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Data for Atomic Processes of Neutral Beams in Fusion Plasma

Summary Report of the Second Research Coordination Meeting

IAEA Headquarters, Vienna, Austria
18 – 20 February 2019

Prepared by
C. Hill
February 2019

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Prepared by

C. Hill

Abstract

12 experts in the field of atomic collisional physics and neutral beam modelling for magnetic confinement fusion devices, together with IAEA staff met at IAEA Headquarters 19 – 21 February 2019 for the Second Research Coordination Meeting of an IAEA Coordinated Research Project on *Data for Atomic Processes of Neutral Beams in Fusion Plasma*. They described progress with their research since the previous project meeting in June 2017, discussed open issues and made plans for continued coordinated research and code comparison during the remaining years of the project. The proceedings of the meeting are summarized in this report.

February 2019

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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. The first Research Coordination Meeting (RCM) of the CRP was held in June 2017 and the summary report is available online (report INDC(NDS)-0743, September 2017 at https://www-nds.iaea.org/publications/indc/indc-nds-0743.pdf). This previous summary report and the CRP website provide more information about the background and the objectives of the project. Please see:

https://www-amdis.org/CRP/neutral-beams

There were 12 research groups represented in the second RCM, including a remote presentation from Maarten De Bock, an external expert in the ITER diagnostic team on active beam spectroscopy. Those attending were O. Marchuk from FZJ, Germany on the topic of atomic data and collisional-radiative modelling of neutral beams in eigenstates, J. Ko (NFRI, Rep. of Korea) on the topic of experimental validation of atomic data for motional Stark effect diagnostics, B. Grierson (PPPL, USA) on the topic of neutral beam analysis codes used on NSTX-U and DIII-D, G. Pokol (Wigner Research Centre, Hungary), K. Tőkési (ATOMKI, Hungary) on the topic of study of atomic beam interactions in fusion plasmas using BES diagnostics, M. O'Mullane (University of Strathclyde, UK) on the topic of quantification of the contribution of collisional processes to the ADAS beam model, A. Dubois (Sorbonne Université, France) on the topic of electronic collisional cross section evaluation with a semiclassical non-perturbative approach, T. Kirchner (York University, Canada) on the topic of basis generator method calculations for ion-atom collision systems of relevance to neutral beams in fusion plasma, A. Kadyrov (Curtin University, Australia) on the topic of 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 fully stripped impurity ions, Y. Wu, (IAPCM, China) on the topic of state-resolved cross section calculations for excitation, ionization and charge transfer in collisions between hydrogen neutrals and the principal fully stripped impurity ions and C. Illescas (UAM, Spain) on the topic of theoretical studies of ionization, charge transfer and excitation in ion-H, He collisions in the 25-500 keV/amu energy range.

The proceedings of the meeting are summarized in Section 2 and the discussions are summarized in Section 3. Work plan updates are provided in Section 4. The list of participants is in Appendix 1 and the meeting agenda is given in Appendix 2. Summaries of presentations are presented in Appendix 3.

2. Proceedings

Presentation materials for all talks are available through the meeting web page:

https://www-amdis.org/meetings/neutral-beams-rcm2/

The meeting was opened by A. Koning, Head of the Nuclear Data Section, and participants introduced themselves. This was followed by a review of the CRP goals and meeting objectives by the scientific secretary C. Hill. Participants presented their work and research plans during the first period of the CRP and discussion sessions were arranged after these presentations.

The first morning's session concerned the modelling of neutral beams in fusion plasmas. O. Marchuk described the use and implementation of different calculational approaches to such modelling, with a focus on the limitations and pitfalls involved in the so-called "statistical", "*nl*-resolved" and "parabolic state" approaches. B. Grierson presented a review of comparisons of atomic data in simulations of the NSTX and DIII-D tokamak devices with experiment. J. Ko spoke about ongoing studies at NFRI to validate atomic data for motional stark effect (MSE) diagnostics with experiment and reported on the recent application of the ALCBEAM code to modelling of the KSTAR device.

The second session focussed on the provision and validation of fundamental atomic data to fusion modelling. M. O'Mullane, representing the Atomic Data and Analysis Structure (ADAS) organisation, described research efforts towards the quantification of the relative contributions made by various atomic collisional processes to the overall beam stopping and emission observed experimentally. Beam modelling by the RENATE code was the topic of a presentation by G. Pokol, which was followed by a related talk by K. Tőkési on the classical trajectory Monte Carlo (CTMC) simulation of ionization, capture and excitation processes in ion-atom collisions relevant to such modelling.

The second day of the meeting concerned the provision and validation of the fundamental atomic data used in neutral beam codes. In the first of two sessions on atomic data, Y. Wu described work carried out at IAPCM in applying the fully quantum-mechanical molecular-orbital close-coupling method (MOCC) with the two-centre atomic-orbital close-coupling method (AOCC) to ion-atom and ion-molecule collisions in the low- to intermediate-energy range. C. Illescas reported on her group's recent studies on ionization and electron capture processes in p^+ + Ar collisions from 100 eV to 200 keV collision energies using both "switching" Classical Trajectory Monte Carlo (CTMC) and semiclassical techniques. T. Kirchner reported on recent progress with applying the two-centre basis generator method (TC-BGM) to collision systems of interest to fusion plasma research, in particular target ion excitation, electron capture, and ionization in proton collisions from excited hydrogen atoms. The final presentation of the session, by A. Kadyrov, concerned the wavepacket continuum-discretisation approach to the calculation of excitation, ionization and electron-capture cross sections for protons colliding with atomic hydrogen in excited states.

The second atomic data session started with A. Dubois' description of his group's use of non-perturbative semiclassical techniques in the treatment of one- and two-active electron processes in ion-atom/molecule collisions. This was followed by a short presentation by C. Hill on the IAEA's recently-established Global Network for the Atomic and Molecular Physics of Plasmas (GNAMPP); for more details see https://www-amdis.org/GNAMPP/.

On the final day participants reviewed their work plans for the remaining period of the CRP and discussed other follow-up actions including plans for the third RCM. These are summarized in the next section of this report.

3. Discussion and Conclusions

The following are notes from the discussion sessions. In many cases questions are raised for further study.

3.1 Data needs for neutral beam modelling and diagnostics

A review of the current status of atomic data used for modelling neutral beams and their diagnostic applications was presented in Section 3.1 of the report on the previous RCM (INDC(NDS)-0743, September 2017). Here are presented additional fundamental data requirements identified by the participants of the present RCM.

