IOP Institute of Physics

AMIG 2017 Summer Meeting

Thursday 7th September

13:00 Lunch (Terrace)

14:00 Welcome (Botanic Suite)

Session 1: Chair: Nigel Badnell

14:10 **4d – 4f photoabsorption in laser-produced thulium plasmas**
(Invited) Emma Sokell, University College Dublin, Ireland

15:00 **Stimulating electron competition with XUV-initiated high harmonic generation**
Kathryn Hamilton, Queens University, Belfast, UK

15:20 **Quantum trajectory electron holography in above threshold ionisation**
Andrew Maxwell, University College London, UK

15:40 **The trans-iron distorted wave opacity project (TIDWOP)**
Simon Preval, University of Strathclyde, UK

16:00 Refreshment break (Botanic Foyer)

Session 2: Chair: Simon Preval

16:30 **The R-matrix with time-dependence method for strong-field, atomic physics**
(Invited) Hugo van der Hart, Queens University Belfast, UK

17:20 **Positron and electron scattering from H_2O in a field-free interaction region**
Rina Kadokura, University College London, UK

17:40 **Ground state configurations and theoretical soft x-ray emission of highly charged actinide ions**
John Sheil, University College Dublin, Ireland

18:00 Poster session (Terrace)

19:30 Conference dinner (Botanic Suite)

Friday 8 September

(Botanic Suite)
Session 3: Chair: Carla Faria

09:00 **Photoelectron spectroscopy with high harmonics: source development and applications**
(Invited) - Emma Springate, Rutherford Appleton Laboratory, UK

09:50 **Laser and microwave spectroscopy of antihydrogen atoms**
Daniel Maxwell, University of Swansea, UK

10:10 **Study of Tokamak divertor detachment using atomic physics and spectroscopy**
Daljeet Gahle, University of Strathclyde, UK

10:30 **Ab initio surface-hopping simulations of CS_2 photodissociation dynamics**
Darren Bellshaw, University of Edinburgh, UK

10:50 Refreshment Break (Botanic Foyer)

Session 4: Chair: Connor Ballance

11:20 **Quantifying the many collisional processes in high energy neutral beam models for magnetic fusion application**
(Invited) Martin O'Mullane, University of Strathclyde, UK

12:10 **Unraveling the soft X-ray emission from the Sun**
Giulio del Zanna, University of Cambridge, UK

12:30 **Pump-probe simulation of CS_2 and CHD: time-dependent photoionization**
Maria Tudorovskaya, University of Edinburgh, UK

12:50 **Exploring the fundamental physics of X-ray backscatter imaging by simulation with a hemisphere detector**
Anna Vella, University of Cranfield, UK

13:10 **Electron-impact ionisation of Mo and Mo+ Using the R-matrix with pseudostates method**
Michael Turkington, Queens University Belfast, UK

13:30 Lunch (Terrace)

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(invited) 4d – 4f photoabsorption in laser-produced thulium plasmas

E Sokell[1], R Stefanuik[1], P Dunne[1], E Long[1] and P Hayden[2]

[1]University College Dublin, Ireland, [2]Dublin City University, Ireland

The dual laser plasma (DLP) technique exploits the continuum emission from one laser produced plasma to probe the ions present in a second plasms (Costello et al, Phys. Scr., 1991, T34, 77). By varying the time delay between the formation of the plasma containing the ions to be observed and the creation of the continuum, it is possible to probe successively lower stages of ionisation. Typically the absorbing plasma is formed as a column in which the plasma electron temperature is below 5 eV. Within laser produced plasmas of this kind, successive ionisation occurs by electron impact ionisation (Colombant and Tonan, J. App. Phys., 1973, 44, 3524).

The output of a Q-switched laser (EKSPLA 512, 5 Hz, 450 mJ at 1064 nm) was focused tightly onto a planar hafnium target to produce a backlighting continuum source, hafnium yields an essentially line-free continuum at these wavelengths. This is due to the extremely high numbers of weak lines which are buried in plasma continuum and bremsstrahlung radiation.The output of a second Nd:YAG laser (Continuum Surelite II, 10 Hz, 600 mJ at 1064 nm) was focused to form a line plasma containing thulium of width 1.4 mm via a cylindrical lens.

