscopy can be divided in several sections: atomic data used to simulate the beam penetration only, atomic data used for fast ion diagnostics, the data for the charge-exchange recombination spectroscopy and finally the atomic data for the beam-emission spectroscopy and Motional Stark effect.

During the last few years significant progress was achieved in understanding the processes leading to the beam excitation in fusion plasmas. As a result of this CRP exceptionally high quality data on the excitation of fast beam atoms by collisions with plasma ions became available [1]. One should nevertheless keep in mind that the *eigenstate* of the beam atoms are parabolic states [2] (if one neglects the week Zeeman splitting [3]) due to the strong electric field which exist in the rest frame of the atoms. The major problem is therefore to connect the new available cross sections with the excitation of new eigenstates. The approach is based on the density matrix formalism and includes two transformation between the wavefunctions [4].

In the second part of this CRP we succeeded in presenting the analytical representations of cross sections in parabolic states in the collisional energy range of 20 – 1000 keV/amu. The excitation cross sections are shown in the closed analytical formulas invoking the elements of the density matrix elements calculated using the AOCC approach [5]. An example of the fitting of the cross sections is shown in the Figure 1 for $n = 2$.

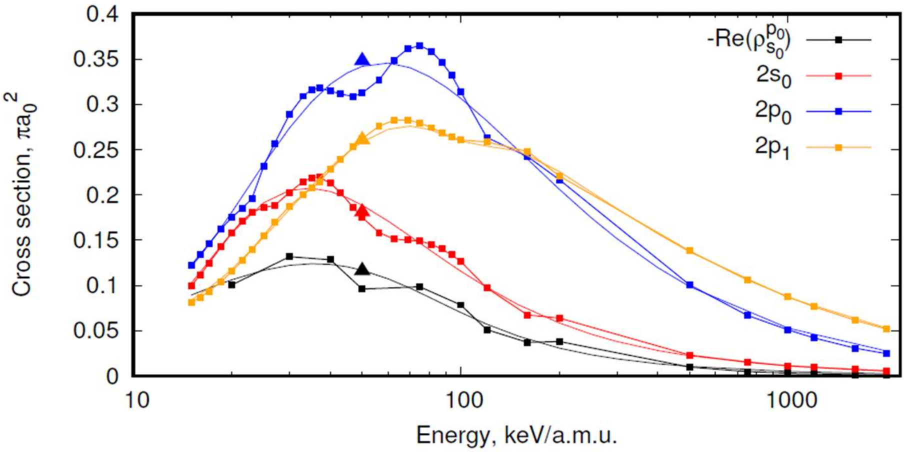


*Figure 1. Fitting of the excitation cross sections to the n=2 levels by ion impacts from 20 keV*

The results of the fit for *n = 3* excitation are shown in Figure 2. Here, in contrast to the *n = 2* level excitations, the number of the off-diagonal elements increases. The Table 1 shows the summary of the coefficients necessary to calculate the cross sections in parabolic states. We point out that the formulas include, for instance, the type of excitation e.g. the dipole and non-dipole excitation or the case of the off-diagonal term of the density matrix. The connection between the cross sections in spherical and parabolic states are as follows:

$$\sigma_{n=2} = \sigma_{s0} + \sigma_{p0} + 2\sigma_{p1} = \sigma_{210} + \sigma_{2-10} + 2\sigma_{201},$$

$$\sigma_{n=3} = \sigma_{s0} + \sigma_{p0} + \sigma_{d0} + 2\left(\sigma_{p1} + \sigma_{d1} + \sigma_{d2}\right) = \sigma_{320} + \sigma_{3-20} + \sigma_{300} + 2\left(\sigma_{3-11} + \sigma_{311} + \sigma_{302}\right)$$

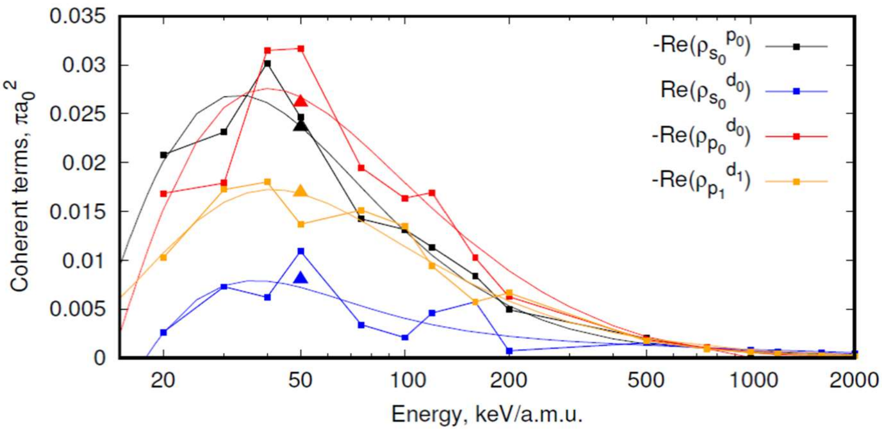


*Figure 2. The coherent terms of the density matrix. Excitation of hydrogen atoms by proton impact.*

The cross sections in parabolic states can be approximated using this table and the expression for the transformation between the spherical and parabolic wavefunctions [5].