3.1.1 High-*n* charge transfer processes: $H^+ + H(n > 1)$

Brian Grierson presented the rate coefficients that are used on DIII-D and NSTX for the C-VI (8-7) emission line at 2590.5 Angstroms from both $n = 1$ and $n = 2$ beam neutral donors. The rates used on both tokamaks are the same. Grierson also showed that when DIII-D performs experimental analysis with high voltage beams and these rate coefficients, considering carbon as the primary impurity species, that the total plasma stored energy and neutron rates tend to be in reasonable agreement within measurement uncertainty. This indicates that there are no egregious errors in the use of $n = 1$ and $n = 2$ rates, neglecting higher-*n* states under typical operating conditions. However, Grierson also presented results from DIII-D that show anomalously high inferred impurity densities when the neutral beam voltage is reduced from 80 kV to 50 kV. This is significant because the higher-n states are more important for lower energy beam voltages (and for 1/2 and 1/3 energy components) because unlike $n = 1$, then $n = 2$ rate is larger at lower energy. This observation of anomalously high inferred impurity densities at low accelerator voltage may indicate that neglecting higher-n bean neutral donors may be to blame. Another indication that higher-*n* processes are occurring in the DIII-D conditions was show, which is consistent with previous work by Ron Bell (PPPL) on TFTR that was shown at RCM1. On DIII-D, the use of a wide wavelength high resolution spectrometer provides observation of the C-VI (8-7) line, as well as a blended line with both C-VI (14-10) + Li-III (7-4) at 5167 Angstroms. By tuning to the spectrometer to this wavelength range prior to the injection of any lithium on DIII-D, the ratio of

C-VI (14-10) to C-VI (8-7) can be determined with high accuracy. For DIII-D, this ratio is found to be approximately 1/30. On TFTR, this ratio was found to be 1/28, which is nearly the same as on DIII-D. If the population of these two transitions were from n = 1 and n = 2 beam neutrals only, this ratio should be significantly smaller.

An area of further study for all CX processes is the role of halo neutrals to the observed CX emission intensities. Recent work by McDermott [1] on ASDEX-Upgrade shows that halo neutrals can contribute up 20% of the observed total CX emission. On DIII-D and NSTX, which have higher Zeff from carbon, this percentage should be smaller (10% or less), but still large enough to be systematic and important when determining the impurity densities. This is the subject of future follow-on work.

[1] R. M. McDermott et al., "Evaluation of impurity densities from charge exchange recombination spectroscopy measurements at ASDEX Upgrade", *Plasma Phys. Control. Fusion* **60** (2018) 095007.

3.1.2 Atomic data needs for halo modelling

In addition to the atomic related directly with the penetration to the beam into the confined plasma region there is also an increasing need for the atomic data for halo modelling. The halo is a cloud of neutrals (H) created as a result of charge-exchange reaction between the neutral beam and protons or deuterons.

$$H^+ + H_b \rightarrow H + H_b^+$$

The halo atoms provide additional contribution to the charge-exchange signal increasing it by 10% as shown on DIII-D and NSTX. Nevertheless, the effect of halo has also a negative impact. First, the (n,l) distribution of the charge-exchange cross section is different from the beam atoms. The halo atoms populates the low l-values, where l is the orbital quantum numbers. Second, the volume of halo atoms is larger as the beam volume as the halo has a thermal velocity of ions in the plasma core. Second, the charge-exchange cross section between the halo atoms and impurity ions has to take into account the relative motion of atoms and impurity ion [1]. In case of neutral beam atoms it can be to a great extent ignored. The atomic data for halo atoms requires not only the proton impact data but also the electron collisional data at high energies. It is expected that the electron collisional cross sections are known with high precision. The detailed calculations for the population of halo atoms will be performed and the effect of relative velocities on the creation and loses of halo atoms will be exemplified in the near future.

[1] M. von Hellermann et al., *Atoms* **7**, 30 (2019): doi:10.3390/atoms7010030

3.1.3 W(I) emission lines

It is expected that the IETR and future fusion reactor contain divertor made of W [1]. The high fluxes of heat and particles sputter the W atoms. As a result one observes not only the highly ionized stages of W ions (e.g. Ne-like W) in the plasma core but also the low ionization stages of W at the plasma edge. The W I-II lines of W could potentially appear in the spectral range of the CXRS spectral lines. It is foreseen to investigate this effect at the PSI-2 linear plasma using the spectroscopy. Though it is obvious that the line intensities from linear plasma could hardly reproduce the experimental conditions at ITER, etc… such measurements provide additional reliability for the CXRS diagnostic. It is foreseen to exploit the existing spectroscopic setup at PSI-2 for the spectral range of CXRS spectral lines (C, He, Be, Ne and Ar as well as the BES and MSE diagnostic). One should note that only the wavelength of W I lines could be analyzed here, as the experimental conditions are quite different.

[1] T. Hirai et al., *Nucl. Mat. Energy* **9**, 616 (2016)
[2] O. Marchuk et al., *J. Phys. B.: At. Mol. and Opt. Phys* **51**, 025702 (2018)

3.1.4 Cross section data for beam-into-gas processes

To minimize systematic errors in motional Stark effect (MSE) diagnostics in a tokamak, the calibration procedure where polarization measurements are made for the beam emission excited in a neutral gas filled in a torus is executed. In this kind of beam-into-gas calibration, however, a certain amount of beam neutrals are ionized, confined by the vacuum magnetic field, and charge-exchanged with the neutral gas (usually, D_2 gas). Some of these 'secondary' beam neutrals emit inside the MSE viewing volume with a random Lorentz electric field orientation due to their random gyro-phase at the time of the emission. This can result in an erroneous polarization angle against that from the primary beam neutral emission.

The contaminating effect of the secondary beam neutrals has been observed in several tokamaks such as Alcator C-Mod and KSTAR. In order to experimentally minimize the secondary neutral effect, the operating torus pressure should be extremely low, which contracts practical engineering setups very often. Interpretation and analyses of the beam-into-gas experimental data in addition to simulations require precise atomic-physics data. In particular, it should be noted that there are differences in collisional *l*-mixing of the beam atoms traveling through a D_2 gas versus a plasma. A limited amount of literature to address this issue includes:

- M. Glass-Maujean *et al.*, *J. Phys. B*, **33**:4593, 2000

- S. Lauer *et al.*, *J. Phys. B*, **31**:3049, 1998

- E. Flemming *et al.*, *J. Chem. Phys.*, **103**:4090, 1995

Though these previous works contain *l*-mixing cross-sections for $H^* + H_2$ collisions, they are for slowly moving excited atoms in unperturbed states, extrapolating much smaller cross sections for high-energy neutral atoms. No experimental cross-section data exist that are applicable to the MSE measurement conditions.

In addition to the secondary neutral emission issue, several tokamaks such as TFTR and Alcator C-Mod have observed that upper state populations (n = 3) are non-statistical in their beam-into-gas calibration experiments. This means that σ lines are not completely perpendicular to the Lorentz electric field. It may not be a critical issue as far as the measurement is made only for π components, but practically, a finite amount of σ lines smears into the bandpass filter, resulting in a low polarization fraction and another source of systematic errors.

It was recognized that only very limited data are available for collision systems like $H + H_2$ and $Li + H_2$. Improving the situation and filling the gap requires further investigation of these systems. New classical simulations are planned by the groups of K. Tőkési and J. Ko to calculate cross sections for collisions between Li, Na and H_2.

3.2 Status of ion-atom collision data assembled during the CRP

The table below summarizes the current status of data assembled within this CRP as of 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. 90% of the high-priority data sets have been calculated or have calculations underway; in most cases more than one computational technique has been employed. 67% of all the desired data sets have been calculated or have calculations underway.

