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Data for Atomic Processes of Neutral Beams in Fusion Plasma

Summary Report of the First Research Coordination Meeting

IAEA Headquarters, Vienna, Austria

19-21 June 2017

Report prepared by

Hyun-Kyung Chung
IAEA Nuclear Data Section

September 2017

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Abstract

The First Research Coordination Meeting of the CRP on Data for Atomic Processes of Neutral Beams in Fusion Plasma was held on 19–21 June 2017 at IAEA in Vienna with thirteen participants from ten countries (Australia, Canada, China, Germany, France, Hungary, South Korea, Spain, UK and USA). Neutral beam injection is a standard method to heat and control the plasma in fusion experiments and a diagnostic method of plasma conditions. The Coordinated Research Project (CRP) is planned to provide evaluated and recommended data for the principal atomic processes relevant to heating and diagnostic neutral beams in fusion plasmas. At this meeting, CRP participants presented their current and future research plans, and discussed coordinated activities to produce and evaluate atomic data needed for neutral beam injection. The proceeding of the meeting is summarized in this report.

September 2017

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1. INTRODUCTION

Neutral beam injection is a standard method to heat the plasma in fusion experiments and it is intended to be used for power control in ITER and perhaps in a reactor. Neutral beams also have important diagnostic uses, both via photoemission from the beam neutrals due to interaction with the plasma and via photoemission from plasma impurities after interaction with the beam. Modelling of beam penetration into the plasma and of the spectroscopic signals relies on detailed data for atomic processes that involve the neutral beam particles. In spite of the importance of the data there are quite significant gaps, especially related to processes starting from an excited state of the neutral atom. On the other hand, for processes starting from the ground state of the neutral atom there are often several different families of calculated or measured data, obtained using different approximations or experimental methods, and it is important to assess their uncertainties and to recommend best data.

The Coordinated Research Project (CRP) on Data for Atomic Processes of Neutral Beams in Fusion Plasma is organized to provide evaluated and recommended data for the principal atomic processes relevant to heating and diagnostic neutral beams in fusion plasmas. The primary emphasis is on processes of hydrogen (H, D, T) neutral beams in the high temperature core plasma. The preparatory meeting was organized on 17-18 March 2016 to define the scope of the CRP and identify scientific groups and the first Research Coordination Meeting (RCM) was held on 19-21 June 2017 at IAEA headquarter in Vienna.

The first RCM brought 10 CRP research groups represented by 13 participants and 2 consultants. CRP participants were O. Marchuk of FZJ, Germany on the topic of atomic data and collisional-radiative modelling of neutral beams in eigenstates, J. Ko, NFRI, Korea on the topic of experimental validation of atomic data for motional Stark effect diagnostics, D. Stotler, PPPL, USA on the topic of neutral beam analysis codes used on NSTX-U and DIII-D , G. Pokol, Wigner Research Centre, O. Asztalos Oers and T. Karoly, ATOMKI, Hungarian Academy of Sciences, Hungary on the topic of study of atomic beam interactions in fusion plasmas using the RENATE synthetic BES diagnostic, M. O'Mullane, U of Strathclyde, UK on the topic of quantification of the contribution of processes in the ADAS beam model, N. Sisourat and J. Gao, UPMC, France on the topic of electronic processes cross sections evaluation with 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 energy range of 25-500 keV/amu. Y. Ralchenko of NIST, USA and Christian Hill of University College of London, UK participated as consultants to the meeting.

Section 2 summarizes the proceedings of the meeting and Section 3 summarizes discussions among participants. Section 4 describes the proposed work plans by each CRP group. The list of participants is presented in Appendix 1 and the Agenda is provided in Appendix 2. The summaries of presentations are provided in Appendix 3 where presentation materials for this meeting are found through the web page https://www-amdis.iaea.org/CRP/NeutralBeams/RCM1.

2. PROCEEDINGS

The Head of Nuclear Data Section, A. Koning opened the meeting by welcoming participants and emphasizing the importance of recommended and evaluated atomic data for fusion applications. The Scientific Secretary and the Head of Atomic and Molecular Data Unit, H.-K. Chung, presented the scope of CRP and the meeting objectives. The agenda was adopted. Participants presented their work and research plans during the period of CRP and discussion sessions were arranged after presentations.

On the first day, presentations on fusion modelling and a review of current issues and data needs with neutral beam diagnostics modelling were arranged. Dr Stotler presented the neutral beam analysis codes used on the NSTX-U and DIII-D tokamaks such as NUBEAM (part of TRANSP) and FIDAsim. Dr Marchuk described the linear Stark and Zeeman effect for the H atom in the plasma used for plasma spectroscopy and presented collisional-radiative (CR) model in parabolic states and atomic data sets used in the CR model. Dr Ko reviewed experimental validation methods of atomic data and models for motional Stark effect implemented at KSTAR tokamak and addressed issues important to experimental validation such as polarized lights and multiple ion sources. Prof Pokol reviewed the RENATE simulation code (CR model) used for beam emission spectroscopy (BES) diagnostics and planned activities in the course of the CRP. Prof Tőkési, a co-worker of Prof Pokol presented classical methods to calculate ionization, state selective capture and excitation cross-sections. Dr O'Mullane presented quantification of the contribution of processes in the ADAS beam model, particularly emphasizing the motivation and areas of focus related to neutral beam diagnostics. The first day closed with a review session on current issues and data needs with neutral beam diagnostics model, which is summarized in Section 3.

The second day proceeded with presentations on atomic data relevant to neutral diagnostics. Prof Sisourat described a semi-classical non perturbative approach to evaluate electronic processes cross-sections and presented a new implementation using multi-center Gaussian type orbitals and results of Li^{3+} - H collisions. Dr Wu presented theoretical methods to calculate state-resolved cross-sections for excitation, ionization and charge transfer in collisions between hydrogen neutrals and the fully stripped impurity ions as well as x-ray spectra from highly charged ion collisions. Prof Illescas presented CTMC (Classical Trajectory Monte Carlo Method) and GTDSE (Grid Time Dependent Schrödinger Equations) methods to study ionization, charge transfer and excitation in ion-hydrogen (helium) collisions in the energy range of 25-500 keV/amu. Prof Kirchner described BGM (Basis Generator Method) calculations for ion collisions with H and He atoms. Prof Kadyrov presented a convergent close-coupling (CCC) approach to accurately calculate state-resolved cross-sections for excitation, ionization and charge transfer in collisions of hydrogen isotopes with protons, deuterons, tritons and impurity ions existing in fusion plasma. Dr Ralchenko presented atomic data for W^{64+} + H and collisional-radiative modeling to simulate tungsten charge exchange recombination spectra for ITER diagnostics. After presentations, the current status of ion-atom collision data was reviewed.

The third day was devoted mostly for discussions on future plans. The two review sessions on the previous two days were summarized by Dr O'Mullane and Prof Kirchner. Dr Ralchenko shared his experience on the NLTE (non-local thermodynamic equilibrium) code comparison workshops. The NLTE workshop series bring code developers together for a week long workshop where code results submitted for defined test cases are discussed for their underlying assumptions and technical details in order to understand differences and discrepancies when comparing code results. Generally test cases are defined a few months in advance and code results are submitted before the workshop. The workshop led to a significant understanding of atomic processes in plasmas, which are difficult to validate and verify experimentally. After the presentation, participants were grouped to discuss the code comparison workshops for neutral beam penetration codes and for ion-atom collision codes. Conclusions of discussion sessions during and after meetings are summarized in Section 3.