**Table 1.** Table of fit coefficients for the excitation cross sections and the real part of coherence terms for excitation to $n = 2$ and $n = 3$. Expression (12) is applied to fit the atomic orbital close coupling (AOCC) data for all elements except the $2p_1$, $3p_1$, and $3d_1$ cross sections in which case the expression (13) must be used. We note that the real part of all coherence terms is negative except for $s_0d_0$ excitation.

| | $A_0$ | $A_1$ | $A_2$ | $A_3$ | $A_4$ | $A_5$ | $A_6$ | $A_7$ | $A_8$ | B |
|---|---|---|---|---|---|---|---|---|---|---|
| $2s_0$ | 3.49+01 | 3.05+01 | 1.01-03 | 5.33-01 | −2.78+00 | −9.33-03 | 3.18+00 | 1.07-02 | 1.03+00 | 0 |
| $2p_0$ | 5.51+01 | 5.89+01 | 9.31-05 | 1.52-01 | −1.66+00 | 1.45-05 | −2.69+00 | 8.48-01 | −8.81+00 | 0 |
| $2p_1$ | 5.23+00 | 7.37+01 | −6.02-34 | 1.89-01 | −1.95+01 | 2.79-02 | 9.40+00 | 1.86-02 | 7.25-01 | 2.12+01 |
| $-s_0p_0$ | 4.96+00 | 5.17+01 | 0 | 0 | 0 | 2.75-02 | 7.84+00 | 5.56-05 | 2.29+00 | 0 |
| $3s_0$ | 3.79+00 | 6.55+01 | 1.19-04 | 5.67-02 | −1.72+00 | −3.55-04 | 6.25+01 | 3.41+10 | −1.29+01 | 0 |
| $3p_0$ | 9.52+00 | 6.30+01 | 4.03-05 | 1.28-01 | −1.88+00 | −9.51-05 | 4.04+03 | −7.13+12 | −1.85+01 | 0 |
| $3p_1$ | 1.70-01 | 6.37+01 | −6.92-01 | 3.50-02 | 1.80-01 | 3.55-01 | 2.38+00 | 5.33-03 | 9.40-01 | 1.14+01 |
| $3d_0$ | 5.24-01 | 8.52+01 | 4.31-04 | 3.74-02 | −1.57+00 | 9.84-05 | −3.05+01 | 3.49+10 | −6.75+00 | 0 |
| $3d_1$ | 1.03-02 | 6.37+01 | −1.30+00 | 2.68-01 | −1.52+00 | 1.54+00 | 2.23+00 | 1.50-03 | 1.64+00 | 1.14+01 |
| $3d_2$ | 5.45-01 | 8.11+01 | 0 | 0 | 0 | 5.24-05 | −9.22+01 | 9.67+11 | −8.67+00 | 0 |
| $-s_0p_0$ | 4.58+00 | 2.95+01 | 0 | 0 | 0 | −7.93-03 | −7.40-02 | 5.24-03 | 1.07+00 | 0 |
| $s_0d_0$ | 2.84e+00 | 2.73e+01 | 0 | 0 | 0 | −1.40e-02 | −7.71e-02 | 5.04e-03 | 1.20e+00 | 0 |
| $-p_0d_0$ | 4.33+00 | 3.28+01 | 0 | 0 | 0 | −2.17-02 | −7.53-02 | 4.83-01 | 5.51-01 | 0 |
| $-p_1d_1$ | 5.25e-02 | 1.23e+02 | 0 | 0 | 0 | 3.03e+01 | 5.47e+01 | 1.34e-01 | 1.39e+00 | 0 |

*Table 1. The table summarizes the fitting coefficients for excitation of atoms by proton impact.*

We should point out that, until now, the formulas for the cross sections in parabolic stattes were obtained only for excitation from the ground state. Thus, the line ratio of the Stark components could be analytically calculated in the *low-density limit* only.

The new calculation demonstrate some others interesting features. Thus, for instance it is proven that in the case of MSE diagnostic in fusion plasmas for instance, the line intensities of $\sigma^+$ and $\sigma^-$ components as well as of the $\pi^+$ and $\pi^-$ must be symmetrical. However, in the case of excitation in the laboratory plasma discharges such as the cathode rays the symmetry breaks. It is shown in the next Figure. The MSE conditions are the most favorable ones as the all (±) components are symmetrical. The frequently observed asymmetry in the experimental MSE spectra are connected with the geometry of the observation such as the angles between the line-of-sight, beam direction and the magnetic flux surfaces.