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
	Be^{4+}		CI	CI	CI, YW	CI
	C^{6+}	AK	AK, CI	AK, CI	AK, YW, AD-limited	AK
	Ne^{10+}		CI	CI	CI, YW	
	H(1s)	(CI), KT, AD	(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	AK, (CI), (TK)	AK, (CI), TK, KT	AK, (CI), KT, TK	AK, (CI), KT, TK
	He^{2+}	(TK)		(TK)	(TK)	(TK)
	Be^{4+}	(TK)		(CI) (TK)	(CI) (TK)	CI (TK)
	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	(CI), KT	(CI), KT
	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)		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)		KT, YW, (AD), (TK)	KT, YW, (AD), (TK)	KT, YW, (AD), (TK)
Na (3s) + …	bare ions, E_{tot} <= 50 keV	(TK)		KT, (AD), (TK)	KT, (AD), (TK)	KT, (AD), (TK)

3.3 Code Comparison Workshop on Beam Penetration

The workshop will be organized in Debrecen, hosted by MTA ATOMKI. The provisional date is 26 – 28 August 2019. Main purpose of the workshop will be to evaluate and discuss the benchmark of the different collisional radiative models (CRMs) used for beam-plasma modelling around the world. Benchmark cases have been discussed and substantially reduced compared to the original proposal by Gergo Pokol. The test cases are to be finalized in an exchange of e-mails. The purpose of the benchmark is to evaluate the CRMs from the point of view of used atomic data, required complexity and treatment of missing atomic data.

Remote participation will be enabled, but personal participation is encouraged.

3.4 Code Comparison Workshop on Electron Dynamics of Atomic Collisions

Theoretical approaches, methodologies and their computer implementations to describe electronic processes in ion-atom collisions are now fairly mature when considering one-electron or quasi-one-electron systems. And this is true in the intermediate energy domain where the use of non-perturbative approaches is unavoidable. A huge number of experimental results are also available for such systems. In general, all these results agree quite well, with however some localized discrepancies, as for the ionisation cross section for about 50 keV in the simple H^+ + H(1s) system. For the same kind of systems, this is not the case when considering collisions with initially excited targets, of interest for fusion plasma modelling and diagnostics. Very few *ab-initio* calculations exist and no experimental data exist. These systems are characterized by very large cross sections but present the drawbacks from the theoretical point of view to require very large number of states (and angular momenta) and a lot of different calculations to cover the different states available in the considered shell.

Due to the present lack of independent data, we propose during the workshop to attack such a system, using the different methods developed in the Spanish, Hungarian, Canadian, Australian and French teams, i.e. SC MO close coupling, classical CTMC, CCC, semiclassical BGM close-coupling and SC AO close coupling. The aim is to produce and compare data for a collision system in order to produce a consistent set of data, with evaluation of their accuracy, through the observed differences and the convergence checks done independently in each group. We chose Be^{4+} + H collision systems and three projectile energies (20, 100 and 500 keV/u) of interest for fusion plasmas and which present overlap between the typical validity range of the different methods. We planned to do the comparison for ground state (1s) and excited (2s, $2p_m$) hydrogen target and considering total capture, ionization and excitation, cross sections as well as the state selective ones (for the dominant channels). End of year 2019 has been chosen as a tentative date to merge the different results. An informal meeting between the participants can be set during the International Symposium on Ion-Atom Collisions, to be held in Paris in July 2019.

4. Work Plans

4.1 Work Plan Reviews

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

Parallel with an important effort of code development, for speed-up, RAM use and optimization of algorithms to be able to handle high angular momenta, we have followed the plan drawn in the last meeting:

- We have published total capture cross sections for H^+–H(*nl*) collisions from semiclassical (up to $n = 3$) and classical (up to $n = 7$) approaches. We developed and checked scaling rules for such systems for the 0.01 – 100 keV projectile energy range [1].

- We have computed cross sections for total ionization and sub-shell selective excitation and capture processes for H^+–H(*nl*) for $n = 1 – 3$, using the SCAOCC method. The accuracy of the cross sections has also been evaluated. The projectile energy domain covers by this study is 1 – 100 keV. The paper consists mainly on tables and is submitted to Atomic Data and Nuclear Data Tables.

[1] *Classical and semiclassical non-perturbative treatments of the electron transfer process in the collisional system proton-hydrogen involving initial excited states*, A. Taoutioui, A. Dubois, N. Sisourat and A. Makhoute, *J. Phys. B* **51**, 235202 (2018).

Brian GRIERSON, Daren STOTLER, Princeton Plasma Physics Laboratory (PPPL)

- Atomic rate coefficients from C-VI (8-7) used on both NSTX and DIII-D were collected and reviewed. Both ground state (n = 1) and the first excited state (n = 2) rates were compared for both machines. Both machines are using the same rate coefficients for both n = 1 and n = 2. The rate coefficients for n = 1 and n = 2 are each higher than the standard adf12 file `qef93#h/qef93#h_c6.dat`. These rate coefficients were produced by V. Soukhanovskii for NSTX and J.M. Munoz-Burgos for DIII-D, and use the same fundamental atomic data.
- Initial assessment of the consistency of this data was reported and for nominal operating conditions on DIII-D the n = 1 and n = 2 rates, as well as the assumption of carbon being dominant, do not display disagreement with other verification metrics such as plasma stored energy, neutron rate, visible bremsstrahlung emission and SXR emission.
- An assessment of the discrepancy in the deduced impurity density between full voltage and reduced voltage NBI was presented. It was found that operating of the neutral beam at 50 kV can produced up to a factor of two error in the inferred impurity density based on the n = 1 and n = 2 rates. This may be due to neglecting higher-n (n > 2) atomic processes, as described in Sec. 3.1.1
- NUBEAM calculations were performed with ‘simple’ and ADAS excited state rates for neutral beam stopping and deposition. It was shown that for nominal operating conditions (volume averaged density of 5.7×10^{19} m^{-3}) that 10 – 15% differences may be expected in the neutral beam deposition from charge-exchange. The total stopping was more weakly affected, and the power flows and neutron rates were largely unaffected for these conditions.
- Inconsistency with the nitrogen effective emission coefficient was presented. During DIII-D nitrogen seeding experiments where a large concentration of nitrogen was introduced, the nitrogen density appears to be over-estimated by a factor of two. This estimate was obtained using both stored energy and neutron rates on DIII-D, and remains an anomaly.

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

Since the first Research Coordination Meeting (RCM) held in June 2017 the proposed studies have been slightly modified. As mentioned in the original plan for the third year, in relation with the explicit treatment of the two active electrons of the target, the following progress has been achieved:

- We have applied the recently developed switching Classical Trajectory Monte- Carlo (s-CTMC) method to the study of proton- argon collisions for 10 keV < E < 400 keV. We have obtained a classical stable description of a multielectronic atom through independent systems, yielding to electron capture (H formation) and electron production cross sections in good agreement with experiment, besides a significantly improvement of the double capture (H- formation) description, i.e. electron capture processes when two electron are involved has been demonstrated. We have realized that the main limitation is the choice of the many-electron interpretation, similarly to what happens in the case of the one-electron calculations.

- We have applied a semiclassical method with a close-coupling expansion in terms of many-electron molecular functions (MFCC) with eight active electrons to calculate single and double electron capture cross sections for energy collisions ranging from 100 eV to10 keV. The total cross sections obtained were in reasonable agreement with experiments. This work has been published in Journal of Physical Chemistry.

A. Jorge, Clara Illescas, L. Méndez, I. Rabadán, "Ionization and single and double capture ion Proton-Ar collisions". *J. Phys. Chem.* **122**, 2523 (2018).