3. DISCUSSION AND CONCLUSIONS

3.1 Review of current status of atomic data used for modelling the beam and its diagnostic capabilities

General remarks

- Many codes are in use for modelling beam stopping and emission.
- CXRS analysis on plasma impurities (for light elements) is well established.
- Data come from similar databases of fundamental processes.
- Atomic data for a beam model are primarily *n*-resolved.

- Atomic data for the CX (Charge Exchange) model should be *nl*-resolved
- MSE (Motional Stark Effect) spectral feature interpretation requires *nlm* cross sections, but they are not readily available.

- Data in use may not be the latest and hence needs evaluation.
- There is no routine use of data uncertainty in the fundamental data.
- There are models and observations for high-Z CXRS to build experiences for ITER diagnostics.
- There is progress in work on synthetic diagnostics addressing the complications of halo, plume, overlapping features from multiple beams and geometry effects.

Atomic processes in model for Hydrogen (H/D/T) beams in 10 keV-1MeV energy range

- Atomic structure and A-values are known to very high precision.
- Electron impact ionisation from n=1: data is good but not a significant process.
- Ion impact ionisation from n=1:
  - The principal process in stopping.
  - Recent publications show progress in refining the cross section
  - A recommended cross section with error bars is a priority.
- Electron impact excitation (between n=1-5): good data but not a significant process.
- Ion impact excitation data (between n=1-5): could be better and recommended data is essential.
- Ion impact ionisation from excited levels:
  - They are very poorly known from n=2,3,4,5 (observable from BES)
  - Recommended data for these processes is essential.
- Ion and electron impact excitation data between high-n levels are needed.
- Projectile ions required are protons, He^{2+}, Be^{4+}, C^{6+}, Ne^{10+} , Ar^{18+} and Z^{z+}

Charge exchange recombination spectroscopy and Motional stark effect model

- MSE spectral feature modelling to complement/replace polarization methods”
  - *nlm* cross sections with density matrix elements for 2s, $2p_0$, $2p_1$ are needed
  - No easily available data for these exists but the capability for producing it is in the codes.
- CXRS/CHERS required *nl* partial cross sections.
- Review of existing light elements (He, Li, Be, C, N, Ne, Ar) to identify any gaps in coverage or precision should be performed.
- High-Z CX, ie tungsten, is almost a new field of study. Need to assess the data, the models and the observations.

Atomic processes in model for Lithium and Sodium beams in 50 keV energy range

- Atomic structure and A-values are known to very high precision.
- Electron processes are more important than for H beams.
- High n contributions are also less significant.
- Projectile ions required are protons, He^{2+}, Be^{4+}, C^{6+}, Ne^{10+} , Ar^{18+} and Z^{z+}

3.2 Priority list of ion-atom collision data to be assembled during the CRP

The objective of this CRP is to come up with evaluated and recommended data.

Collision systems

A. H(1s) + H^+, He^{2+}, Be^{4+}, C^{6+}, Ne^{10+} , H(1s), H_2 at 10 keV – 1 MeV
B. H(2s, $2p_0$, $2p_1$) + H^+, He^{2+}, Be^{4+}, C^{6+}, Ne^{10+} , H(1s), H_2 at 10 keV – 1 MeV
C. H(n>2) + H^+, He^{2+}, Be^{4+}, C^{6+}, Ne^{10+} , H(1s), H_2 at 10 keV – 1 MeV
D. He($1s^2\,{}^1S$), He(1s2s ${}^3S$) + bare ions (at & up to 70 keV total energy)
E. Li(2s), Na(3s) + bare ions (at & up to 50 keV total energy): partially stripped ions are of lower priority

Quantities of interest

- Excitation probabilities and cross-sections (m-resolved) : A
- Density matrix elements : A
- Ionization probabilities and cross sections: A, B, C (D, E)
- Charge exchange probabilities and cross-sections: A, (B, C, D, E)
- nl-resolved excitation probabilities and cross-sections: (B, C), D, E

Priorities

- H^+-H(1s) : target excitation (m-resolved, n=2,3)
- H^+-H(1s) : ionization + charge exchange
- H^+-H^*
- A^{q+} - H(1s), H^*

3.3 Discussion on code comparison workshop on neutral beam penetration and beam-based photoemissions

There exist many codes that simulate neutral beam penetration and beam-based photoemissions. The photoemissions are used in diagnostics including beam emission spectroscopy (BES) and the motional Stark effect (MSE) diagnostic, which both rely on photoemissions from the beam neutrals, and charge exchange recombination spectroscopy (CXRS or CHERS), which relies on photoemissions from plasma impurities. The beam codes employ a variety of atomic models and data and the comparison exercise would help the code developers to identify possible concerns with the atomic data and to identify important sensitivities of the simulations of beam penetration and beam-based emissions to uncertainties in the atomic data. Therefore, the principal objective of this code comparison exercise is to identify the range of differences among various codes, each implementing some set of atomic physics data, for simulations of beam penetration and beam-based photoemissions. As a result of this comparison it may be found that some atomic data really need attention. However, this code comparison workshop is not set up to assess the uncertainties in the atomic data or to recommend best data. The background and scope of the workshop on neutral beam penetration and beam based photoemissions can be found at https://www-amdis.iaea.org/meetings/CCW2017NeutralBeamEmissions/. CRP participants discussed the possible exercise cases as summarized here.

Beam penetration

- Ionization + CX data Beam emission (yes\no)
- CX spectra

Proposal: Uniform plasma and codes calculate attenuation (dependence on magnetic field?), mono-energetic beam.

Exercise 1. Hydrogen. Beam penetration only. *Atomic data (Rates) must be visible.*

- Modify the code if require (the author must be able to do this)
- Parameter set:
  - density(cm-3): 1e10, 1e13, 1e14
  - temperature(eV): 100, 1000, 10000
  - Beam energy(keV): 25, 50, 100, 500, 1000
  - Length (cm): first point 0 (beam intensity 1), 1000 points .. last point 5 m
  - Impurity(individual)): (H^+) (He^{2+}) (Be^{4+}) (C^{6+}) (Ne^{10+}) ($Ar1^{8+}$)
  - Impurity(Zeff=2): H + X (X =He, BE, C, Ne, Ar; all are fully ionized)
- Output: Populations: total, n=1, n=2, n=3, all states that are in the model...

Exercise 2. Realistic scenarios. ITER-Scenario2. Input from HU.

- Profiles are specified by the Input table (HU)
- pure H plasma
- DT plasma scenario
- Impurities from input table….
- Output: Populations as in the exercise 1.

Exercise 3. Beam – emission modelling

- Results from exercise 1
- Results from exercise 2
- Output: L-alpha, H-alpha, beta, gamma
- KSTAR-Experiment
  - Input from HU... preferable the same conditions as for MSE-KSTAR

Exercise 4. MSE Data.

- Hydrogen
  - Temperature(eV): 1000
  - Beam energy (keV): 50, 100, 500
  - Density (cm-3): 1e10,1e13, 1e14
  - Magnetic field (T): 0, 1, 3, 5 (magnetic field is perpendicular to the beam)
- Output: Impulses at L-alpha, H-alpha, beta, gamma, populations of substates.
- KSTAR-Scenario , Input from KO
  - Beam into gas as well
  - Pressure of the D2 molecules, energy of the beam, magnetic field

Testing: Plasma would be semi-infinite (0.le.x), uniform, normally including a uniform magnetic field in the y-direction. Plasma electron density might be 1e14/cm3 always; bulk species is deuterium. Plasma temperature might be 100 eV, 500 eV, 2 keV, 10 keV. If there is an impurity then we might agree that Z_eff=2 in each case, and there is only a single impurity; say Be, C, N, Ne or Ar. (Need some care if the impurity would not be fully stripped.) Maybe consider some tungsten impurity as well.