In this work, spectra revealing photoabsorption due to Tm, Tm^{+} and Tm^{2+} ions has been observed in the spectral region between 6 and 8 nm where 4d to 4f photoabsorption is the dominant process. These ions are of particular interest as they have a $4d^{10}4f^{13}6s^{n}$ (n = 2, 1 & 0 for Tm, Tm^{+} and Tm^{2+}, respectively). Thus the 4d – 4f transitions are of the form $4d^{10}4f^{13}$ - $4d^{9}4f^{14}$ with the 6s electrons effectively playing a spectator role where present. Only photoabsorption from the lower $^{2}F_{7/2}$ term in neutral thulium has been observed prior to this work (Radtke, J. Phys. B: Atom. Molec. Phys 1979 12 L71]. For each ion stage the absorption profile can be explained in terms of two spin-orbit components based on the was observed in this region, peaking at ≈ 7 nm which is maintained through all ion stages.

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Stimulating electron competition with XUV-initiated high harmonic generation

K Hamilton, H van der Hart and A Brown

Queen's University Belfast, UK

High harmonic generation (HHG) is a well established technique for both attosecond pulse production1 and time resolved spectroscopy2. The usefulness of HHG however is limited by its reliance on IR radiation as a driver as, in such fields, usually only the outermost valence electron can be ionised. By initiating the HHG process with an XUV pulse, we allow more deeply bound electrons to be driven by the IR field. We recently showed that inner-valence electrons in neon were the source of high energy harmonics in a combined XUV/NIR laser field,3 and, in this work, we apply XUV initiated HHG (XIHHG) to an argon atom and elucidate the signatures of electron correlation present in the resulting spectra.

Among ab-initio, computational methods, only the R-matrix with time-dependence (RMT) approach4 combines the efficiency required to capture electron dynamics driven by long-wavelength (NIR) radiation, with the accuracy required to properly represent atomic structure and multi-electron correlations. The method has been demonstrated in calculations of HHG in the NIR regime5, electron rescattering in negative ions6, attosecond transient absorption spectroscopy of core- and doubly-excited states in neon7 and XIHHG from neon3.

We excite the 3s3p6nl Rydberg states of Argon with a 27 eV pulse and drive HHG from these excited states with a few-cycle 1800 nm pulse. In addition to an extension of the plateau (due to the higher binding energy of the 3s electron) we observe a resonant boost in the cut-off harmonics. This feature disappears if we neglect either the ionisation of the inner valence electron, or the 3s23p4ndnl correlation orbitals suggesting that both are involved in the XIHHG mechanism. We propose that this resonant boost is due an auto-ionisation pathway involving both the 3s and 3p electrons. A 3s electron is temporarily promoted into the 3s3p6nl Rydberg series by the XUV pulse. It subsequently refills the 3s vacancy, and the energy released allows a 3p electron to be ionised and driven by the IR field leading to the observed increase in harmonic yield.

XIHHG presents an attractive means of studying electron interactions in atomic systems. Where previous studies have focused either on the extension of the HHG spectrum, or the efficiency gains offered by XIHHG8, we here demonstrate the technique's promise for investigating electron correlation in ultrafast dynamics.

[1] M. Chini, K. Zhao and Z. Chang, Nat. Photon. 8, 178-186 (2014).
[2] L. He et al., Phys. Rev. A 92, 043403 (2015).
[3] A. C. Brown and H. W. van der Hart, Phys. Rev. Lett. 117, 093201 (2016).
[4] L. R. Moore et al., Mod Optics 58, 1132 (2011).
[5] O. Hassouneh, A. C. Brown, and H. W. van der Hart, Phys. Rev. A 90, 043418 (2014).
[6] O. Hassouneh, S. Law, S. F. C. Shearer, A. C. Brown, and H. W. van der Hart, Phys. Rev. A 91, 031404 (2015).
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[8] C. Buth, Eur. Phys. J. D 69, 234 (2015).