Alisher KADYROV, Faculty of Science and Engineering, Curtin University

The following progress has been achieved within the CRP since the 1st RCM:

- Developed a single-centre convergent close-coupling (CCC) approach to ion collisions with helium. The approach is based on wave-packet continuum discretisation. It has been applied to electron capture, excitation and single and double ionisation of helium in collisions with antiprotons and energetic protons. A comprehensive set of benchmark results for the fully differential single ionisation of helium has been generated. The calculated results for 1-MeV proton impact are in excellent agreement with recent experimental measurements [Gassert *et al.*, Phys. Rev. Lett. **116**, 073201 (2016)] for all considered geometries.
- Developed a two-centre CCC approach to ion-atom collisions including elastic scattering, excitation, ionisation, electron capture and electron capture into the continuum. The approach has been used to calculate the double differential cross section for ionisation in proton collisions with atomic hydrogen. Overall good agreement with experiment of Laforge *et al*. [Phys. Rev. Lett. **103**, 053201 (2009)] is obtained for all considered cases without convolution.
- Using the 2-centre CCC approach calculated excitation, ionisation and electron-capture cross sections for proton collisions with n = 2 states of atomic hydrogen, where n is the principal quantum number. Calculated cross sections for scattering on the metastable 2s state are compared with other theoretical results obtained using other approaches. Considerable disagreement with previous calculations has been found for some transitions at various incident energies. The density matrix elements required for fusion plasma modeling and diagnostics have been calculated for proton scattering on the initial 2s, $2p_0$ and $2p_1$ states of hydrogen.
- Developed a two-centre CCC approach to ionisation and electron capture in collisions of multiply-charged ions with hydrogen. So far the method has been used to ionisation, electron capture and excitation in collisions of C^{6+} ions with atomic hydrogen. Calculations have been performed for the projectile energy range from 1 keV/amu to 10 MeV/amu. Excellent agreement with experimental data for the total electron-capture cross section over the entire energy range is obtained. However, the calculated total ionisation cross section somewhat overestimates the only available experimental point. The singly and doubly differential ionisation cross sections at 1 and 2.5 MeV/amu are in good agreement with the most of the experimental data by Tribedi *et al*. [J. Phys. B 31, L369 (1998)], however some discrepancies remain. The differential cross section calculations are extended to lower energies where perturbative methods are expected to fail.
- Developed an approach to calculate proton beam stopping in hydrogen. The stopping cross section for protons passing through hydrogen is calculated for the energy range between 10 keV and 3 MeV. Both the positive and neutral charge-states of the projectile are accounted for. In other words, interactions of the proton and hydrogen atom (formed due to electron capture) components of the beam with the target are taken into account. The approach is also applied to calculate the charge-state fractions. These are then used to combine the proton-hydrogen and hydrogen-hydrogen stopping cross sections to yield the total stopping cross section for protons passing through hydrogen. This makes the approach fully *ab initio*. The results are in excellent agreement with available experimental data in the entire energy range considered.

The following papers have been published within the CRP since the 1st RCM:

1. J. J. Bailey, I. B. Abdurakhmanov, A. S. Kadyrov and I. Bray, *Proton beam stopping in hydrogen,* Phys. Rev. A (2019) in production.
2. I. B. Abdurakhmanov, K. Massen-Hane, Sh. U. Alladustov, J. J. Bailey, A. S. Kadyrov, and I. Bray, *Ionization and electron capture in collisions of bare carbon ions with hydrogen*, Phys. Rev. A 98 (2018), 062710.
3. I. B. Abdurakhmanov, Sh. U. Alladustov, J. J. Bailey, A. S. Kadyrov, and I. Bray, *Proton scattering from excited states of atomic hydrogen*, Plasma Physics and Controlled Fusion 60 (2018) 095009.
4. I. B. Abdurakhmanov, J. J. Bailey, A. S. Kadyrov, and I. Bray, *Wave-packet continuum-discretization approach to ion-atom collisions including rearrangement: Application to differential ionization in proton-hydrogen scattering*, Phys. Rev. A 97 (2018), 032707.
5. I. B. Abdurakhmanov, A. S. Kadyrov, I. Bray, and K. Bartschat, *Wave-packet continuum-discretization approach to single ionization of helium by antiprotons and energetic protons*, Phys. Rev. A 94 (2017) 022703.

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.
Our progress with the planned studies since the first Research Coordination Meeting (RCM) held in June 2017 has been delayed due to a shortage of resources (man power). Nevertheless, we have accomplished the following:

- As proposed in the original work plan, we have carried out two-center basis generator method (TC-BGM) calculations for proton-hydrogen collisions for 2s and 2p initial states in the 1 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. For H(2s) a set of cross section results has been assembled (and presented at the second RCM in February 2019) and only a few final tests need to be completed before cross section tabulations can be finalized. This work is yet unpublished.
- Closely related to the originally planned activities for year 2, 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 our work was to compare calculated Lyman-line emission counts for both targets with measurements for krypton. The work has been published in Physical Review A [1].
- A similar study with an emphasis on radiative emissions was carried out for slow Ne^{8+} impact on helium atoms and hydrogen molecules [2]. In all these works, relatively large basis sets are necessary to calculate electron capture into high-lying projectile shells.

[1] A. C. K. Leung and T. Kirchner, Phys. Rev. A **97**, 062705 (2018)
[2] A. C. K. Leung and T. Kirchner, Atoms **7**, 15 (2019)

Jinseok KO, National Fusion Research Institute (NFRI)

- A high-precision ($\Delta\lambda \leq 0.05$ nm) spectroscopy suite comprising a 1.33-m Czerny Turner spectrometer, an 1800-g/mm grating and a 2048 × 512 CCD has been constructed with a capability of dispersion self-calibration. The MSE spectrum measurements with this spectroscopy suite were made for the beam-into-gas (both with and without a field) and beam-into-plasma experiments.

- A multi-Gaussian fit procedure combined with the ADAS was done for the MSE spectra from single-ion-source injected plasmas. The internal magnetic field structure from the fit was compared with that from the conventional Photoelastic-Modulator (PEM) MSE instrumentation in KSTAR.
- Through both spectral and polarimetric MSE systems, various factors associated with the polarimetric spectral line shapes have been investigated and characterized. These include the multi-ion-source injection with finite beam width, the smearing and amplification of the σ components, and beam-into-gas secondary neutral beam emissions.