Beam is propagating in the positive x-direction along the x-axis; ignore beam width on entry. The beam species would be deuterium and the energy might be 50 keV, 200 keV, 1 MeV. Initial state is pure, D(1s) or D(2s) or D(2p) in any polarization. Ignore beam density effects; assume independent beam particle model.

Beam emission. L-alpha emission / H-alpha, beta gamma

- Li beam and Na beam, He beam (who else except for Hungary and ADAS, US ?)
- Beam-gas emission (tests)
- Approach reality (KSTAR as working experiment/horse).

The same conditions as in case of Testing.

MSE Codes.

To be discussed later

Emission from “halo” (beam) emission coefficients . But only atomic data

To be discussed later

3.4 Discussion on code comparison workshop on electron dynamics in atomic collisions

The Unit promotes organized activities on uncertainty quantification of theoretical atomic and molecular data and recently published an article on uncertainty quantification of atomic and molecular data. (J. Phys. D: Appl. Phys. Vol 49, p. 363002 (2016) http://iopscience.iop.org/article/10.1088/0022-3727/49/36/363002/meta).One of possible ways to study and understand uncertainties associated with theoretical calculations is to compare different methods, models and implementations. Several methods have been applied to the basic problem of collisions involving one active electron and straight line nuclear motion. There are multiple groups that use classical trajectory Monte Carlo (CTMC). Several groups use Atomic Orbital Close Coupling (AOCC; also the acronym TC-AOCC is used), either based on Slater-type orbitals or on Gaussian orbitals. Several groups evolve the time-dependent Schrödinger equation on a lattice, which can be rectangular or cylindrical, fixed or adaptive, and the acronyms are LTDSE, GTDSE and also just TDSE. Several groups use a Molecular Orbital Close Coupling (MOCC or QMOCC) approach. There are some other keywords as well: Sturm basis or Sturmian functions, time dependent close coupling, distorted wave approach. It appears that there is enough diversity of approaches to have an interesting workshop. The workshop will provide a great opportunity to test different assumptions used by codes and understand uncertainties of calculations for problems where measurements are not possible. More details on the background and scope are found at https://www-amdis.iaea.org/meetings/CCW2017AtomicCollisions/

Five CRP participants discussed the values of having code comparison workshops on ion-atom collision data and the meeting formats. They agreed that the code comparison workshop should bring more experts from the ion-atom collision community in order to make the workshop effective and productive. The IAEA staff and a few CRP participants organized a discussion session at the 25th International Symposium on Ion-Atom Collisions (ISIAC) held in Palm Cove, Australia on July 23-15, 2017 where 19 workshop participants attend the discussion session. They agreed that the code comparison workshop (CCW) on Electron Dynamics in Atomic Collisions is worthwhile doing. It is recommended to attach the proposed CCW to one of upcoming conferences next year in Europe. The candidates are HCI (3-7 September, Lisbon), ICACS (1-6, July, France) and MPS (22-24, August, Budapest). Prof. Tőkési, a CRP participant, agreed to host the CCW in Budapest or Debrecen if MPS is chosen. If HCI or ICACS are chosen, local hosts should be identified in Lisbon (possibly in Madrid) or in Caen (possibly elsewhere in France). Test cases will be determined by e-mail. There are proposals for a few simple cases as well as idealized cases to test various aspects of codes. In order to give enough time for highly sophisticated codes, it is recommended to define test cases in a couple of months.

It is possible for IAEA to provide travel support to participants from eligible countries (up to 5000 Euros total). This is subject to the budget of IAEA upon an official request of local organizer for “IAEA cooperation meeting”.

4. PROPOSED WORK PLANS

Work plans proposed by CRP research groups are summarized in this section.

Proposal from Princeton Plasma Physics Laboratory, Daren Stotler

1st year:

- List atomic physics processes used in project codes,
- Determine sources of cross section or rate data,
- Perform an initial assessment of the consistency and accuracy of these data.
- Recount the assessment and proposed plan of action for the D(n>2)+C^{6+} charge exchange data.

2nd year:

- Perform comparisons of effective rate data from CR models noted above.
- Provide additional details on NUBEAM-FIDAsim benchmark, as requested.
- Document parameters of DIII-D FIDAsim validation tests.
- Report on progress towards understanding inconsistencies in DIII-D impurity injection and beam voltage variation experiments.

3rd year:

- Document outstanding data needs, if any, identified in first two years of the project
- Revise atomic physics data according to input provided by other CRP participants.
- Update progress towards understanding inconsistencies in DIII-D impurity injection and beam voltage variation experiments.
- Assess status of data required for NUBEAM simulation of helium beam penetration.

Proposal from NFRI, Jinseok Ko

1st year:

- Construction of self-calibrated high-precision (d(lambda) less than 0.05 nm) spectral diagnostic
- Development of a single-ion-source-injection fitting routine and interface for existing atomic data and modeling packages (such as NOMAD, ADAS, etc.)

2nd year:

- Introduction of the polarization-distortion effects to the spectral analysis suite
- Systematic comparison with the PEM-base MSE

3rd year:

- Evaluation and assessment of the atomic data used in the spectral analyses
- Optimization of the spectral analysis suite for ITER application

Proposal from University of Strathclyde, Martin O’Mullane

The overall contribution to the research project is to improve ADAS beam population model by providing error surface data for beam stopping, beam emission and CX emissivity coefficients and making these available via ADAS and OPEN-ADAS.

Year 1:

- Rank, in a quantitative way, using the existing ADAS model and data, the relative importance of the various atomic processes to the final stopping coefficients, BES and MSE spectra for representative JET and ITER conditions.
- Ascribe an arbitrary, but realistic, error bar to each quantity/process and propagate these uncertainties through the beam population model.

Year 2:

- Explore the consequences of relaxing any in-built assumptions such at Te=Tion and the data reduction choices.
- Explore the effect of beams with significant birth populations in excited states by adapting the model to give relevant cross coupling coefficients. Explore the effect of these on the attenuation profiles and BES, MSE and CHERS spectra.
- Evaluate the asymptotic behavior of the model at MeV energies.
- Incorporate data from RCM activity.

Year 3:

- Include the improved fundamental data generated during the coordinated research activity into the beam and CXRS models and propagate the recommended uncertainties through the models to produce recommended coefficients with accompanying error surfaces.

Proposal from FZJ, Oleksandr Marchuk

1st year

- Calculation of the MSE Line intensities (L_alpha, H_alpha, H_beta) for the reference cases based on the available data
- Redistribution of the code in the eigenstates between some of participants/experiments if required
- Comparison between statistical and non-statistical results for the specific cases

2nd year

- Implementation of the new atomic data in the code
- Coordination of the flow of atomic data if required
- Calculation of the MSE spectra /beam emission/attenuation using the new data
- Verification of the new atomic data against the old and hopefully new experimental data

3rd year

- Final results would be prepared
- Submission and preparation of the final report and/or paper(s).
-

Proposal from Wigner Research Centre for Physics, Hungarian Academy of Sciences, Gergo Pokol

1st year

- Take part in Code Comparison Workshop on Neutral Beam Penetration and Beam-based Photoemissions (https://www-amdis.iaea.org/meetings/CCW2017NeutralBeamEmissions/) using the RENATE Open Diagnostics code 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.
- Take part in estimating sensitivity of attenuation and emissivity on reaction rates by perturbing reaction rates and evaluating the CR model.
- Take part in Code Comparison Workshop on Electron Dynamics in Atomic Collisions (https://www-amdis.iaea.org/meetings/CCW2017AtomicCollisions/) by CTMC modelling by Károly Tőkési. Calculate cross-sections for selected test cases.