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Quantum trajectory electron holography in above threshold ionisation

A Maxwell[1], A Al-Jawahiry[1], T Das[2] and C Faria[2]

[1]University College London, UK, [2]Max-Planck-Institut für Physik Komplexer Systeme, Germany

Recent improvements in lasers allowing finer control of electrons in matter, coupled with a greater understanding and modelling ability of these systems, has paved the way for many new physical applications. One such application is atomic/ molecular imaging using electron holography. An electron is ionised via above threshold ionisation (ATI) by a high intensity low frequency ($I > 10^{13}$ W/cm^2 , $\lambda \approx 800$nm) laser field. In ATI the photoelectron quantum tunnels into the continuum, the archetypal physical picture of this process is in terms of multiple "quantum" trajectories that together mimic the behaviour of the electronic wavepacket. For a given fi- nal momentum, these trajectories interfere and recently it has been shown that this can be used to perform electron holography [1, 2].

Holography is the process where the interference of two waves (often light) are used to image a target; one passes through the target (signal) while one does not (reference). Detailed information is encoded in the interference of the two waves. In ATI some electron paths are direct, while others will be influenced by the ion via soft or hard scattering. Hence, holography can be performed and the interference will encode information about the residual ion. Given this can occur for two orbits that may be separated by less than one laser cycles, it can enable imaging with sub femtosecond temporal resolution.

We perform a detailed analysis of the electron trajectories and their interference using the recently developed quantum orbit strong-field approximation (CQSFA) [4, 5]. This describes the electron tunnelling and subsequent propagation in terms of individual interfering quantum trajectories and yields good agreement with the full solution of the time-dependant Schr¨odinger equation (TDSE), Fig. (1). Using this trajectory description we perform an in-depth analysis of several features such as side-lobes, intra- and intercycle interference [6], which also enables the formulation of analytic conditions. We determine how the electron trajectories are distorted by the Coulomb potential, investigate how this alters the phase and how this manifests itself in the photoelectron angular distribution (PAD). Four different quantum trajectories can be found for ATI [7]. However, two have often been neglected as they were thought to have too low a probability amplitude to be important. We find that one of these trajectories, known as Orbit 3, has a significant effect on the PAD, affecting both the general shape and the interference fringes observed. Hence, we develop the frame work to generalise electron holography to three electron orbits. We also investigate assumptions on the initial conditions of the electron Orbits previously made in the literature.

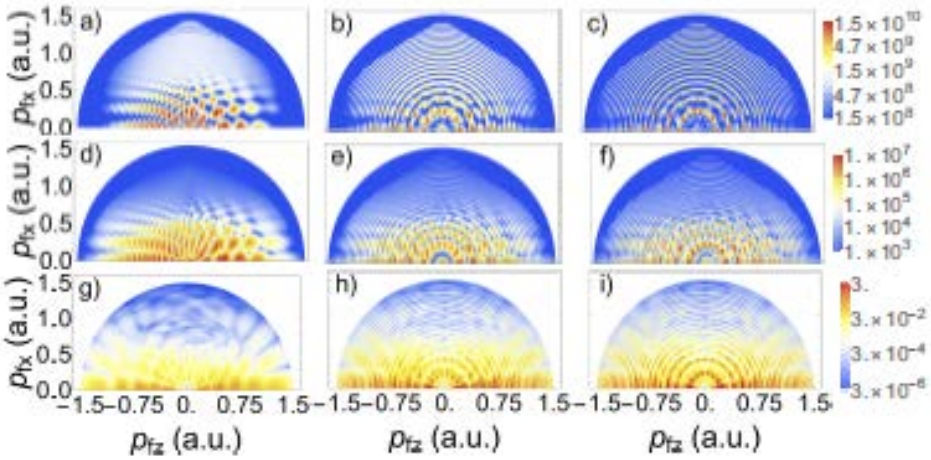

Fig. 1: Photoelectron angular distribution computed using the CQSFA (top two rows) and the time-dependant Schrödinger equation (TDSE) (bottom row), with one two and four cycles (columns left to right), for the TDSE a trapezium pulse was used with an additional half cycle ramp on and off. Calculated for hydrogen with

Ip=0.5 a.u. and field intensity of $I = 2 \times 10^{14}$ W/cm^2 and wavelength $\lambda = 800$ nm. The first and second panels have been computed without and with prefactors, respectively. The TDSE was calculated using the freely available software qprop [3].