List of publications

J Ko and J Chung, "Direct measurements of safety factor profiles with motional Stark effect for KSTAR tokamak discharges with internal transport barriers", *Rev. Sci. Instrum.* **88**, 063505 (2017)

K Lee, J Ko, J H Jo, and J Chung, "Design of a multi-cahnnel polarization-preserving optical system for the KSTAR motional Stark effect diagnostic", *Fusion Eng. Des.* **121**, 301-307 (2017)

J Chung, H S Kim, Y M Jeon, J Kim, M J Choi, J Ko, K D Lee, H H Lee, S Yi, J M Kwon, S –H Hahn, W H Ko and S W Yoon, "Formation of the internal transport barrier in KSTAR", *Nucl. Fusion* **58**, 016019 (2018)

M C C Messmer, J Ko, J Chung, M H Woo, K –D Lee and R J E Jaspers, "Evolution of the central safety factor during stabilized sawtooth instabilities at KSTAR", *Nucl. Fusion* **58**, 016030 (2018)

Y B Nam, J Ko, G H Choe, Y Bae, M J Choi, W Lee, G S Yun, S Jardin and H K Park, "Validation of the full reconnection model of the sawtooth instability in KSTAR", *Nucl. Fusion* **58**, 066009 (2018)

J Ko, "Effect of multi-ion-source injection on motional Stark effect diagnostic", *Rev. Sci. Instrum.* **89**, 10D104 (2018)

J Chung, J Ko, S –H Hahn, H S Kim and S J Wang, "Considerations of the q-profile control in KSTAR for advanced tokamak operation scenarios", *Rev. Sci. Instrum.* **89**, 10D112 (2018)

Oleksandr MARCHUK, Forschungszentrum Jülich (FZJ)

In this period of time the review paper on status of charge-exchange recombination spectroscopy but also the Motional Stark effect diagnostics have been prepared [1]. It summarizes the current status of atomic data for active beam spectroscopy:

- The non-statistical population distribution was implemented in the SOS Code, which is going to be used in the assessment of experimental data in ITER as well as the current design of ITER-Core CXRS System [2].
- We have demonstrated that the averaging the rate coefficient over the distribution function of halo and ion has a dramatic impact on the population of halo atoms in ITER core plasma by modification of rate coefficients.
- The preliminary assessment of the existing rate coefficients of the charge-exchange was performed in this paper.

References

[1] M. von Hellermann et al., *Atoms* **7**, 30 (2019): doi:10.3390/atoms7010030 (2019)

[2] P. Mertens, *Journal of Fusion Energy*, 1 (2018): doi: 10.1007/s10894-018-0202-1

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

A new variant of the ADAS beam population code (adas316) has been adapted to accept a multiplier on each atomic process: ionization and excitation (driven by ions or electrons) and charge exchange. One or multiple atomic processes can be simultaneously varied and energy dependent uncertainties in the cross section can be specified. Initial results show that sampling with a normal error distribution applied to the ionization and excitation processes, produces a slightly skewed normal distribution for the recovered beam stopping (bms) and beam emission (bme, ie Balmer-α 3-2) coefficients. The centre of the distribution of bms and bme coefficients is within 0.5% of the original coefficient. The size of the propagated FWHM error bar responds to the plasma conditions reflecting how each process responds differently. Ranking the contribution of individual processes to bms or bme can be displayed as heat maps.

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

We performed Classical Trajectory Monte Carlo simulations to calculate the cross sections for various channels in collisions between H + H_2 and Li + H_2 for a wide range of projectile energies. Based on the calculated cross sections, a simplified version of the collisional radiative model has been derived. We show that the model is suitable to obtain the beam attenuation in neutral gases outside of the confined plasma region. A strong density dependence has been found for each beam species. This preliminary study only considered ionization channels from the ground state, but has proved the feasibility of more complex calculations of nl-resolved cross-sections and corresponding rate equations for sophisticated beam models [1].

[1] O. Asztalos, B. Szondy, K. Tokesi, G.I. Pokol: "The modeling of atom - neutral collisions for beam emission spectroscopy applications", *European Physical Journal D, in press* (2019)

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

- Benchmark calculations were carried out for the ionization cross sections in electron and Ar system. At first the electron energy was 100 eV. Beside the total cross section also the angular and energy differential cross sections were obtained. Good agreements with the previous works are reported. Further work will include the calculation of state-selective excitation cross sections.
- Code to calculate the cross sections in H(*nl*) + H(*nl*) collisions has been developed. Test calculations were performed for the Li + D system and total cross sections were obtained. More testing is required, especially for the excitation channels.
- The calculations and evaluation of the cross section calculations in H^+ + H_2 and Li+ H_2 collisions were completed [1]. The simulations were performed in 4 body approximation, i.e. the Li atom and the H_2 molecule were mimic as two body system. The focus was on total cross section calculations for all possible reaction channels. Initially, cross sections were obtained for a ground state target when the projectile was also in ground state.
- Test calculations were performed for ionization cross sections of carbon by electron impact, and the ionization cross section calculations of carbon by electron impact were finalized. Work with the Ne and N targets continues.

[1] O. Asztalos, B. Szondy, K.Tőkési, G.I.Pokol, "Application of collisional radiative models in Beam Emission Spectroscopy (BES) modeling for fusion plasma density diagnostics", *Eur. Phys. J. D, to be published* (2019).

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

State-resolved cross section calculations for excitation, ionization and charge transfer in collisions between hydrogen neutrals and the principal fully stripped impurity ions

As proposed in the work original plan, we have performed cross section calculations for excitation, ionization and charge transfer in collisions between hydrogen neutrals and highly charged ions, as summarized in the following:

- We have carried out two-center Atomic orbital close-coupling method calculations for Ne^{q+}-H(q=7-9), C^{4+}-He and Ar^{8+}-He collisions in energy region from about 1keV/amu to 1MeV/amu, both total and state-selective cross sections have been obtained. The work of Ne^{q+}-H(q=7-9) have not been published yet.
- We have carried out molecular orbital close-coupling method calculations for B^{4+}-H and O^{q+}-H(q=6-7) in energy region from a few eV/amu to about 5 keV/amu, both total and state-selective cross sections have been obtained. The paper of O^{7+}-H collisions now is in preparation.
- Related to the work plan in the first 2 years, we have also performed calculations of He^{+}-H/He collisions, combining Atomic orbital close-coupling method and molecular orbital close-coupling method.
- In addition, the previous studies of our group on highly charged ions collisions with He/H have been summarized, including H^{+}/He^{2+}/Be^{4+}/C^{6+}/O^{8+} collisions with neutral hydrogen in ground state.

List of publications

[1] J W Gao, Y Wu, J G Wang, A Dubois and N Sisourat, Double Electron Capture in H^{+} + H^{-} Collisions, *Phys. Rev. Lett.* **122** 093402 (2019)

[2] J W Gao, Y Wu, J G Wang, N Sisourat, A Dubois, State-selective electron transfer in He^{+} + He collisions at intermediate energies, *Phys. Rev. A* **97** 052709 (2018)

[3] J W Gao, Y Wu, N Sisourat, J G Wang, A Dubois, Single- and double-electron transfer in low- and intermediate-energy C^{4+} + He collisions, *Phys. Rev. A* **96** 052703 (2017)

[4] L Liu, X H Lin, Y Wu, J G Wang, R K Janev, Cross sections for state-selective electron capture and excitation in He^{+}-H collisions, *EPJD* **71**, 9, 70520-5(2017)

[5] Ab initio study of charge transfer in low energy collisions of B^{4+} with H, C H Liu, J G Wang, *EPJD* **71**, 6, 80020 (2017)

[6] Single-electron capture in 3-keV/u Ar^{8+} -He collisions, R T Zhang, X L Zhu, X Y Li, L Liu, S F Zhang, W T Feng, D L Guo, Y Gao, D M Zhao, J G Wang, X Ma, *Phys. Rev. A* **95** 042702 (2017)

[7] Radiative charge transfer and association in slow Li^{-} + H collisions, X H Lin, Y G Peng, Y Wu, J G Wang, R Janev, B Shao, *A&A* **598**, A75 (2017)

4.2 Work Plan Updates

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

- Complete our calculations concerning collisions between Li and Be ions and H, in ground and excited states; Visit systematically low charge projectile-He collisions.
- Optimize our 2-electron, multi-center (molecular) targets code;
- Visit collision systems involving multi-electron (up to 4) target/projectile, focusing on population of multi-open shells atomic states though electron transfer or excitation; Probe approximations (as frozen core approx.) used in the past when multi-electron transitions could be described in ab initio non perturbative approach.