2nd year

- 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).
- If benchmarks show applicability of the method, extend available energy range of excitation and ionization cross-sections for Li and Na by CTMC modelling.

3rd year

- Attempt calculation of nl-resolved excitation and ionization H0+H0 collisions by CTMC modelling.
- Attempt calculation of nl-resolved excitation and ionization of H0+Li collision by CTMC modelling.
- Evaluate the effect of neutrals on beam modelling using the freshly calculated set of cross-sections for H0+H0 collisions.
- Modell beams shot into gas for calibration purposes provided the cross-sections are available

Proposal from UPMC, Alain Dubois, Nicolas Sisourat

1st year:

- compute state-resolved cross-sections for excitation, ionization and charge transfer processes for collisions between fully-stripped ions, from hydrogen to lithium, and hydrogen in its electronic ground state.
- optimize and parallelize our code.

2nd year:

- compute the state-resolved cross-sections for excitation, ionization and charge transfer processes for collisions between fully-stripped ions, from hydrogen to lithium, and hydrogen in its lowest electronic excited states (H(2s) and H(2p))
- compute state-resolved cross-sections for excitation, ionization and charge transfer processes for collisions between fully-stripped ions, from beryllium to boron (Carbon if possible), and hydrogen in its electronic ground state.

- finalize code for two-active electron systems.

3rd year:

- compute the state-resolved cross-sections for excitation, ionization and charge transfer processes for collisions involving two-electron systems.

Proposal from York University, Tom Kirchner

1st year:

- In the first year of the CRP we will focus on the calculation and evaluation of proton-hydrogen cross section data in the 1-1000 keV impact energy range. For neutrals in the ground state, two-center basis generator method (TC-BGM) calculations have already been carried out, but will be re-assessed and partly repeated. For excited initial states new TC-BGM calculations with larger projectile basis sets will be performed and the convergence properties of the results will be studied. Comparisons with other available results (published or generated by other participants of the CRP using different methods) will aid this process.

2nd year:

- In the second year the focus will be on multiply-charged-ion collisions from hydrogen neutrals in the 1-1000 keV/amu impact energy range. The case of bare berylium 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.

3rd year:

- In the third year we will generate effective potentials for partially-stripped projectiles and carry out TC-BGM calculations for the 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.

Proposal from Universidad Autónoma de Madrid, Clara Illescas

1st year:

- Calculation of ionization and total and partial charge exchange cross sections in collisions of neutral H and some principal fully stripped impurity ions (Be, B, C and Ne; also probably Ar and Kr) using Classical (CTMC), semi classical (eikonal) Grid numerical and quantal methods using two-center molecular wave functions will be employed in order to cover a wide range of collisional energies and to assess associated uncertainties in the data produced.

2nd year:

- Calculation of cross sections for excitation, charge-transfer and ionization in collisions of fully stripped ions with excited states of H. This application will require a good description of the neutral excited state. We also intend to compare the results of different theoretical approaches; we will start to treat the systems with the CTMC method.

3rd year:

- Study of the inelastic processes of fully stripped low charged ions (He, Be, C) with He with an explicit treatment of the two active electrons of the target.

Proposal from Curtin University, Alisher Kadyrov

1st year

- We will start from calculations of the Balmer-alpha (n=3 to n=2) emission when a hydrogen or deuterium beam is injected into the fusion plasma. This requires accurate calculations of the cross sections for excitation of 3s, 3p and 3d states of the neutral atom. Almost 90% of the Balmer-alpha emission comes from 3s and 3d states. In addition, since the plasma contains protons and dueterons, electron transfer to 3s, 3p and 3d states of hydrogen and deuterium atoms will also contribute. Currently, there is a disagreement between experimental measurements and theoretical calculations for the Balmer-α emission. Our aim is to resolve this discrepancy by providing accurate data on cross sections of all underlying processes.

2nd year

- We will provide accurate data for ion scattering on excited states of hydrogen isotopes. In particular, we will consider further excitation or de-excitation, electron capture and ionisation in proton collisions with H(nlm), where the initial state principal quantum number n can be from 2 to 5. In addition, fully differential and various partial differential cross sections for ionisation, angular differential cross sections for excitation and electron transfer in proton-hydrogen collisions will be calculated.

3rd year

- We will provide state-resolved (nlm) cross sections for excitation and electron transfer and total and differential cross sections for ionization in collisions of hydrogen isotopes and the main impurity ions in fusion plasma. Specifically, we will consider scattering of He^{2+}, Be^{4+}, C^{6+}, N^{7+} and O^{8+} ions with H, D and T.

Proposal from IAPCM, Yong Wu

The AOCC, MOCC and CDW methods will be employed to calculate the excitation, charge transfer and ionization cross section in collisions between hydrogen (H, D, T) and the fully stripped ions of He, Be, C, N, O, Ne, Ar at hydrogen energy from about 1 keV to 1 MeV.

1st year:

- He2+, Be4+, C6+, N7+-H collisions

2nd year:

- O8+, Ne10+ -H collisions

3rd year:

- Ar^{18+} -H collisions

Appendix I: List of Participants

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Appendix II: Meeting Agenda

Monday 19 June 2017 **Meeting Room: M0E24**

09:30 – 09:45 Opening, Introduction of Participants, Adoption of Agenda

09:45 – 10:00 **H. Chung** “Meeting Objectives”

Session I: Fusion Modeling (Chair: H. Chung)

10:00 – 10:40 **D. Stotler** “Neutral beam analysis codes used on NSTX-U and DIII-D”

10:40 – 11:00 *Coffee break*

11:00 – 11:40 **O. Marchuk** “Atomic data and collisional-radiative modelling of neutral beams in eigenstates”

11:40 – 12:20 **J. Ko** “Experimental validation of atomic data for motional Stark effect diagnostics”

12:20 – 14:00 *Lunch*

Session II: Fusion Modeling and Data (Chair: D. Stotler)

14:00 – 14:40 **G. Pokol** “Study of atomic beam interactions in fusion plasmas using the RENATE synthetic BES diagnostic”

14:40 – 15:20 **M. O’Mullane** “Quantification of the contribution of processes in the ADAS beam model”

15:20 – 15:40 *Coffee break*

15:40 – 17:00 Review of current issues and data needs with neutral beam diagnostics modeling

19:00 *Dinner*

Tuesday 20 June 2017

Session III: Atomic Data (Chair: Y. Ralchenko)

09:00 – 09:40 **N. Sisourat** “Electronic processes cross sections evaluation with semiclassical non perturbative approach”

09:40 – 10:20 **Y. Wu** “State-resolved cross section calculations for excitation, ionization and charge transfer in collisions between hydrogen neutrals and the principal fully stripped impurity ions”

10:20 – 10:50 *Coffee break*

10:50 – 11:30 **C. Illescas** “Theoretical studies of ionization, charge transfer and excitation in ion-H, He collisions in the energy range of 25-500 keV/amu ”

11:30 – 12:10 **T. Kirchner** “Basis generator method calculations for ion-atom collision systems of relevance to neutral beams in fusion Plasma”

12:10 – 14:00 *Lunch*

Session IV: Atomic Data (Chair: T. Kirchner)

14:00 – 14:40 **A. Kadyrov** “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”

14:40 – 15:20 **Y. Ralchenko** “Atomic data for W^{64+} and H”