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The Trans-Iron Distorted Wave Opacity Project (TIDWOP)

S Preval, and N Badnell

University of Strathclyde, UK

The Opacity Project (OP, Seaton et al. 1994) was, and still is, the authoritative source for photoionization cross section data for use in opacity calculations. Using sophisticated R-Matrix methods, the OP calculated atomic data for "astrophysically relevant" atoms and ions up to iron. Nowadays, observations of metals heavier than iron are routinely made in the atmospheres of stars, such as germanium, barium, and even xenon (Vennes et al. 2005, Rauch et al. 2014, Werner et al. 2015). Stellar atmosphere codes such as TLUSTY (Hubeny 1988, Hubeny & Lanz 1995) typically assume the photoionization cross sections (PICS) of such metals to be hydrogenic. However, this approximation can lead to large uncertainties in measured atmospheric abundances, and the synthetic stellar flux (Preval et al. 2017). Clearly, more realistic data are required.

Multiple methods exist for calculating PICS. The two most widely used are the R-Matrix method, and the distorted wave method. While R-Matrix methods are very accurate and include Fano resonances, they are limited in scope due to their complexity and large computational demands. Calculations using the distorted wave method are quicker, and allow a wide range of configurations to be included, offering an efficient way of generating data for multiple ions. To realise this data requirement, we propose The Trans-Iron Distorted Wave Opacity Project (TIDWOP). In this talk, I will describe the project in more detail, and highlight the aims and methodologies of the project. I will also present examples of test calculations.

[1] Hubeny, I., 1988, CPC, 52, 103.
[2] Hubeny, I., Lanz, T., 1995, ApJ, 439, 875.
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[4] Rauch, T., Werner, K., Quinet, P., Kruk, J. W., 2014, A&A, 566, A10.
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[7] Werner, K., Rauch, T., Ringat, E., Kruk, J. W., 2012, ApJL, 753, 7.

(invited) The R-matrix with time-dependence method for strong-field, atomic physics

H van der Hart and A Brown

Queen's University, UK

The R-matrix with time-dependence (RMT) method is one of the leading approaches to laser-atom interaction studies in contemporary computational physics [1]. While other approaches have been developed to address either multi-electron systems or electron dynamics in strong, long-wavelength fields, the RMT method sits at the intersection of atomic physics and ultrafast science, giving it unrivalled capability in the description of strong-field processes. This capability is of particular importance when fine details of the atomic structure become pronounced in experiment (e.g. in attosecond transient absorption spectroscopy [2]) and has enabled success in leading theoretical understanding of photoionisation time delays [3], and XUV-assisted high-harmonic generation for inner-shell electrons [4].

As with other R-matrix approaches, RMT is based on the idea of the division of space [5]. In an inner region, close to the nucleus, multi-electron correlations including exchange are described in full detail. We assume that a single electron can be ionised, and thus in an outer region far from the nucleus, we describe this single electron moving in the long-range potential of the residual ion and neglect electron-exchange. This allows the time-dependent Schrödinger equation to be solved in a large region of space by confining the computationally intensive electron exchange calculations to a relatively small region. Thus we have an inner region which is small but computationally arduous, and an outer region which is relatively less intensive, but quite large.

The strength of RMT compared with other implementations of the time-dependent R-matrix theory is the use of numerical techniques most appropriate to each region. Thus in the inner region where correlation is most important, the wavefunction is described using accurate B-spline basis set techniques. In the outer region, where the size of the configuration space is the limiting factor, an efficient grid-based technique is used. This approach, coupled with clever parallelisation of the code, allow us to address systems beyond the reach of competing methods, in particular addressing detailed atomic structure effects and dynamics in the challenging near-IR wavelength regime [6].

In this talk I will give an overview of the method and introduce some of the ground-breaking science it has facilitated. In particular I will report on recent results addressing XUV-initiated High Harmonic Generation [4].

[1] L. R. Moore, et al. J. Mod. Optics, 58, 1132 (2011)
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[3] L. R. Moore, et al. Phys. Rev. A, 84, 061404 (2011)
[4] A. C. Brown and H. W. van der Hart. Phys. Rev. Lett., 117, 093201 (2016)
[5] P. G. Burke. R-matrix Theory of Atomic Collisions. Springer Berlin Heidelberg (2011)
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Positron and electron scattering from H_2O in a field-free interaction region

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Synopsis Total cross section measurements of positron scattering from H_2O and preliminary results of electron scattering from H_2O have been investigated using an electrostatically guided beam with a field-free interaction and detection region, enabling a high angular resolution of ≈1° against forward scattered projectiles. The precision and accuracy achieved by our present measurements allow us to make a direct comparison between the two probes, as well as directly compare experimental values against theoretical determinations.