Brian GRIERSON, Daren STOTLER, Princeton Plasma Physics Laboratory (PPPL)

- Document and report outstanding data needs from DIII-D and NSTX for intrinsic and seed impurities
- Calculate contributions from halo neutrals to the impurity emission at high and low neutral beam voltage to determine if the fraction of halo-induced emission increases as the neutral beam voltage decreases
- Test neutral beam stopping and emission rate coefficients with newly installed spectroscopic sightlines on DIII-D for assessing strong neutral beam attenuation to the high-field side of the tokamak
- Revise atomic physics data according to input provided by other CRP members and perform comparisons with existing calculations and self-consistency tests

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

Before the third RCM we plan to:

- Collect, re-visit and complete our calculated (CTMC and semiclassical grid numerical) ionization and total and partial electron capture cross sections of H^+, He^{2+}, Li^3+ Be^{4+}, B^{5+} and C^{6+} in collision with neutral H, providing opacity functions, bP(b), as functions of the impact parameter, b, for selected energies, with the aim of assessing associated uncertainties in the data produced.

- Apply the CTMC method to the study of collisions of fully stripped ions with first excited levels of the hydrogen atom. We particularly will look at the excitation cross sections as well as capture and ionization for ion-H *(n = 2*) and ion-H (*n = 3*) at the intermediate energy range, 10 keV/amu < E < 500 keV/amu.

- Extend our switching-CTMC approach to the study of inelastic processes in collisions of low stripped ions with Li targets, and also perhaps with small molecules of interest in Fusion research.

Alisher KADYROV, Faculty of Science and Engineering, Curtin University

Before the 3rd RCM we are planning to:

- Apply the two-centre CCC approach to He^{2+}, Li^{3+} and Be^{4+} collisions with hydrogen. Calculate integrated and various differential cross sections for electron capture, excitation and ionisation. Provide density matrix elements for excitation of the first several states of the target and the one-electron ion formed after electron capture.
- Extend the CCC approach to ion collisions with 2-electron targets to incorporate charge exchange. Calculate integrated and various differential cross sections for proton-impact excitation and ionisation of He and electron capture.
- Re-visit the controversial C^{6+} + He ionisation in the perpendicular plane geometry [Schulz *et al*., Nature **422**, 48 (2003)] using more accurate two-centre CCC approach.

In a longer perspective, possibly beyond the current CRP, we plan to:

- Extend the CCC approach to multi-electron targets. Calculate excitation, charge exchange and ionization in proton collisions with alkali atoms.
- Calculate excitation, charge exchange and ionization in proton collisions with noble gas atoms.

- Extend the CCC approach to molecular targets. Calculate excitation, charge exchange and ionization in proton collisions with H_2^+ and H_2 molecules.
- Calculate excitation, charge exchange and ionization in proton collisions with H_2O molecule.

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.

- In the next few months we will focus on the completion of the proton-hydrogen calculations for excited target states. In particular, the results for the 2p initial states (calculated already) need to be analyzed carefully and compared with recent results of other participants of the CRP. Once this step has been completed we plan to write up the proton-hydrogen work in a publication (and make the cross section data available).
- Subsequently, we will continue with the original plan and focus on further multiply-charged-ion collisions from hydrogen neutrals in the 1-1000 keV/amu impact energy range. The case of bare beryllium ions will be given particular consideration given its importance and the availability of published theoretical data for detailed comparisons. We will first consider collisions starting from the hydrogen ground state and then look at excited initial states, which pose heavy demands on the number of projectile states to be included in the TC-BGM basis sets. We will systematically study the level of convergence that can be achieved with increasing projectile charge.
- In the final year of the CRP we will generate effective potentials for partially-stripped projectiles and carry out TC-BGM calculations for collisions of these ions with hydrogen neutrals. The role of the projectile electrons will be analysed. We will also use our suite of density functional theory based models to deal with the few-electron neutrals helium and lithium and generate required cross section data for them.

Jinseok KO, National Fusion Research Institute (NFRI)

- Further analysis on the beam-into-gas and beam-into-plasma spectra integrated with the NOMAD database structure.
- Measurement and calibration of the background polarized light utilizing the newly installed MSE background polychrometer system.
- Measurement of ion temperature and rotation from the main-ion charge exchange components of the beam emission spectra.
- Full 3D calculation of the beam penetration and benchmark of the atomic data utilizing the KSTAR version of the ALCBEAM code.

Oleksandr MARCHUK, Forschungszentrum Jülich (FZJ)

It is foreseen to explore the effect of correct averaging the rate coefficients for the direct charge-exchange reaction. In further studies I am going to analyze and incorporate in the atomic beam model in parabolic states the recent calculation of density matrix elements and excitation to and from magnetic levels [1]. On the other hand, I am going to compare the recent experimental data from the KSTAR tokamak [2] with collisional radiative model NOMAD in parabolic states [3]. Finally the same procedure is going to be applied to the beam-into gas experiments (DIII-D, KSTAR) and compare these results with the new data for H-H collisions. Finally, I am going to demonstrate the effect of magnetic and electric field on the charge-exchange recombination cross-sections.

References
[1] B. Abdurakhmanov et al. *Plasma Phys. Control. Fusion* **60** 095009 (2018)
[2] J. Ko and J. Chung, *Rev. Sci. Instrum.* **88**, 063505 (2017)
[3] O. Marchuk et al, *J. Phys. B: At. Mol. Opt. Phys.* **43,** 011002 (2010)

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

In the next period, we will generate beam stopping and emission coefficients with error bars formed by propagating uncertainties on the fundamental cross sections, and apply these to a simple beam attenuation model. Extend the analysis to other stopping elements. Use the cross sections produced during the CRP for realistic assessment of the uncertainties.

We will participate in the code comparison workshop and will validate the deliberately simple code against CHEAP analyses of JET beam behaviour to separate the atomic questions from the complications of a full analysis.

The contribution of charge transfer from n>2 excited levels from the neutral beam have been identified as important. We will review the current data and perform a similar uncertainty propagation analysis on the CXRS emission coefficients.

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

- Organize the Code Comparison Workshop on Neutral Beam Penetration and Beam-based Photoemissions. Participate with RENATE and RENATE Open Diagnostics codes and possibly further codes made available by our collaborating partners. Results to be compared consist of beam attenuation and wavelength-integrated emissivity of H, Li and Na beams injected into plasmas of H isotopes with trace impurities.

- Participate in model error estimation. 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).

- Attempt calculation of *nl*-resolved excitation and ionization $H^0 + H^0$ and $H^0 + H_2$ collisions by CTMC modelling.

- Evaluate the effect of neutrals on beam modelling using the freshly calculated set of cross sections for $H^0 + H^0$ collisions.

- Attempt calculation of *nl*-resolved excitation and ionization of $Li + H^0$, $Li + H_2$, $Na + H^0$ and $Na + H_2$ collision by CTMC modelling.

- Model beams shot into gas for calibration purposes provided the cross-sections are available.