15:20 – 15:50 *Coffee break*

15:50 – 17:00 Review of current status of ion-atom collision data

Wednesday 21 June 2017

Session V: Code Comparison Workshops

09:00 – 09:30 **Y. Ralchenko** “Code Comparison Workshops”

09:30 – 10:30 Discussion on code comparison workshop on neutral beam penetration and beam-based photoemissions

10:30 – 10:50 *Coffee break*

10:50 – 12:00 Discussion on code comparison workshop on electron dynamics in atomic collisions

12:00 – 13:30 *Lunch*

Session VI: Conclusions

13:30 – 15:00 Development of work plans during the CRP period

15:00 – 15:20 *Coffee break*

15:20 – 17:00 Sketch of meeting report

17:00 – *Adjournment of Meeting*

Appendix III: Summary of Presentations

Neutral Beam Analysis Codes Used on the NSTX-U and DIII-D Tokamaks

Daren Stotler

Princeton Plasma Physics Lab, Princeton, New Jersey, United States of America

Beam related codes and diagnostics in use on two tokamaks in the US are described in the presentation. DIII-D is a medium size tokamak with 4 beam boxes, two beam lines each; NSTX-U has two beam boxes with three sources each. These beams all have maximum energies of around 90 keV. The maximum core plasma temperatures in DIII-D can exceed 10 keV; 1 keV is typical for NSTX-U. The maximum core plasma densities for the two devices are $\sim 10^{20}$ m^{-3} .

The project CSI (Stotler) is the principal developer of the DEGAS 2 Monte Carlo neutral transport code. The relevant expertise he brings to the project is his familiarity with H atomic physics processes and collisional radiative (CR) models. The secondary CSI, Brian Grierson, is the DIII-D Neutral Beam Physics Leader and winner of a 2014 DoE Early Career Research award. The latter supported his development of the DIII-D main ion (deuterium) charge exchange recombination (CER) spectroscopy system, a key diagnostic for this project.

The NUBEAM routine at the heart of the TRANSP interpretive and predictive transport analysis code is one of the project's principal codes. It performs a Monte Carlo beam deposition calculation, including a 3-D, multiple generations, tracking of halo neutrals. Only the newest, ADAS based models in NUBEAM are being considered for the project.

The FIDAsim code, developed by Bill Heidbrink and co-workers at the University of California, Irvine, is similar to NUBEAM in that it performs a Monte Carlo beam penetration calculation. The beam attenuation on electrons, main and impurity ions is handled by its own time dependent, CR model, tracking excited states up to n=6. The code uses charge exchange data for the lower excited states that are available in ADAS; other data are from the Janev, Reiter, Samm Juel-4105 compendium. The latter is also the source of the code’s excitation and ionization data.

The NSTX-U Charge Exchange Recombination Spectroscopy (CHERS) diagnostic, maintained by Ron Bell, provides measurements of C^{6+} density, temperature, toroidal, and poloidal velocity. The data for ground and n=2 state deuterium donor atoms are taken from ADAS. However, Bell finds that n>2 states make significant contributions; cross sections for these reactions are needed.

Fred Levinton and Howard Yuh of Nova Photonics are participating in the project with the goal of ensuring that they have the most accurate data available for the Motional Stark Effect (MSE) systems on NSTX-U and for the one being designed for ITER. Because these diagnostics rely on the Stark Effect generated structure in the hydrogen spectrum, their CR model requires *nl*resolved cross sections, i.e., more detailed than those used by standard beam attenuation codes.

A recent benchmarking of the NUBEAM-FIDAsim codes could serve as a valuable test case for other project participants. Although targeted at verifying NUBEAM's new 3-D halo simulation capability, the tests evaluated all aspects of beam deposition in the codes. With both codes run using "ground state only" atomic physics, their beam and halo densities matched well. However, with their default atomic physics options (including excited beam atom states), the beam and first generation halo densities matched, but the total halo density obtained by NUBEAM was 20% larger than that from FIDAsim.

Data from the DIII-D CER system has been used to successfully validate FIDAsim calculations of beam component and FIDA densities, as well as of detailed spectra and the halo density. This comparison could also be the basis for a reference beam deposition model test case.

The project's scope will be primarily limited to the deuterium beam injection systems installed on NSTX-U and to the aforementioned diagnostics. Both machines have predominantly carbon plasma facing components so that the principal plasma impurity is carbon. Light emission from carbon ions is also used by both charge exchange recombination spectroscopy systems. The FIDA and MSE systems utilize only Balmer-α light. Exceptions to the above include the use of seeded nitrogen and neon in DIII-D. Also, a helium beam simulation capability is being developed for NUBEAM.

Experimental validation of atomic data for motional Stark effect diagnostics

Jinseok Ko

National Fusion Research Institute, Daejeon, Korea

The research activities on the experimental validation of atomic data for motional Stark effect (MSE) diagnostics are twofold: (1) High-precision (spectral resolution < 0.05 nm) measurements of beam-emission spectra from KSTAR plasma discharges; and (2) Development of a spectral analysis tool with a modulated interface for atomic data. The MSE spectral analysis that will ultimately be capable of inferring the magnetic pitch angles is to take into account various factors that can distort the polarization characteristics of incident signals, therefore, introducing both systematic and statistical uncertainties. These factors include the mirror reflections, Faraday rotation, polarized background light, and multi-ion-source neutral beam injection.

The conventional photo-elastic-modulation (PEM) MSE that has been operational at KSTAR since 2015, will play an important role in the development of the spectral MSE [1, 2]. This PEM approach has been calibrated against most of the factors that introduce systematic errors mentioned above and is expected to provide the spectral approach with reliable inputs for the validation of various atomic data codes. Preliminary spectral analyses have already been performed for the measured spectra, in particular for the band-pass filters calibration procedures of the diagnostic. The existing MSE diagnostic has been producing pitch angle and safety factor measurements in various plasma conditions such as sawtooth instabilities and internal transport barriers [3, 4].

Starting with the construction of self-calibrated high-precision spectral diagnostic suite and the development of a single-ion-source-injection fitting routine and interface for the atomic data and modelling packages such as NOMAD and ADAS in the first year of the CRP, the inclusion of various polarization-distortion effects and the comparison with the PEM MSE results will be made in the following year. Finally, the third year activities will include the evaluation and assessment of the atomic data used in the spectral analyses and the optimization of the spectral analysis suite for ITER applications.

[1] Chung et al, Rev. Sci. Instrum. 85, 11D827 (2014)

[2] Ko et al, Fusion Eng. Des. 109-111, 742 (2016)

[3] Ko, Rev. Sci. Instrum. 87, 11E541 (2016)

[4] Ko et al, Rev. Sci. Instrum. 88, 063505 (2017)

Quantification of the contribution of processes in the ADAS beam model.

Martin O’Mullane

University of Strathclyde, Glasgow, United Kingdom

Neutral beams in magnetically confined fusion plasmas are a mature technology and are essential for fuelling (both deuterium and tritium), heating the plasma via collisions, shaping the current profile and are one of the most reliable ways of switching the plasma into the high confinement regime (H-mode). The diagnostic capabilities of neutral beams were recognized immediately, in particular the localized nature of the beam-plasma interaction volume. Charge exchange recombination spectroscopy (CXRS or CHERS), where the charge transfer reaction between the high energy, mono-energetic beam and the thermal plasma impurities, is routinely used to measure profiles of ion temperature, plasma rotation and impurity content.