The present total cross section (σ_T) results of positron scattering from H_2O are presented in figure 1, along with previous experimental and theoretical determinations. The current work spans the energy range (10 – 300) eV. The higher angular discrimination of the present work [1] [2] with respect to earlier experiments has yielded values of σ_T which are 50% - 100% higher than previous direct measurements [3]. Agreement among experiments is achieved once allowance is made for forward elastic scattering using the theoretical differential elastic cross section calculated using the (rotationally summed) R-matrix method [4].

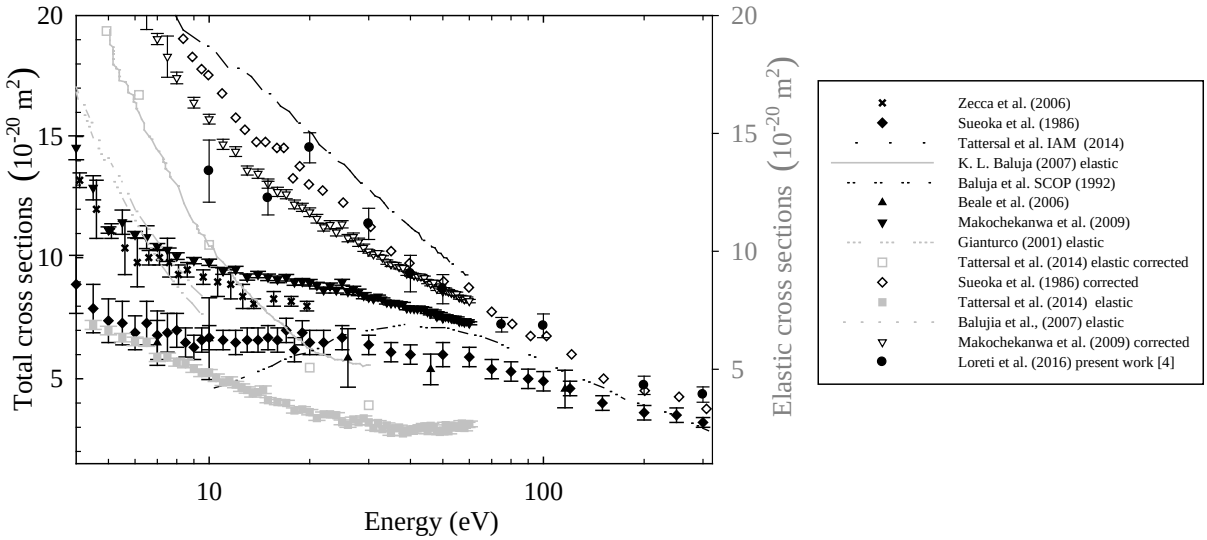

Fig 1: Cross sections for e^+ scattering from H_2O. Solid symbols denote direct measurements, hollow symbols denote measurements corrected for forward-angle elastic scattering, and lines denote theories.

The same beam is now being used to measure σ_T of (e^- + H_2O) scattering. Although measurements for this system have been carried out since early in the 20th century, some discrepancies remain among experimental and theoretical results at low energies e.g. [5]. Preliminary results will be presented at the meeting.

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[2] A. I. Williams et al. 2015, J. Appl. Phys. 118 105302
[3] A. Loreti et al. 2016 Phys. Rev. Lett. 117 253401
[4] J. Tennyson private communication
[5] Y. Itikawa and N. Mason 2005 J. Phys. Chem. Ref. Data, 34

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Ground state configurations and theoretical soft x-ray emission of highly charged actinide ions

J Sheil[1], L Liu[2], D Kilbane[1], P Dunne[1] and G O'Sullivan[1]