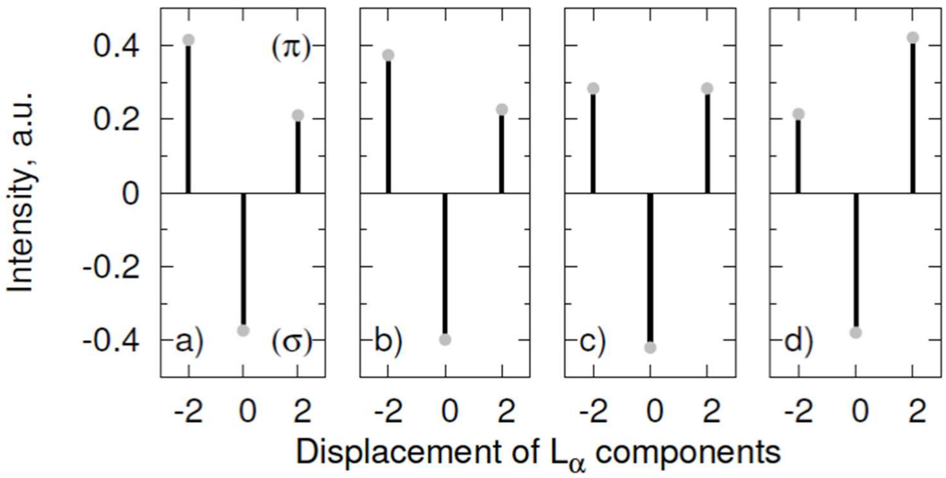


*Figure 3. Intensity of $L_\alpha$ components for different angles of orientation between the electric field and the velocity of atom (proton ion is at rest). For (a) the angle is 0c, (b) the angle is 45°, (c) the angle is 90° and (d) the angle is 180°.*

The obtained asymmetry in the excitation of $L_\alpha$ or $H_\alpha$ components is qualitatively confirmed from the first results on Stark effect in plasma discharges. The line intensities are changed depending on the angle of orientation between the electric field and electrons velocity. Usually the excitation at 0° and 180° degree was detected.

The obtained results provide the user with the possibility to estimate the line ratios between different components in the low density limit. The obtained data were already implemented in the SOS code [6]. At the same time, the results could be used in the modelling of the spectra measured at KSTAR, JET, ITER, etc. The new magnetically resolved data such as [1] could be further incorporated and presented in the form attractive for the experimental studies of the Motional Stark Effect. By increasing the plasma density the line ratios move towards the statistical limit achieving it at the plasma densities of $10^{14}$ $cm^{-3}$. The presented result could be further extended also for the excitation of $n = 4$ levels or the levels between $n = 2$, $n = 3$ and $n = 4$. Here $n$ is the principal quantum number. Also the excitation of hydrogen atoms by impurity ions of $He^{2+}$ or $Be^{4+}$ in parabolic states can be considered in the future.

Much more difficult is to provide the closed expression for the collisions within the same principal quantum number. In this case the energy between the levels depends on the energy of the ions therefore more accurate and complex formulas are required to provide the cross sections between these quantum states. Up to now this problem can only be solved numerically.

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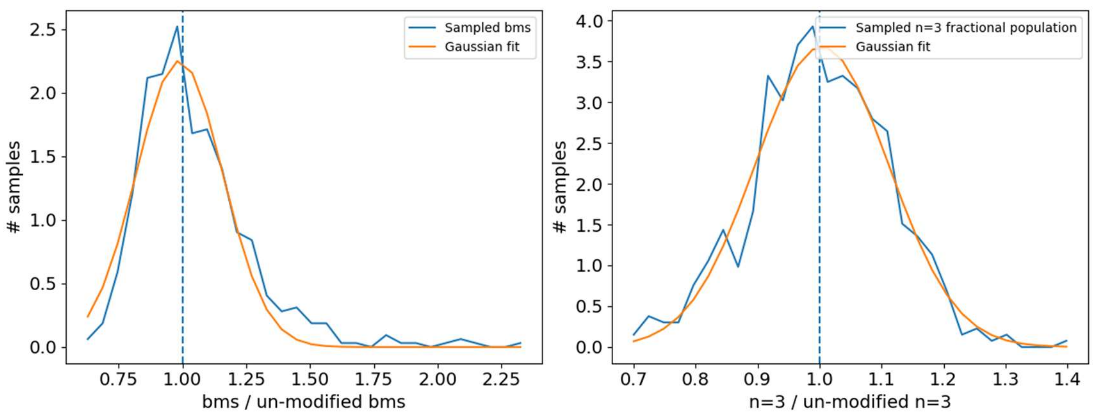
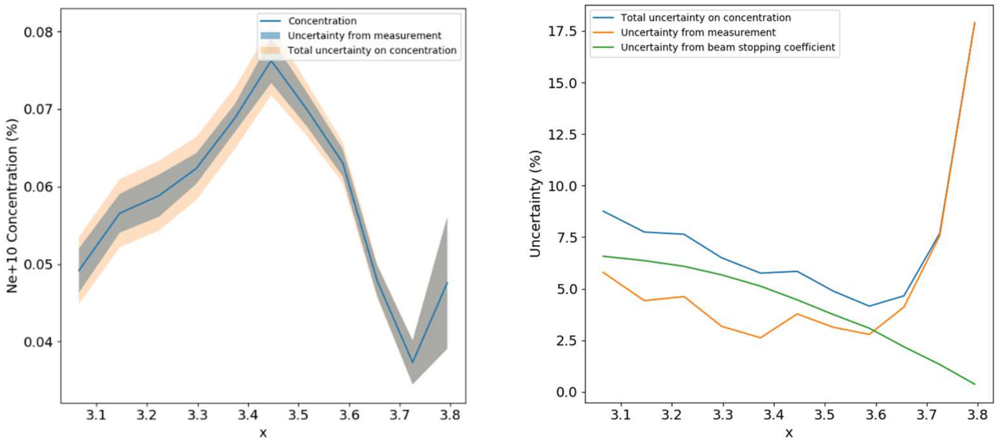
## Martin O'MULLANE, Department of Physics, University of Strathclyde

The ADAS beam stopping and emission coefficient production code (`adas316_mc`) was upgraded to allow simultaneous variation of multiple processes. Proton impact ionization and excitation and charge exchange cross section data may be varied over separate normal distributions, within a user-defined uncertainty envelope. The resulting spread in coefficients is fitted with a Gaussian to recover the nominal (mean) value and the propagated error is taken as the FWHM. Although the shape of the spread is a slightly skewed Gaussian, the value of the mean is typically within 2% of the non-sampled nominal value when fitted with a simple Gaussian. Therefore, the propagated uncertainty may be provided as a simple error bar.