ADAS has a bundle-n resolution code to calculate the beam stopping and beam emission coefficients which can be included in shine-through/attenuation models, where the geometry and orientation effects are considered. Another ADAS code calculates the emissivity coefficients for CXRS analysis. The beam stopping, emissivity and CX driven emission are closely intertwined and a goal of any analysis is to have self-consistency between the different measurements and with complementary observations such as Z_{eff} and bolometry. Other ADAS data and models can be used to predict the spectral emission arising from other parts of the plasma, predominately the edge region, which may be in the line of sight of the spectrometers viewing the beam.

Despite being a well established technique in routine use, there are still questions. JET has a ‘neutron deficit’ problem (H Weisen *et al*, Nucl. Fusion, **57** (2017) 076029) where the measured neutron rate is lower than that predicted by codes such as TRANSP. One possible explanation put forward is that the neutral beam deposition may be overestimated. The conclusion of the analysis was that this was not considered to be a significant effect since two codes differed by 2-4% and the power deposited on the beam-dump, as measured by an IR camera with/without the plasma, matched expectations. From the viewpoint of data and code validation, the agreement of the codes may be because they use the same, or similarly benchmarked, atomic data. Quantification of how well the fundamental data is known will give greater confidence in comparing code outputs.

The ADAS beam model is a bundle-n collisional-radiative calculation which explicitly include levels n=1-12 and then in steps of n=15, 20, 30, 40 .., 100. Interpolation works well to calculate rates between the skipped n levels. The ADAS code has built-in semi-empirical formulae for the various processes required; Vainstein and Lodge formalisms for ion impact excitation, ECIP for electron ionisation, Percival&Richards approach for ion impact ionization and Gaunt factor methods for other quantities. These methods are appropriate and good for the high-n states but are quite poor for the transitions between the lower lying n levels, and ionization losses from these levels. To approach the required precision of ~5% for beam stopping coefficients, significantly better data from sophisticated codes, ideally benchmarked against experiment, must be used for n=1-5.

The last comprehensive review of the data and model for hydrogen was undertaken in 2000 (H. Anderson *et al*, Plasma Phys. Control. Fusion, **42** (2000) p781806). For hydrogen beams there were two updates, as a result of identifying errors: see the ADAS report, http://www.adas.ac.uk/notes/adas_c09-01.pdf and, another refinement soon afterwards reported in, E Delabie *et al*, Plasma Phys. Control. Fusion, **52** (2010) 125008.

The fusion plasma is not pure hydrogen so the ion impact driver population is a set of mixed colliders, with He^{2+}, Be^{4+}, C^{6+}, N^{7+}, Ne^{10+} and Ar^{18+} identified as the most likely encountered. Higher Z elements, such as iron, krypton and tungsten will also be encountered although their contribution to the subsequent effective coefficient is expected to be small. The variation in the stopping coefficient corresponding to a plausible tokamak density range, 10^{18}-10^{20} m^{-3}, is similar to a plausible impurity content of Z_{eff}~2. Therefore ion impact and ionization data from these colliders with the neutral hydrogen beam atoms are identified as crucial data for assessment and error quantification.

The most important and significant process, ionization of the beam atoms by protons, has been the subject of a number of calculations in the past 15 years, eg N. Toshima, Phys. Rev. A, **59**, (1999) p3940, A. Lolakowska et al, Phys. Rev. A, **59**, (1999) p3588, E. Y. Sidky and C. D. Lin, Phys. Rev. A, **65**, (2001) 012711 and T. G. Winter, Phys. Rev. A, **80**, (2009) 032701 and probably others. The difference between the data used in the ADAS model and these newer results is greatest at the JET beam energy (~110kV). The difference is ~10%, although this results in a ~5% change in the shine-through fraction. An expert recommendation, with rigorous error bars is required in order to advance the confidence of the beam models.

CXRS analysis may be outside the scope of the CRP. However there are two aspects where quantifying the error will be helpful. Firstly a re-evaluation of the existing low Z, nl-resolved CX cross section data currently used for He, Li, Be, C, N, Ne, Ar, would be beneficial. An expert recommendation for appropriate error bars is needed with the greater need for the carbon and beryllium data since these are in widespread use and are from data assessments compiled with data calculated/measured in the late 1980's to mid 1990's. Data for the 'more difficult' heavier species were calculated later with present day techniques so may be as up to date as can be achieved. Secondly the effects of charge exchange from heavy species, effectively iron and tungsten (and possibly krypton), on the spectrum observed for beam emission and CXRS analysis must be estimated. ADAS has a universal scaling for producing n and nl resolved CX data which enables predictions for the active signal due to high Z ions. Calculation to check the scaling would give greater confidence in the predications and some work is already underway.

The goal for ADAS participation in this CRP is to improve the ADAS beam population model by providing error surface data for beam stopping, beam emission and CX emissivity coefficients. These will be made available via ADAS and OPEN-ADAS.

Specifically the work falls into three phases. The first is to rank the relative importance of the different processes to the final stopping coefficients, BES and MSE spectra for representative JET and ITER conditions, using the existing ADAS model and data. An arbitrary, but realistic, error can be ascribes to each process and propagated through the ADAS model. The second phase is to explore, and mitigate, the limitation of the assumptions in the ADAS model. Finally the improved atomic data will be incorporated and used to produce coefficients for modeling with accompanying error surfaces.

Atomic data and collisional-radiative modelling of neutral beams in eigenstates.

Oleksandr Marchuk

Institute for Climate and Energy Research, Forschungszentrum Jülich GmbH, Jülich, Germany

In this presentation the following was discussed:

- Brief introduction on the Active H or D beam spectroscopy in fusion plasmas
- Impact of the excited states on the beam –penetration into the confined volume
- Current status of the n –resolved (statistical) CRM models widely used in the beam penetration codes
- Problems with the statistical assumption, e. g., the fact that the statistical assumption for the excited states such as n=2 or n=3 was not really confirmed in experiments
- The true eigenstates of the beam are determined by the Zeeman-Stark effect
- The CRM model in parabolic states was formulated, here the Stark effect was included only
- It was shown how the cross-section between the parabolic states are formed as the linear combination of the cross-sections in the spherical states + non-diagonal terms of the density matrix elements
- Some examples of the calculation of the cross-section in the parabolic states were shown
- The results of the collisional radiative model for the different experimental conditions were shown
- The results of calculation of the CRM model NOMAD and comparison with the experimental data from JET or ALCATOR-C Mod were presented
- Finally, we have shown for the results of the impact of the non-LTE calculation on the derived pitch angle of magnetic field in fusion plasmas (example from ASDEX Upgrade). Here the effect of non-LTE and Zeeman Effect were treated separately and still not self-consistent.
- Discussion on the need of atomic data resolved over the magnetic numbers including density matrix calculations was proposed.

Study of atomic beam interactions in fusion plasmas using the RENATE synthetic BES diagnostic

Gergo Pokol

Budapest University of Technology and Economics, Budapest, Hungary

Hungarian parties represented by Wigner RCP plan to contribute to CRP F43023 on Data for Atomic Processes of Neutral Beams in Fusion Plasma (2016-2020) (Short title: Neutral Beams) in two aspects: 1. The evaluation of the precision of beam modelling by the collisional-radiative model using RENATE rate equation solver and the BES synthetic diagnostic [1]. 2. Cross-section modelling using the CTMC method. Present talk considered the first aspect.

Core of RENATE is a collisional-radiative (CR) model solver with options to use rates: 1. Quasi-static for H from Open ADAS (2010). 2. Bundled-n for H from ALADDIN (2010) with corrections from E. Delabie, et al. PPCF 2010 [2]; benchmarked with O. Marchuk's CRM (2011). 3. nl-resolved for Li from J. Schweinzer, et al. Atomic Data and Nuclear Data Tables 1999 and some earlier publications [3,4,5] benchmarked with J.Schweinzer's simula (2007) [6]. 4. nl-resolved for Na from K. Igenbergs, et al. Atomic Data and Nuclear Data Tables 2008[7].