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It is well known that the lanthanide and actinide elements are formed by the filling of 4f and 5f subshells which occurs after the filling of 5d and 6d subshells, respectively, has begun. With increasing ionization one expects the energy levels to eventually regroup to their hydrogenic ordering i.e. in terms of principal quantum number. In the lanthanides, the 4f electron binding energy overtakes that of the 5p near the 6^{th} or 7^{th} ion stage and the 5s near the 14^{th} or 15^{th} leading to dramatic rearrangements of ground state configurations. We report on the results of a study to explore the effects of increasing ionization on the ground state configurations of actinide ions as a result of 5f and 6p or 6s level crossings. It is seen that the effects generally occur later and are more strongly influenced by spin-orbit splitting than in the lanthanides. The near degeneracy of 5f and 6l energies in these stages leads to configuration interaction (CI) amongst configurations with variable numbers of 5f, 6p and/or 6s electrons. The effects of CI on the level complexity are explored for ions along the Rn I sequence and found to lead to the formation of 'compound states' as predicted for the lanthanides. The extreme ultraviolet (EUV) and soft x-ray (SXR) spectra of medium and highly charged lanthanides are dominated by emission from unresolved transition arrays (UTAs) of the type $\Delta n=0$, $4p^6 4d^{N+1}$- $4p^5 4d^{N+2}$+$4p^6 4d^N 4f$ which, in general, overlap in adjacent ion stages of a particular element. Here the corresponding $\Delta n=0$, $5p^6 5d^{N+1}$- $5p^5 5d^{N+2}$+$5p^6 5d^N 5f$ UTAs have been studied theoretically with the aid of Hartree-Fock with configuration interaction calculations. As well as predicting the wavelengths and spectral details of the anticipated features, the calculations show that the effects of configuration interaction are quite different for the two different families of $\Delta n=0$ transitions and once more, spin-orbit interaction effects play a major role.

(invited) Photoelectron spectroscopy with high harmonics: source development and Applications

E Springate

STFC Rutherford Appleton Laboratory, Didcot, UK

The ultrafast pulses of extreme ultraviolet radiation produced through high harmonic generation (HHG) have great potential for applications in photoelectron spectroscopy in gases, liquids and solids. Time-resolved photoelectron spectroscopy is a powerful technique for directly observing electron dynamics, as all states can in principle be ionized. Extending the probe photon energy to the XUV allows observation of more tightly bound states, including important reaction intermediates and products.

In this talk, I will present measurements with a 6 eV pump and 21 eV HHG probe that allow for the unambiguous assignment of the full reaction pathway in a polyatomic molecule. Our measurements follow the dissociation dynamics of CS2, including ground state depletion, population of multiple excited electronic states, dynamics in the initially excited singlet state, subsequent conversion into the triplet manifold of states as well as production of the final dissociation products. The HHG probe allows us to monitor the entire reaction coordinate, in comparison with previous studies which only measured the singlet state, even when 6 - 8 eV probe photons were used.

A key future direction for our work is to use HHG at higher photon energies and higher repetition rates. We are developing a few-cycle source in the infrared at 1700 nm with the aim of generating HHG photons into the water window. I will also present results from this work, including a novel pulse characterisation technique and amplification of these few-cycle infrared pulses in an OPA.

Laser and microwave spectroscopy of antihydrogen atoms

D Maxwell

University of Swansea, UK

The aim of the ALPHA experiment is to perform spectroscopic comparisons between hydrogen and antihydrogen atoms as a test of CPT (charge-parity-time) symmetry [1]. In 2016, the ALPHA collaboration observed the first optical transition in antihydrogen atoms [2], the result of which is consistent with CPT invariance at a relative precision of 2 parts in 10^{10}. We also took further steps towards ground-state microwave spectroscopy, building on the first microwave transitions observed in 2012 [3].

We will present the experimental methods that have made spectroscopy of antihydrogen atoms possible. New techniques developed in antihydrogen trapping mean that we can now trap and perform spectroscopy on tens of antihydrogen atoms simultaneously. Previously, we could only trap around 1 atom on average [4]. The observation of optical and microwave transitions, along with the improved trapping rate, are big steps towards high-precision spectroscopy of antihydrogen. The ultimate aim is to match the levels of precision that have been achieved in hydrogen where, for example, the absolute frequency of the 1S-2S transition has been measured to 4 parts in 10^{15} [5].