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

- Classical simulations in collision between Be^{4+} and H(1s), H(2s) H($2p_0$) H($2p_1$); Calculation of the ionization, the state selective charge exchange cross sections and also the state selective excitation cross sections.

- Calculation of the state selective cross sections in collision between to hydrogen atoms. Simulations to be performed at several impact energies, as follows: 20eV, 30 eV, 40 eV, 60 eV, 80 eV, 100 eV, 200 eV, 500 eV, 1000 eV.
- Classical calculations for the determination of the ionization, the state selective charge exchange and state selective excitation cross sections for the collision system X^{q+} + H(n > 2).

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

State-resolved cross section calculations for excitation, ionization and charge transfer in collisions between hydrogen neutrals and the principal fully stripped impurity ions

- The two-center Atomic orbital close-coupling method will be employed to study the ionization processes in H^+-H collisions in the energy range of 1-1000 keV and the results will be compared with recent results of other participants of the CRP.
- Systematic calculations of charge transfer and excitation cross sections will be performed for H^+/He^{2+}/Be^{4+}/C^{6+}/ N^{7+}/O^{8+} collisions with hydrogen ground state in the energy range of 1 – 1000 keV and a set of recommendation data will be proposed based on comparison with corresponding theoretical and experimental data available.
- In our original plan, only the collisions systems with hydrogen target in ground state are proposed. Due to its importance in neutral beam modeling, the two-center Atomic orbital close-coupling method will be employed to study the collisions of highly charged ions and He/H excited state in the energy range of 1-1000 keV, starting with H(2s) collisions with H^+ and Be^{4+}.

List of Participants

Maarten DE BOCK, ITER Organization, Route de Vinon-sur-Verdon - CS 90 046, 13067 ST. PAUL LEZ DURANCE, FRANCE

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Appendix 2

Agenda

Meeting Room M0E100

Monday, 18 February 2019

09:30 – 10:00 Christian HILL, Arjan KONING: Opening, Introduction of Participants, Meeting Objectives, Adoption of Agenda

Session 1: Fusion Modelling

Chair: Christian HILL

10:00 – 10:40 **Oleksandr MARCHUK**, *Forschungszentrum Jülich (FZJ), Germany*
Atomic data in the active beam spectroscopy of fusion plasmas

10:40 – 11:10 Coffee Break

11:10 – 11:50 **Brian GRIERSON**, *Princeton Plasma Physics Laboratory (PPPL), United States of America*
Comparisons of Atomic Data for NSTX and DIII-D Tokamak Analysis and Simulation with Experimental Validation

11:50 – 12:30 **Jinseok KO**, *National Fusion Research Institute (NFRI), South Korea*
Progress on the KSTAR polarimetric and spectral MSE research

12:30 – 14:00 Lunch

Session 2: Fusion Modelling and Data

Chair: Brian GRIERSON

14:00 – 14:40 **Martin G. O'MULLANE**, *Department of Physics, University of Strathclyde, United Kingdom*
Quantifying the contribution of each atomic process to the overall beam stopping and emission

14:40 – 15:20 **Gergő POKOL**, *Institute of Nuclear Techniques (INT), Budapest University of Technology and Economics (BME), Hungary*
Beam modelling by RENATE Open Diagnostics and proposed test cases for beam model benchmark

15:20 – 15:50 Coffee Break

15:50 – 16:30 **Károly TŐKÉSI**, *Institute for Nuclear Research, Hungarian Academy of Sciences (ATOMKI), Hungary*
Classical simulations of collisions between light particles

16:30 – 17:30 Discussion (all participants): current issues and data needs in neutral beam diagnostics modeling

Tuesday, 19 February 2019

Session 3: Atomic Data I

Chair: Alain DUBOIS

09:00 – 09:40 **Yong WU**, *Institute of Applied Physics and Computational Mathematics (IAPCM), China*
Theoretical study of ion-atom collisions in low and intermediate energy range

09:40 – 10:20 **Clara ILLESCAS**, *Department of Chemistry, Universidad Autónoma de Madrid (UAM), Spain*
Theoretical studies of ionization and single and double electron capture in ion-atom collisions with many active electrons at low and intermediate energies

10:20 – 10:50 Coffee Break

10:50 – 11:30 **Tom KIRCHNER**, *Department of Physics and Astronomy, York University, Canada*
Basis generator method calculations for ion-atom collision systems of indirect and direct relevance to neutral beams in fusion plasmas

11:30 – 12:10 **Alisher KADYROV**, *Faculty of Science and Engineering, Curtin University, Australia*
Proton scattering from excited states of atomic hydrogen

12:10 – 14:00 Lunch

Session 4: Atomic Data II

Chair: Kalle HEINOLA

14:00 – 14:40	**Alain DUBOIS**, *Laboratoire de Chimie Physique – Matière et Rayonnement (LCPMR) at Sorbonne Université, France* Asymptotic basis set semiclassical coupled channel calculations for ion-atom collisions: background and test cases
14:40 – 15:20	**Christian HILL**, *IAEA, Austria* The Global Network for the Atomic and Molecular Physics of Plasmas (GNAMPP)
15:20 – 15:50	Coffee Break
15:50 – 17:00	Discussion (all participants): review of current status of ion-atom collision data
19:30 – 22:00	Social Dinner: Café Ansari, Praterstraße 15, 1020 Wien

Wednesday, 20 February 2019

Session 5: Code Comparison and Uncertainty Quantification

Chair: Gergő POKOL

09:00 – 10:30	Discussion (all particpants): code comparison workshops on: (1) neutral beam penetration and beam-based photoemissions; (2) on electron dynamics in atomic collisions
10:30 – 11:00	Coffee Break

Session 6: Applications: Data Needs at ITER

Chair: Martin G. O'MULLANE

11:00 – 12:30	**Maarten DE BOCK**, *ITER, France* Atomic Needs for ITER CXRS
12:30 – 14:00	Lunch

Session 7: Review and Future Work Plans

Chair: Christian HILL

14:00 – 15:30	Development and review of work plans for the CRP
15:30 – 16:00	Coffee Break
16:30 – 17:00	Drafting of meeting report; adjournment of meeting

Presentation Abstracts

Asymptotic basis set semiclassical coupled channel calculations for ion-atom collisions: background and test cases

A. Dubois

Laboratory of Physical Chemistry – Matter and Radiation, Training and Research Unit of Chemistry, Faculty of Sciences and Engineering, Sorbonne University, Paris, France

In the meeting we shall present the theoretical approach and codes that we use to describe the electronic occurring processes in ion-atom/molecule collisions. Focusing on the intermediate energy range, where the impact velocity is comparable to the classical velocity of the active electron in the initial channel, we use a non perturbative semiclassical treatment allowing the accurate description of the various processes which are likely and couple in the domain. Examples for one- and two-active-electron systems will also be presented, illustrating the power of the method but also the difficulties encountered in the calculations.

Comparisons of Atomic Data for NSTX and DIII-D Tokamak Analysis and Simulation with Experimental Validation

Brian A. Grierson

Princeton Plasma Physics Laboratory, Princeton, USA

In this talk I will cover the rates and procedures for analysis, the rates used in FIDASIM and NUBEAM, and validation with carbon, neon and nitrogen.