Rates are calculated from cross-sections by integrating for the relative velocity distribution assuming Maxwellian for the plasma species. On the top of 1D emissivity calculations, RENATE facilitates 3D beam and observation system modelling making it capable of modelling key features of fluctuation BES systems affecting spatial and time resolution.

Cross-section needs

We study beams of H isotopes, Li and Na. Accordingly, nl-resolved excitation, ionization and charge-exchange cross-sections are of our primary interest, up to the levels that suffer ionization due to the electric field experienced by high velocity atoms in the strong magnetic field. Plasma species of interest are: H isotopes and most common impurities (fully stripped and maybe partially stripped) of He, Li, Be, C, maybe N, Ne, Ar, W. First, a benchmark could be performed to see if present state of the art can produce better cross-sections than the already existing ones. Calibration modelling requires improvement on Li + H [5] collisions and H + H as well.

References:

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[5] D. Wutte, *et al.* ADNDT **65** 155 (1997)

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[7] K. Igenbergs, *et al*. ADNDT **94** 981 (2008)

Cross-section modelling for Beam Emission Spectroscopy – Classical treatment

Károly Tőkési

Institute for Nuclear Research, Hungarian Academy of Sciences, Debrecen, Hungary

Various approaches of classical Trajectory Monte Carlo (CTMC) method were introduced. We demonstrated the validity and accuracy of the classical treatment. We plan to use mainly two models within CTMC. In our first model, the effective static target nucleus charge is used and Coulomb force acts between the colliding particles. In this case we calculate the effective charge of the valance electron by Slater's rules. In the second approach we represented the target (and Projectile) atom(s) with

Garvey model potential. The two parameters of the potential; ξ and η represents quantum mechanical effects by taking into account of the independent particle model.

Classical method (CTMC) reproduces different experiments for collisions between charged particles and atoms, gives accurate cross sections for ionization, capture and excitation. It is valid in wide projectile energy range and also can describe partial cross sections. We are able to calculate cross sections according to the wish list in 3,4,5 and even more body systems.

We plan to calculate for example the ionization cross sections in H+H and Li+H collisions, the state selective excitation cross sections in H+H and Li+H collisions. Accurate simulation in H++ H(nlm) collision system in wide projectile energy range.

Electronic processes cross sections evaluation with a semiclassical non perturbative approach

Nicolas Sisourat, Alain Dubois

Sorbonne Universites, UPMC Univ Paris, CNRS, France

During the talk, we shortly described the straight-line impact parameter method (IPM) which is used to compute cross sections for electronic processes in ion-atom collisions in the collision energy range going from 1 keV/u to 1 MeV/u. In the IPM, one assumes that the relative motion of the projectile and target is described by a classical trajectory defined as $\vec{R}(t) = \vec{b} + \vec{v}t$ (see figure). In the collision energy range of interest this assumption is valid since the impact energy largely exceeds the energy loss from the inelastic electronic processes and the scattering diffusion angle is small. The IPM leads to the Time-Dependent Schrödinger Equation (TDSE) for the electron(s) in the moving field of the nuclei.

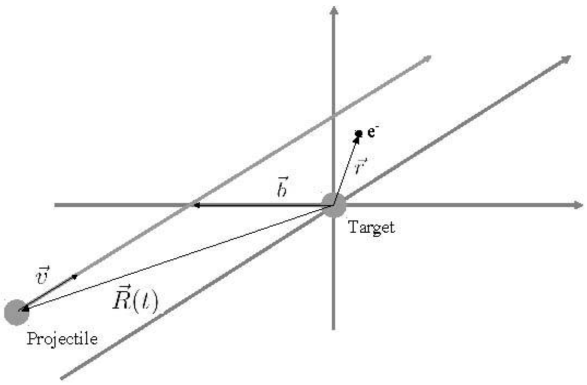

Fig. 1 Collision geometry. The impact parameter $\vec{b}$ and the projectile velocity $\vec{v}$ define the collision plane. The position of the electron with respect to the target center is denoted $\vec{r}$.

After introducing the IPM, our implementation was presented in details. In order to solve the TDSE, the total electronic wavefunction is expanded in the basis of the eigenstates of the isolated target and projectile states. One is then left with solving a set of first order differential equations for the time-dependent coefficients of the expansion. In our implementation, the eigenstates of the collision partners are described as linear combinations of multi-centered Cartesian Gaussian Type Orbitals (GTO). The advantages of GTO were discussed and the choice of the sets of GTO to be employed was reported. Some other details of the implementation were described.

In the second part of the talk, results on Li^{3+} H(1s) obtained with our code was reported. It was shown that there are large discrepancies in the previously published cross sections for excitation, especially for impact energies around 100 keV/u. Using our approach and with a systematic and careful study of the cross sections convergence with respect to the GTO basis set, we have proposed a new set of recommended state-resolved cross sections for excitation up to H(6h). Furthermore, we have provided some explanations for the disagreements between the different previously published cross sections.

Basis Generator Method Calculations for Ion-Atom Collisions of Relevance to Neutral Beams in Fusion Plasma

Tom Kirchner

York University, Toronto, Ontario, Canada

The Basis Generator Method (BGM) was developed more than 20 years ago as a general basis expansion approach to the solution of time-dependent quantum problems [1]. The main idea is that convergence does not require completeness, but can be achieved in a relatively small basis set if the states dynamically adapt to the problem at hand. In a second paper [2], the BGM was formulated more explicitly for ion-atom collisions in the semiclassical approximation. Numerous subsequent publications are testament to the success of the method in applications to a variety of collision problems [3]. In 2005, a full two-centre version (TC-BGM) was implemented to obtain a better description of electron transfer processes, and has become and remained our workhorse ever since [4].

Most applications of BGM and TC-BGM deal with few-electron collision systems and are formulated within an effective single-particle picture. In practice, this often implies usage of the independent electron model (IEM), but it is worthwhile to point out that time-dependent density functional theory (TDDFT) provides a firm footing of the IEM and suggests that in principle an exact treatment of the few-electron problem, including electron correlations, can be achieved by solving single-particle equations. Indeed, a few BGM studies have been devoted to studying electron-correlation effects in collisions in the TDDFT framework. For the p - He and He^{2+}- He systems correlation integrals in the final-state analysis of one- and two-electron processes were investigated [5], while an ongoing work is concerned with an exact-exchange representation of the three-electron He^{+}- He system.

Within the context of the Neutral Beams Coordinated Research Project, atomic hydrogen is the primary collisional target of interest. Elaborating on an earlier study of the so-called integral alignment parameter in p – H collisions [6] the TC-BGM will be used to study all reaction channels (excitation, charge transfer, and ionization) in a number of systems involving ground-state and excited-state atomic hydrogen. A recent test-case study for O^{6+} - H showed very good agreement with published molecular and atomic orbital close-coupling calculations [7]. Helium and lithium targets are of interest in the fusion-plasma context as well and will be addressed building on the previous and current works mentioned above.

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Theoretical studies of ionization, charge transfer and excitation in ion-H, He collisions in the energy range of 25-500 keV/amu

Clara Illescas

Universidad Autonoma De Madrid, Spain

In this talk I begin to mention the need of accurate total and partial cross sections to model the impurity density of the plasmas. Therefore, ionization, charge transfer and excitation processes in ion-atom collisions of interest in fusion research will be studied.