[1] T. Hansch et al., Hyperfine interact. 76, 47-57 (1993).
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Study of Tokamak divertor detachment using atomic physics and spectroscopy

D Gahle[1,2], S Henderson[1], J Harrison[2] and M O'Mullane[1]

[1]University of Strathclyde, UK, [2]Culham Centre for Fusion Energy, UK

Divertor detachment is currently the leading solution to the steady-state heat flux problem in magnetic confinement fusion devices. The plasma heat exhaust in a burning fusion reactor is expected to be several times the engineering limit of the target surface, hence this understanding is a necessary step for continuous operation.[1] Detachment is the separation of upstream plasma and vessel surface conditions; and results in gas displacing the plasma from the surface of the vessel.

The physics of detachment is not well understood and yet to be accurately modeled by current codes. As the energy loss mechanisms in the plasma are dominated by atomic and molecular processes, such as bremsstrahlung, charge exchange and recombination, spectroscopy can be used to analyse the plasma and better understand detachment.

The electron temperature, T_e, can be inferred through a detailed analysis of high-n deuterium Balmer emission intensity, T_e, and the electron density, n_e, from the shape of the high-n Balmer lines, typically dominated by Stark broadening at low T_e, high ne conditions that are typically observed during detachment onset.[2]Furthermore, the spatial distribution of spectral emission from multiple low to mid-Z impurity charge states, for example from nitrogen or carbon, can be used to infer T_e across the divertor.[1]

The characteristic electron temperatures and densities in the divertor range from 0.1 to 100 eV and 10^{18} to 10^{22} m^{-3}. This results in the need of collisional radiative models to interpret the atomic spectra which is done using ADAS (Atomic Data and Analysis Structure).[3] This work is made increasingly complicated by none equilibrium atomic charge states and line of site integration effects which can reduce the effectiveness of spectroscopy as a diagnostic.

This contribution describes current developments in preparation for MAST Upgrade operation in 2018. The first experiments will explore the relationship between magnetics configurations with detachment onset and continuation. This will be done using a spectrometer with multiple viewing chords will be used to monitor passive spectral line emission from the divertor with high spatial resolution (~1cm) and time resolution (<20ms) in order to evaluate the spatial distribution of n_e and T_e across the divertor. Comparison of these measurements with the state-of-the-art SOLPS simulations can identify plasma physics that the code cannot full explain or express.[4]

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[2] Lipschultz, B. et al., Phys. Rev. Lett **81**, 1007 (1998)
[3] Summers, H. P. (2004) The ADAS User Manual, version 2.6 http://www.adas.ac.uk
[4] Havlickova, E. et al., Plasma Phys. Control. Fusion **57**(2015) 115001

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Ab initio surface-hopping simulations of CS_2 photodissociation dynamics

D Bellshaw and A Kirrander

University of Edinburgh, UK

The rapid photodissociation dynamics of CS2 following UV excitation into the $^1B_2$(S2) state is dictated by the complex interplay between multiple excited electronic states in a crowded manifold of potential energy surfaces. The reaction results in the production of a ground state CS($X\,^1\Sigma^+$) molecular fragment alongside atomic sulfur in either an excited spin-allowed state (^{1}D) or the spin-forbidden ground state (^{3}P). The latter channel is mediated via the spin-orbit coupling arising from the presence of the sulfur atoms. Although the exact branching ratio has proven difficult to measure accurately, the spin-forbidden product is seen to dominate in most experimental studies [1], highlighting the importance of spin-orbit coupling in this photochemical process.

We present here the first simulations of CS_2 photodissociation that account for spin-orbit coupling. We use the SHARC code (**S**urface **H**opping including **Ar**bitrary **C**ouplings) [2] interfaced with the Molpro suite of electronic structure programs [3]. Based on the fewest switches surface-hopping (FSSH) algorithm, SHARC accounts for spin-orbit coupling through a reformulation of the standard surface-hopping scheme in terms of a unitary transformation matrix and has previously been used to study the importance of spin-orbit coupling and branching ratios in systems such as IBr [2].

These simulations are compared to new time-resolved photoelectron spectroscopy measurements performed by experimental collaborators. This demonstrates that it is now possible to carry out *on-the-fly* dynamics calculations such that we are able to explain the shifting and narrowing of the photoelectron spectrum in terms of the bending motion of the vibrational wavepacket, and track population changes between the singlet and triplet manifold, with excellent agreement between experiment and theory [4].