These error bars have been used in the Charge Exchange and Analysis Package (CHEAP) code to add an 'atomic error' to the usual instrumental and viewing geometry uncertainties for a number of JET discharges. The derived concentration of $Ne^{10+}$ shows that this error increases towards the core of the plasma, since evaluating beam attenuation accumulates the error at each step. The balance between the atomic and other errors also changes but it never becomes the dominant error.




Electron impact excitation plays a minor role in beam stopping and is not fully in scope for the CRP but we have new calculations for transitions up to $n = 8$ which show better asymptotic behaviour than the current data.

The conclusion of this work is to use the new collision data produced during the CRP to assess an appropriate uncertainty interval and to propagate this through the ADAS and CHEAP codes for gauge the effect on routine impurity concentration measurements over a JET experimental campaign.

### Gergő POKOL, Wigner Research Centre for Physics, Budapest University of Technology and Economics (BME), Hungarian Academy of Sciences

During the course of 2020 and 2021, the codes participating in the benchmark (RENATE, RENATE-OD, BBNBI, FIDASIM, SOS, CHERAB, CRM by O. Marchuk) provided many new and corrected data, and initial comparison results were presented at the EPS2021 conference [1].

Calculations of cross sections needed to evaluate the effect of neutrals on beam modelling were done by K. Tőkési for $H^0 + H^0$ and Li + $H^0$ and formatted so that it is accessible for the RENATE-OD rate equation solver.

Future work includes:

- The Code Comparison Workshop on Neutral Beam Penetration and Beam-based Photoemissions was successful in starting up the benchmarking effort, and the results will be published soon: a journal paper will to be submitted to *Journal of Physics B*. Data for Li and Na beams is not available, so only include H beam attenuation and photoemission will be included.
- Participation in a model error estimation exercise: RENATE can handle quasi-static and bundled-*n* models with different number of levels considered for heating beams. *nl*-resolved and *nlm*-resolved cross sections are handled by codes by collaborating parties. Optimal levels of modelling details are to be determined for different purposes (beam penetration, integrated BES emissivity, MSE spectrum).

- Evaluation of the effect of neutrals on beam modelling using the freshly-calculated set of cross sections for $H^0 + H^0$ and $Li + H^0$ collisions using RENATE-OD.
- Calculation of *nl*-resolved excitation and ionization of $Li + H_2$, $Li + D$, $Li + D_2$, $Na + H^0$ and $Na + H_2$ collision by CTMC modelling at 50 keV impact energies.
- Validation of beam-to-gas simulations by actual measurements.

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## Károly TŐKÉSI, Institute for Nuclear Research, Hungarian Academy of Sciences (ATOMKI)

### *Summary*

#### Three-body type simulations

Within the classical trajectory Monte Carlo (CTMC) and Quasi-Classical Monte Carlo (QCTMC) models, we 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.

A significant improvement was reached 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., $\alpha_H$ and $\xi_H$. We have achieved this goal by analyzing the radial and momentum distributions of the target electron. We found that our 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, we compared our results with quantum-mechanical approaches for various channels. We found that our results are very close and are in good agreement with the previously obtained quantum-mechanical results. Also, for $H^+ + H(1s)$ system, we found excellent agreements between our QCTMC ($\alpha_H$= 3.5, $\xi_H$ = 0.9354) results with previous experimental data as well as quantum-mechanical ones. We also generated a database for state-selective electron capture cross sections in the collision between bare ions and ground state hydrogen atom. We believe that our 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 as follows:

We 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, we 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. we found that for ground state hydrogen, the reasonable range of $\alpha_H$ is expected to be $\alpha_H \geq 3.5$ in the QCTMC model.

b) We considered three calculation schemes during the investigation of the effect of the Heisenberg correction term between the bodies. We 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) We calculated the cross sections for various exit channels, like excitation, ionization, and electron capture, and compared them with previous quantum-mechanical and experimental results. We obtained excellent agreement between our QCTMC ($\alpha_H$= 3.5, $\xi_H$ = 0.9354) results and previous ones in $H^+$+H(1s) collision.

We 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. We found that the QCTMC method can reasonably describe the state-selective cross sections in a wide projectile energy range. Our calculations provide a reliable estimation of fusion related state-selective cross sections, especially in low impact energies.

We presented the electron capture cross sections into $n$ = 3, 4, 5, 6, 8, 10 and $nl$ = 3$l$, 4$l$, 5$l$ states of the projectile in $Be^{4+}$ + H(1s) using CTMC and QCTMC models. We 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, we have shown that our 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.

We 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. we 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. We compared our results with the theoretical approaches. We 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.

We 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 $n$, $l$, $m$.

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## Four-body type simulations

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 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, 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. Our 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.