In the frame of the CRP F43023 on *Data for Atomic Processes of Neutral Beams in Fusion Plasmas* we present our two purposes:

1. Obtaining detailed data for atomic processes involving neutral hydrogen employing the Classical Trajectory Monte Carlo (CTMC) [1-2] and the Grid Time Dependent Schrödinger Equation (GTDSE) [3] methods.
2. Description of atomic processes involving neutral beams of He and Li. In order to carry out these studies, we propose to use the CTMC switching approach, which has been especially designed to classically treat more than one active electron systems [4].

A description of the Eikonal CTMC method is given noting the importance of the phase space initial distributions that can be used for H(1s) and H(n=2) targets (beams). The results obtained in our group for stripped ions A^{q+} + H (A= B, C, N) are presented [5], as well as, as data of highly charged ions such $Ar^{16+, 17+, 18+}$, Kr^{36+} and W^{60+} + H(1s), focusing on capture to very high-lying states of the projectile, which trigger the visible radiative lines. Scaling for total and n-partial cross sections at collision energies ranged 25-200 keV/amu [6] is also shown.

The second part of this talk is dedicated to the introduction of a new classical approach recently developed to treat systems with two-active electrons and two nuclei. First, the classical stable description of the H^- anion is shown, and the possible extension to other multi-electronic atoms, such He, Li, Be, is presented. The study of the H + H and H^+ + H^- collisions recently proposed [4] is presented, observing the good agreement obtained for projectile H^- formation cross sections in the first system and for mutual neutralization process in the case of the second reaction.

We conclude by summarizing our work using CTMC methods for the treatment of electronic collisions of one and two active electrons in the intermediate impact energy range.

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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.

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- We will use the two-centre convergent close-coupling (CCC) approach to ion-atom collisions to calculate various cross sections. The CCC approach incorporates all underlying processes.
- As a result the approach is capable of providing accurate state-resolved (nlm) cross sections for all these processes including excitation and ionization of the atom, electron transfer into bound and continuum states of the ion.

- Two distinct versions of the CCC approach will be applied: fully quantum-mechanical and semi-classical. This will allow to independently verify the accuracy of obtained results.
- We will start from calculations of the Balmer-alpha emission when hydrogen or deuterium beam is injected into the plasma.
- The relative populations of the n=3 states will be calculated as they may affect polarisation measurements in fusion plasma diagnostics known as a motional Stark effect (MSE).
- One of the important objectives of the proposed research is to provide data for ion scattering from excited states of the atom.
- We can provide data for any initial state H(nml) [for n within reasonable limits].

Following topics were presented:

- Convergent close-coupling approach to ion-atom collisions
    - Single-centre CCC
    - Two-centre CCC (including rearrangement)
- CCC approach to proton scattering including electron capture to continuum (ECC)
    - Quantum-mechanical: QM-CCC
    - Semi-classical: SC-CCC
    - Wave-packet: WP-CCC
- Proton-hydrogen collisions:total and differential ionisation cross sections
- Single ionisation of helium by protons
- Multiply-charged ion collisions with hydrogen

Processes of interest are:

- Fully differential breakup calculations of p + H
- Single ionisation of helium in p + He
- Multiply-charged ion collisions with hydrogen: He^{2+} and C^{6+}

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

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Recent works on ion-atom/molecule collisions in the IAPCM atomic and molecular physics group were presented. Various theoretical approaches have been developed and applied to treat ion-atom/molecule collision processes in a large energy range from a few eV/u to 1MeV/u, including molecular orbital close-coupling (MOCC), atomic orbital close-coupling (AOCC), time-dependent DFT (TDDFT), time-dependent Schrödinger equation (TDSE), multi-reference time-dependent Hartree (MCTDH) and Continuum distorted wave (CDW) methods *etc*. These methods are appropriate to different systems and different collisions energies.

As examples, presented were some results of different collisions systems, including the following processes:

The charge transfer processes between highly charged ions and H:

- Be^{2+} $(1s^2)$ +H(1s)→$Be^{+}(1s^2 nl)$+H^+,
- B^{3+} $(1s^2)$ +H(1s)→$B^{2+}(1s^2 nl)$+H^+,
- Ne^{10+} +H(1s)→$Ne^{9+}(nl)$+H^+,
- Ne^{9+} (1s) +H(1s)→$Ne^{8+}(1snl)$+H^+,
- Ne^{8+} $(1s^2)$ +H(1s)→$Ne^{7+}(1s^2 nl)$+H^+,
- C^{5+} (1s) +H(1s)→$C^{4+}(1snl)$+H^+,
- O^{6+} $(1s^2)$ +H(1s)→$O^{5+}(1s^2 nl)$+H^+.

The ionization processes between ion and atom/ion:

- He^{2+} +H(1s)→He^{2+}+H^++e,

- He^{2+} +C^{5+}(1s)→He^{2+}+C^{6+}+e;

The collision processes of excited target atom

- H^+ +Li(2pσ,$\pi^\pm$)→H(2*l*)+Li^+;

The charge transfer process between anion and atom

- $H^-(1s^2)+Li(1s^22s) \rightarrow H(1s)+Li^-(1s^22s^2)$

  $\rightarrow H(1s)+Li^-(1s^22s2p)$;

The electron capture and ionization processes between H^+ and H_2O, as well as the charge transfer processes between He^{2+} +H collisions in external magnetic field.

Accurate scattering cross sections have been computed and provided, including total, *n*-resolved and *nl*-resolved cross sections.

Atomic data for W^{64+} and H

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Neutral beam injection is to be one of the primary heating techniques for the international tokamak ITER. In addition, another lower energy beam will be used for diagnostic purposes to analyze ITER plasma properties from the beam emission and its interaction with other plasma particles. One of the important mechanisms to bring about new spectral features in various spectral ranges will be the charge exchange (CX) between the beam neutral particles (H and D) and plasma impurities of which tungsten will be the most abundant. This work discusses the charge exchange recombination spectra (CXRS) due to collisions between Ne-like W^{64+} and H in a wide range of collision energies, from 10 keV/u to 1000 keV/u.

For typical densities and temperatures of the ITER core, on the order of 10^{14} cm^{-3} and 20 keV, respectively, the Ne-like W^{64+} will be the most abundant ion of tungsten, and therefore analysis of its CXRS becomes the most important topic. The previous investigations on CX between fast neutral beams and impurity ions (e.g., Marchuk et al, J.Phys. B 42, 165701, 2009) were based on a detailed time-dependent collisional-radiative (CR) modeling of impurity interactions which was possible due to a relatively small size of the model. However, for highly-charged tungsten one has to include many thousands of atomic states in order to adequately describe the ensuing spectra, and thus time-dependent simulations become impractical. That is why here the effort was restricted to a steady-state simulation for one ionization stage only.

The CX cross sections were calculated with two modifications of the Classical Trajectory Monte Carlo method, namely, pCTMC (microcanonical) and rCTMC (hydrogenic). These two methods generally agree quite well for high energies also disagreement increases toward smallest energies in this study. Both *nl* and *n* state-selective cross sections were calculated and compared. This data was then used as an input to an extensive CR model for Na-like W^{63+} that is produced during CX with a neutral beam. The model takes into account major physical processes affecting populations of atomic states under typical conditions of the ITER core plasma, such as electron- and proton-impact excitation and ionization, radiative processes, autoionization and dielectronic capture into autoionizing states, radiative recombination, and charge exchange. The spectra under steady-state conditions were calculated from 1 Å to 10,000 Å for different beam energies and densities. We discussed the observed modifications and new spectral features due to CX and applications of this CXRS technique to diagnostics of ITER plasma.

This work was performed in collaboration with D.R. Schultz (University of North Texas, USA).

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