Theoretical studies of ionization and single and double electron capture in ion-atom collisions with many active electrons at low and intermediate energies

Clara Illescas

Departamento de Química, módulo 13. Facultad de Ciencias. Universidad Autóniomа de Madrid, Spain

At the first RMC meeting we introduced the switching CTMC approach, especially designed to classically treat more than one active electron systems [1], with the aim to describe atomic processes involving neutral beams with more than one active electron.
In this talk I will report our recent studies on ionization and electron capture processes in proton+ Ar collisions from 100 eV to 200 keV collision energies [2]. We have applied two methods, the swithching CTMC and a semiclassical treatment with a molecular expansion [3] in a basis of electronic wave functions of the ArH^+ quasimolecule and we have tried to accurately represent two-electron processes, in particular, the double electron capture which cross sections are very small. I will show the general good agreement of the calculated cross sections and I will also discuss the limitations of both type of calculations.

[1] A Jorge *et al.*, Phys. Rev. A **94** 022710 (2016)
[2] A Jorge *et al.*, J. Phys. Chem. A **122** 2523 (2018)
[3] P Barragán *et al.*, Phys. Rev. A **82** 030701 (2010)

Proton scattering from hydrogen atom in excited state

A. S. Kadyrov

Curtin Institute for Computation and Department of Physics and Astronomy, Curtin University, GPO Box U1987, Perth, WA 6845, Australia

We have developed a wavepacket continuum-discretisation approach to calculate excitation, ionization and electron-capture cross sections for protons colliding with atomic hydrogen in excited states [1]. The approach assumes a classical motion for the projectile and is based on the solution of the three-body Schrödinger equation using the two-center expansion of the total scattering wave function. The scattering wave function is expanded in a basis set made of negative-energy eigenstates and wavepacket pseudostates representing the continuum of both the target atom and the atom formed by the projectile after capturing the electron. Calculated cross sections for scattering on the metastable 2s state are compared with other theoretical results obtained using atomic-orbital close-coupling and classical trajectory Monte Carlo approaches. Considerable disagreement with previous calculations has been found for some transitions at various incident energies.

[1] I. B. Abdurakhmanov *et al*., Plasma Phys. Control. Fusion **60**, 095009 (2018)

Basis generator method calculations for ion-atom collision systems of indirect and direct relevance to neutral beams in fusion plasmas

T. Kirchner

Department of Physics and Astronomy, York University, Toronto, Canada

I will report on recent progress with two-center basis generator method (TC-BGM) calculations for collision systems that are of indirect and direct interest in the context of fusion-plasma research. In the *indirect* category we have studied low-impact-energy C^{6+} and O^{8+} collisions from hydrogen and krypton atoms [1]. The work was motivated by recent measurements of Lyman-line emissions after capture from krypton into those ions. Since krypton and hydrogen have very similar (first) ionization potentials it was argued that the krypton measurements may be compared with calculations for hydrogen targets. Our results for both targets and both ions suggest that this is in general not a terribly good idea [1].

More recently, and in the *direct* category, we started to look into the problem of target excitation, electron capture, and ionization in proton collisions from excited hydrogen atoms. Not surprisingly, larger basis sets than for ground-state target atoms are required to achieve reasonable convergence. Preliminary results will be presented and compared with recent wavepacket convergent close-coupling [2] and previous theoretical calculations.

[1] A. C. K. Leung and T. Kirchner, Phys. Rev. A **97**, 062705 (2018)
[2] I. B. Abdurakhmanov *et al*., Plasma Phys. Control. Fusion **60**, 095009 (2018)

Progress on the KSTAR polarimetric and spectral MSE research

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Aiming at the experimental validation of atomic data for motional Stark effect diagnostics under the CRP, the following polarimetric and spectram MSE analysis activities are reported - Application of single-ion-source-injection fitting routine to the beam-into-gas MSE spectra and comparison with two-ion-source-injection fitting analysis; System errors introduced from multi-ion source injection with finite beam width and non-focused signals; and characteristics of background polarized spectra and their effect on the MSE measurements. In addition, a little progress on a new item is reported - Application of ALCBEAM to KSTAR and its preliminary results.

Atomic data in the active beam spectroscopy of fusion plasmas

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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.

Whereas the *eigenstates* of the beam atoms in fusion are the solutions of the Schrödinger Equation for hydrogen atom in the crossed electric and magnetic fields the different approximations are used to describe the beam atoms in the plasma:

The *statistical* models are until now the most common and the simplest models describing the ground and excited levels of the beam. The second type of models are the so called *nl* resolved model. These models provide more accurate descriptions for the beam –emission data, however, they can be not applied for the population's calculations. Finally, the most accurate type of models used now is the model using the parabolic states. The advantage of this model is also the application of the field ionization induced by the electric field.

The transitions between different atomic models, limitations, pitfalls and current status of the collisional atomic data will be shown in this work.

Quantifying the contribution of each atomic process to the overall beam stopping and emission

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We will outline the ADAS approach to beam population calculations and the corpus of fundamental data on which it relies. A preliminary ranking of the contribution of these process to the beam stopping and beam emission coefficients is outlined. A comparison of the influence of other drivers, such as the plasma impurity mixture, to the size of possible errors in the hydrogen coefficients is given. We also report on work on l-changing collisions which may be of interest to this problem.

Beam modelling by RENATE Open Diagnostics and proposed test cases for beam model benchmark

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RENATE Open Diagnostics (RENATE-OD) is an open source beam emission modelling tool that is being developed to serve as synthetic diagnostic in the ITER Modeling and Analysis Suit (IMAS). The beam model is based on the previously validated beam emission modelling tool RENATE. Status and further plans of development for RENATE-OD are presented. In the second half of the talk the proposed test cases for the beam model benchmark are presented, along with preliminary ideas on the physics question to be addressed.

Classical simulations of collisions between light particles

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The classical trajectory Monte Carlo (CTMC) method is quite successful in dealing with ionization, capture and excitation processes in ion-atom and in ion–molecular collisions. In the last decades a Software package of the classical trajectory Monte Carlo (CTMC) codes using 3-4-5 and many-body systems was developed.
Collisional radiative models used in the modeling of beam emission spectroscopy diagnostics recently neglect the atom-atom collisions due to a lack of these atomic cross section data. Filling this scantiness we performed a classical trajectory Monte Carlo simulations to calculate the cross sections for various channels in collisions between H + H_2, Li + H_2 and Li^+ + N_2 in wide range of projectile energies. I show simulation results for various cross sections from the total till the multi-differential ones of these systems. The results of the simulations will be compared with other theoretical and available experimental data.

Co-workers
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Theoretical study of ion-atom collisions in low and intermediate energy range

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The collisions between ions and atoms/molecules exit extensively in various environments, such as low temperature plasma, fusion plasma and the interstellar atmospheres etc. Therefore, the scattering cross sections and rate coefficients are the fundamental atomic data needed in the simulation and diagnosis of these plasma.

In this talk, I will report our recent studies of the charge transfer processes in ion-atom/molecule collisions in low and intermediate energy range. Combining the fully quantum-mechanical molecular-orbital close-coupling method (MOCC) with the two-center atomic-orbital close-coupling method (AOCC), the electronic correlations effects in charge transfer processes can be well treated and the charge transfer cross sections can be obtained at high precision in a large impact energy range. At the end of the talk, I will briefly introduce the recent progresses of the atomic and molecular database in IAPCM.

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