We summarize the new results as follows:

We calculated the classical ionization and excitation probabilities as a function of the projectile impact energy and determined the impact parameter dependent probabilities in collisions between two hydrogen atoms. We presented total cross-section data for ionization and excitation. We found excellent agreement with the previous data, especially in high-energy regions.

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

a) We analyzed and optimized the influence of the choice of the model potential parameters ($\alpha$, $\xi$) on the initial radial and momentum distribution of the electron.
b) We 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) We 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. We presented total cross-section data for ionization. We found excellent agreement between our data and the previous experimental data.

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

a) We 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. We found that for the case of the reduced calculations the enhancement in the cross sections disappeared, emphases the importance of electron-electron repulsion.

We 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 50 keV to 50 MeV, 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.

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## Yong WU, Institute of Applied Physics and Computational Mathematics (IAPCM)

### *Short summary*

In the past five years, extensive studies on ion-atom/molecule collisions have been carried out in the IAPCM group under the support of CRP project and various theoretical methods have been applied to treat the collisions at different energy range.

For low energy range (less than a few keV/u) collisions, MOCC calculations have been performed for the systems of $O^{6+}/O^{7+}$ – H[1], $N^{4+}/N^{5+}$ – He[2-3], $Li^{-}$ – H[4], $He^{2+}$ – Ne[5], $Rb^{+}$ – Rb[6] etc., in which the ab initio potential curves and non-adiabatic coupling matrix elements are computed by using the multi-reference single- and double-excitation configuration-interaction method. It is found that the pseudo states are also important to obtain the convergent results for high charged ion collisions, especially in the low-energy region. Total and state-selective cross sections charge transfer cross sections have been obtained and recommended cross sections can be given based on the present calculations and experimental and theoretical data available.

For intermediate energy range (~100 eV/u < $E$ < ~100 keV/u) collisions, AOCC calculations have been performed for a large number of systems and charge transfer cross section have been obtained for $Ne^{q+}$ – H ($q$ = 6 – 10)[7], $Be^{4+}$ – H (1s, 2s, 2p)[in preparation], $C^{4+}$ – He[8], $Li^{3+}$ – Li ($1s^2 2s$, $1s^2 2p$) [9], $He^{+}$ – He($1s^2$;$1s2l\ ^{1,3}L$)[10-13], $H^{+}$ – $Be^{+}$[14], $H^{+}$ + $H^{-}$[15], $N^{5+}$ – $H_2$[16], $H^{+}$ – Mg[17-19] etc., excitation cross sections have been obtained for $Be^{4+}$ – H (1s, 2s, 2p) [in preparation] and $Be^{3+}$ – Li[20], and ionization cross sections have been obtained for $Be^{4+}$ – H (1s, 2s, 2p) [in preparation] and antiproton – helium[21]. For high charged ions or excited state target, very large basis sets are needed to obtain convergent results; and for excitation and ionization processes, even larger basis sets are needed for convergence. Total and state-selective electron capture, excitation and ionization cross sections are computed for a large energy range. Furthermore, TDDFT calculation has been performed to study $Ar^{8+}$-induced dissociation of $C_2H_2$ molecule at 1.2 MeV [22]. It is found that molecular dissociation depends strongly on the ionization at the initial stage and the collision configuration. A detailed analysis shows a correspondence between the charge state of $[C2H2]^{q+}$ and the final fragments. The comparison between various exchange-correlation functions reveals that electrons' correlation and self-interaction do not significantly impact the initial ionization and fragment distribution in the present study.

Except the works on ion-atom/molecule collisions, other atomic and molecular processes have been studied, including the dissociation of $N_2Ar$, ArCO, $SO_2$ and $H_2O$ etc. [23-27], the photodissociation of $BeH^+$ [28-29], predissociation of $HF^{2+}$[30], molecular Opacity of $HLi^+$[31], as well as the electron collision ionization of O II – IV[32], $Fe^{12+}$(33), electron collision excitations of $H_2O$[34], as well as the Bremsstrahlung of $W^{74+}$[35] etc. Moreover, the free-free Gaunt factors of hydrogen-like ion in plasma [36-37] have also been studied systematically. Please see the corresponding publications for detail.

## *Outlook*

Despite extensive studies of highly charge ions collision with H have been performed in the past five years and sets of high-quality cross section data have been obtained under the support of CRP project. However, the studies of collisions of complex atom/molecule species are still very few and the treatments of multi-electron systems remain a challenging problem in the community of atomic and molecular physics. The corresponding cross sections, especially state-resolved cross sections, are very scarce and can't meet the atomic data requirement in related studies of fusion since and astrophysics. For example, for the collisions of $W^{q+}$ ions, only CTMC calculations are performed to obtain the charge transfer cross sections up to now and the reliability and precision of the data are very limited. Therefore, how to improve the reliability of the cross section data is a vital issue in the future work and it is necessary to develop some sophisticated theoretical models or methods to treat the ion-atom/molecule collisions, in which the multi-active-electron AOCC or DFT-based molecular dynamics methods are two promising ones. Meantime, high-precision experiments are highly expected to benchmark the theoretical methods developed. On the other hand, how to apply the today's popular techniques, for example the machine learning method, would be very helpful to increase the capacity to treat the collisions of complex atom/molecule.

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## 5. Future Activities

A Consultancy Meeting, to be held in person at IAEA Headquarters, was tentatively arranged for late May 2023 to review progress on the Code Comparison Workshops and to finalise plans for the CRP final report; this meeting could be held online should the COVID situation forbid an in-person event.

A database, CollisionDB, is under development by the AMD Unit at https://db-amdis.org/collisiondb/ – data will be deposited in this resource as they become available, providing they can be associated with a DOI for a peer-reviewed and published article. A suitable format in which data providers may submit their data was discussed and agreed; it is anticipated that the experience of populating the database over the next few months will improve this data format, and details will be published on the above website.

An Application Programming Interface (API) will provide access to CollisionDB by CR codes to assess relative importance of different cross sections – this work will be carried out by AMD Unit staff with the assistance of Ö. Asztalos (Wigner Research Centre for Physics).

The Neutral Beam modelling code comparison exercise will be completed in the first half of 2022 and published; further benchmarking activities relating to calculated data within the CRP may be considered as an extension of this exercise.

With the finalisation of the CRP and publication of its final report, the CRP will be closed through the usual mechanisms of the IAEA's Committee for the Coordination of Research Activities.

A Working Group on Neutral Beams data will be considered for inclusion within AMD Unit's Global Network for the Atomic and Molecular Physics of Plasmas (GNAMPP, https://amdis.iaea.org/GNAMPP/)

There is a growing consensus in the community that the currently used cross sections relating to p + $H^0$ collisions (particularly ionization) are too small; updated data from the calculations and comparisons of this system made within the CRP will be recommended, probably in the project's final report.

Appendix 1

## List of Participants

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Appendix 2

# Agenda

*Virtual Meeting held using Webex*

## Wednesday, 24 November 2021

| | |
|---|---|
| 10:15 – 10:30 | Christian HILL and Kalle HEINOLA: Opening of the meeting; Welcome and introductions |
| 10:30 – 11:00 | **Alisher KADYROV**, *Faculty of Science and Engineering, Curtin University, Australia*<br>Recent progress in convergent close-coupling approach to ion–atom collisions |
| 11:00 – 11:30 | **Yong WU**, *Institute of Applied Physics and Computational Mathematics (IAPCM), China*<br>Theoretical study on ion-atom collisions in low and intermediate energy range |
| 11:30 – 12:00 | **Károly TŐKÉSI**, *Institute for Nuclear Research, Hungarian Academy of Sciences (ATOMKI), Hungary*<br>Atomic cross section in collision between hydrogen atom, carbon and lithium ions with hydrogen atom |
| 12:00 – 13:00 | Break |
| 13:00 – 13:30 | **Clara ILLESCAS**, *Department of Chemistry, Universidad Autónoma de Madrid, Spain*<br>Classical and semiclassical calculation of cross sections of $Be^{4+}$ + H(1s) and H(2s) collisions at 20, 100 and 500 keV/u |
| 13:30 – 14:00 | **Nicolas SISOURAT**, *Laboratoire de Chimie Physique – Matière et Rayonnement (LCPMR), Sorbonne Université, France*<br>Electronic collision cross section evaluation with a semiclassical non-perturbative approach |
| 14:00 – 14:30 | **Károly TŐKÉSI**, *Institute for Nuclear Research, Hungarian Academy of Sciences (ATOMKI), Hungary*<br>Investigation of cross sections of $Be^{4+}$ and hydrogen atom collisions using classical models |

### Thursday, 25 November 2021

12:00 – 12:30 **Tom KIRCHNER**, *Department of Physics and Astronomy, York University, Canada*
Basis generator method calculations for ion-atom collision systems of relevance to neutral beams in fusion plasmas: November 2021 update

12:30 – 13:30 Evaluation and comparison of Atomic Collisions Code Comparison Workshop activity; Discussion Session.

13:30 – 14:00 Break

14:00 – 14:30 **Jinseok KO**, *Korea Institute of Fusion Energy, South Korea*
Progress on the KSTAR beam emission spectra research

14:30 – 15:00 **Oleksandr MARCHUK**, *Forschungszentrum Jülich (FZJ), Germany*
Atomic data for calculation of the intensities of Stark components of excited hydrogen atoms in fusion plasmas

15:00 – 15:30 **Gergő POKOL**, *Institute of Nuclear Techniques, Budapest University of Technology and Economics, Hungary*
Progress in RENATE-OD synthetic diagnostic and benchmark

15:30 – 16:00 **Martin O'MULLANE**, *Department of Physics, University of Strathclyde, United Kingdom*
Adding uncertainties to the ADAS beam model and implications for diagnostic measurements

### Friday, 26 November 2021

11:00 – 12:00 Updates and evaluation of the Atomic Processes of Neutral Beams in Fusion Plasma Code Comparison Workshop activity; Discussion session.

12:00 – 13:00 Planning of the CRP Final Report; Meeting conclusion.

# Presentation Abstracts

# Classical and semiclassical calculation of cross sections of $Be^{4+}$ + H(1s) and H(2s) collisions at 20, 100 and 500 keV/u

*Clara Illescas, A. Jorge, L. Méndez and I. Rabadán,*
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A computational study of $Be^{4+}$ + H(1s) and H(2s) collisions has been carried out. Two computational models have been employed: The Classical Trajectory Monte Carlo (CTMC) method and the numerical solution of the Time-Dependent Schrödinger Equation (GTDSE). The integral $n$ and $nl$ partial cross sections for H excitation and electron capture, obtained with both methods,
will be compared for both systems.

In the case of H(2s), we will compare our results at two energies: 20 and 100 keV/u. It will be shown that the CTMC, with an improved hydrogenic initial distribution, provides excitation cross sections in good agreement with the numerical calculation for excitation to H($n$) with $n > 3$. The agreement between the corresponding $nl$ partial cross sections from both methods is less satisfactory at 100 keV/u. The electron capture cross sections calculated with the CTMC method do not depend on the initial distribution and show a reasonable agreement with the GTDSE ones, which supports the use of the CTMC method to calculate electron capture cross sections into highly excited levels and total cross sections.

Similarly, integral $n$ and $nl$ partial cross sections obtained with both methods for the case of $Be^{4+}$ + H(1s) will be shown. Classical total ionization cross sections will be also presented for both systems.

# Recent progress in convergent close-coupling approach to ion-atom collisions

*Alisher Kadyrov*
*Department of Physics and Astronomy, Curtin University, Perth, Australia*

We review recent progress in applications of the wave-packet convergent close-coupling (WP-CCC) approach to ion-atom collisions relevant to the CRP on Data for Atomic Processes of Neutral Beams in Fusion Plasma. In particular, we will present:

- A computationally more efficient one-centre approach to two-centre rearrangement collisions involving single and multielectron targets [1]. The method is tested on proton-hydrogen system and then applied to proton-lithium collisions.
- The angular differential cross sections of elastic scattering, excitation, and electron capture, as well as the ionisation cross sections singly differential in the ejected-electron angle, and in the ejected-electron energy [2] in proton-hydrogen collisions.
- The angular differential cross sections for direct scattering and electron capture [3], and various singly differential cross sections for ionisation [4] in proton-helium collisions.
- An effective single-electron treatment of ion collisions with multielectron targets that does not use the independent-event model [5]. The method is applied to calculate single-electron capture and single-ionisation cross sections for proton collisions with alkalis.
- We also report on calculations of the total and state-selective cross sections for bare beryllium ion collisions with hydrogen in its ground state [6], and update on the status of similar calculations for the excited states of hydrogen.

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# Basis generator method calculations for ion-atom collision systems of relevance to neutral beams in fusion plasmas: November 2021 update

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I will report on our recent progress with two-center basis generator method (TC-BGM) calculations for collision systems of interest in the context of fusion-plasma research. Two items have been addressed:
(i) collisions of $Be^{4+}$ ions with atomic hydrogen in ground and excited initial states, (ii) collisions of bare and partially-stripped triply charged ions ($Li^{3+}$, $C^{3+}$, $O^{3+}$) with ground-state hydrogen.

In subproject (i) we have focused on the collision energies of 20, 100, and 500 keV/amu, as agreed upon in a previous meeting, and have calculated target excitation, electron capture, and total ionization cross sections. Reasonably well-converged results are obtained for H(1s) and H(2s) initial states, but not for H(2p).

For the triply-charged ions we have looked at collision energies from 1 to 100 keV/amu and have compared our calculations with previous work, where available. For the $C^{3+}$ case we have checked that our cross-section results do not change dramatically if different effective potentials are used to represent the projectile. Moreover, our calculations do not indicate that the projectile electrons play an active role in the collision dynamics.

# Progress on the KSTAR beam emission spectra research

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Several progresses have been made for both polarimetric and spectral motional Stark effect (MSE) diagnostic systems in KSTAR. We have developed a new and effective beam-into-gas calibration technique applicable to superconducting tokamaks to calibrate out major systematic uncertainties such as Faraday rotation and secondary neutral beam effects [1, 2]. A systematic methodology has been devised to evaluate the effect of multi-ion-source neutral beam injection on polarimetric MSE measurements, which in turn, can be used to benchmark the spectral MSE method under the same situations [3]. The spectral MSE approach under development has been tested with a wide range of plasma densities and its sensitivity has been compared with that of the polarimetric MSE. The study of the beam emission spectra has been extended to the thermal Balmer alpha region to detect the ion thermal temperature, utilizing the main ion charge exchange with the neutral atoms. Finally, the KSTAR version of the beam penetration code (originally, ALCBEAM) has been developed (KSTARBEAM) and used to evaluate impurity carbon ($C^{6+}$) density profiles associated with the effective charge exchange emission rates from ADAS.

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# Atomic data for calculation of the intensities of Stark components of excited hydrogen atoms in fusion plasmas

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Motional Stark effect (MSE) spectroscopy is a unique diagnostic tool for the measurements of magnetic field and its direction in fusion plasmas. The primary excitation channel for fast hydrogen atoms in injected neutral beams in the range of 25 – 1000 keV are collisions with protons and impurity ions (e.g., $He^{2+}$ and heavier impurities). As a result of such excitation, at the particle density of $10^{13} – 10^{14}$ $cm^{-3}$, the line intensities of the Stark multiplets do not follow statistical expectations (i.e., the populations of fine-structure levels within the same principal quantum number $n$ are not proportional to their statistical weights). Hence, any realistic modeling of MSE spectra has to include the relevant collisional atomic data. A general expression for the excitation cross sections in parabolic states within $n = 3$ for an arbitrary orientation between the direction of the motion-induced electric field and the proton-atom collisional axis will be presented. The calculations make use of the density matrix obtained using different calculation methods. The results can be applied to other collisional systems (e.g., $He^{2+}$, $Be4^{+}$, $C^{6+}$, etc.). We point out that the asymmetry detected in the first classical cathode ray experiments between the red- and blue-shifted spectral components can be quantitatively studied using the proposed approach.

# Progress in RENATE-OD synthetic diagnostic and benchmark

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The RENATE Open Diagnostics has been upgraded with two main features: 1. Detailed noise modelling was added, and the effect of detector noise on the measured statistical properties of plasma fluctuations was studied. 2. Rate calculator module was added, motivated by the benchmark showing discrepancies at high beam energy.

The benchmark includes more-or-less complete set of data from BBNBI (both ADAS and Suzuki), CHERAB, FIDASIM, RENATE and RENATE-OD. Some test cases needed to be dropped, others show reasonably good agreement. Further plans are to be discussed.

# Electronic Processes Cross Section Evaluation with a Semiclassical Non-Perturbative Approach

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In the talk, I will summarize the recent theoretical developments our group has made in the context of the Coordinated Research Project on Data for Atomic Processes of Neutral Beams in Fusion Plasma:

- We have developed, implemented and employed a semiclassical non-perturbative approach for one and two-electron collision systems [1-4].
- We have calculated electron capture, excitation and ionization cross sections for collisions of fully stripped hydrogen, helium and lithium ions with atomic hydrogen in the ground state and in all excited states up to n=3 [5]. Collision energies between 1 and 100 keV/u were considered. Furthermore, we provide estimates of the accuracy of the cross sections. The set of data presented in this work represent the first complete and consistent quantum study of these collision systems, which can be used in the modeling and diagnosis of thermonuclear fusion plasma reactors.
- In the context of the code comparison we have calculated the cross sections for collisions of fully stripped beryllium ions with atomic hydrogen in the n=2 excited states.

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# Investigation of cross sections of $Be^{4+}$ and hydrogen atom collisions using classical models

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In recent decades, reactors such as the International Thermonuclear Experimental Reactor (ITER) have taken a significant step in supplying energy cleanly and safely by developing power plants whose energy is produced due to the nuclear fusion process. Due to the unique thermophysical properties and low atomic number, beryllium is defined as a plasma-facing material. Therefore, it plays a key role in the wall structure of next-generation fusion reactors. On the other hand, impurities are one of the main problems in controlled thermonuclear fusion plasmas. As a common plasma impurity, Be ions also play a role in the loss of radiant energy that causes the plasma to cool when colliding with the primary plasma components such as neutral hydrogen atoms. To determine the Be impurities in the plasma, knowledge of the cross section for various channels of interaction such as ionization, electron capture, excitation, and state-selective electron capture is very important.

The standard three-body classical trajectory Monte Carlo method (CTMC) cannot compete with quantum calculation in many aspects because of lacking the quantum feature of the collisions [1]. Therefore, we developed a three-body quasi-classical Monte Carlo model taking into account the quantum features of the collision system, where the Heisenberg correction term is added to the standard three-body classical trajectory Monte Carlo model [2]. In our research work, we use both the standard CTMC and the QCTMC-KW models to show the ionization [3], electron capture [3] , excitation [3], and state-selective cross sections in $Be^{4+}$ and H(1s) collisions [4-6]. The calculations were performed in the impact energy range between 10-1000 keV/amu. We show that the QTMC-KW model may have an alternative of the quantum-mechanical models providing the same results with maybe low computation efforts [7].

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# Atomic cross section in collision between hydrogen atom, carbon and lithium ions with hydrogen atom

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The hydrogen atoms generated by ion recombination on the fusion reactor's wall and other plasma-facing components [1-5] play a significant role in the beam emission spectroscopy (BES), which is an active plasma diagnostic tool used for density measurements in fusion research [1]. The cross sectional data of H-H atom collisions act as raw data for BES modeling. Besides hydrogen atoms, the impurities such as carbon, lithium, oxygen, deuterium, and tritium have existed in the plasma edge area [4, 5]. As comprehensive studies, the interactions of carbon and lithium ions with neutral hydrogen atoms were also investigated [4, 5], where carbon composites are used in first wall tiles [6-8] and lithium ions were used as a potential solution to solve the fusion reactor diverter heat flux. The ionized lithium ions can form a highly radiative layer of plasma, thus could significantly reduce the heat flux to the diverter surfaces [4, 9]. This work is created toward developing a theoretical description of inelastic interactions such as ionization and excitation processes that can give the total cross section accurately. In addition it is also contribute to creating a database for total cross sections as raw data for the BES modeling [10].

Classical calculations for determining atomic collision cross sections have received a great deal of interest in the past 20 years. There was a great revival of the CTMC calculations applied in atomic collisions involving three or more particles [2-5]. The CTMC method is a non-perturbative method, where classical equations of motions are solved numerically [2-5]. For a better description of the classical atomic collisions, the quasi-classical trajectory Monte Carlo model of the Kirschbaum and Wilets (QCTMC) improves the results of the standard CTMC model [3-5].

We present ionization, excitation, and electron capture cross sections in collisions between hydrogen atom, carbon and lithium ions with hydrogen atoms. We found a reasonably good agreement between classical results and the previously obtained experimental data.

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