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(invited) Quantifying the many collisional processes in high energy neutral beam models for magnetic fusion application

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Beams of neutral hydrogen, with high velocities, are used in magnetically confined fusion plasmas 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). Now a mature technology, the diagnostic capabilities of neutral beams was recognized immediately, where the localized nature of the beam-plasma interaction volume provides a direct measurement of internal plasma properties. Charge exchange recombination spectroscopy (CXRS), 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. Emission from the beam is used to monitor its penetration into the plasma and the motional Stark effect (MSE) is used to measure the profile of the magnetic field.

Modelling the beam plasma interaction involves many collision processes – principally ion impact driven excitation and ionization, but also electron collisions and charge exchange. The presence of strong magnetic fields introduces directional effects. We describe the ADAS beam model which is a bundle-n collisional-radiative calculation with explicit inclusion of 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. Using the highest quality data for all atomic processes between these lower lying levels is essential.

We report on the current state of the atomic collision data required for neutral beam needs. Quantifying the effect of uncertainties in these data, and in their propagated influence through the ADAS model, allows us to give an overall error in terms of machine operational parameters. The fundamental atomic data come from many different theories, calculation techniques and with some experimental benchmarks. Techniques for assessing a usable uncertainty in such a diverse set of data are discussed and areas where improved data would be most beneficial are identified.

Unraveling the soft X-ray emission from the Sun

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Solar and stellar coronae produce soft X-rays (5-15 nm), dominated by emission lines, mostly from Iron, formed between 1 and 15 MK. Until recently, the soft X-rays were largely unknown, compared to the other regions of the electromagnetic spectrum.

I will describe how I unraveled some of the mysteries in this spectral region using a combination of solar and laboratory observations together with state-of-the-art atomic physics calculations carried out within the UK APAP network, a collaboration between the University of Strathclyde, the Cambridge University and University College London (UK).
Since 2010, we have for the first time continuous monitoring of the solar corona in two soft X-ray bands. In one of them, several spectral lines were unknown. The first identifications of Iron lines were carried out in the 1930's by Edlen, who became famous because they were then used to identify the visible forbidden lines, and the discovery that the solar corona has a few million degrees. Continuing Edlen's work required running large-scale electron-ion scattering calculations for all the coronal iron ions, which produced a number of surprising results.

Pump-probe simulation of CS_2 and CHD: time-dependent photoionization

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We are reporting a new tool for analyzing a pump-probe experiment involving molecular excitation and photoionization. The photoelectron spectrum is a function of time and quantum molecular dynamics. We used Dyson Orbitals (DO)-based approach calculating to find the ionization rate. We consider 1,3-cyclohexadiene (CHD) and carbon disulfide (CS2). The former exhibits ring opening and can be considered prototypical for a range of photochemical reactions. The latter is important as a synthesis intermediate for carbon tetrachloride, used in cellophane production or as an insecticide, and other applications.

For CHD, we make use of previously calculated reaction trajectories and their relative weight to find out which scenario is the most probable, and how the total photoionization spectrum looks like.

A lot remains unknown if CS2 is not in its equilibrium state at the moment of ionization. We conduct accurate *ab initio* simulations [2] of the pump pulse and introduce the concept of the “average trajectory” for the dissociative and non-dissociative scenario.

We find that the photoionization spectrum allows to judge about structural changes in molecules and electron structure changes.

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Exploring the fundamental physics of X-ray backscatter imaging by simulation with a hemisphere detector

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Images of concealed objects can be generated using the X-rays backscattered from an illuminating X-ray source, with a dependency on the X-ray properties of the materials involved. Although analytical expressions and data exist for material cross-sections, the properties of the backscatter image are difficult to predict without simulation.

PENELOPE [1] was used to model a novel all-in-one hemispherical detector for studying the fundamental physics of X-ray backscatter imaging. This type of detector has the advantage of discriminating the different kind of interactions occurring within the material thicknesses, by exploring which phenomena are predominant against the others at the different scattering angles. In synthesis, unlike a real experiment, this model describes the fundamental physics of X-ray backscatter in a single simulation.

The model was designed using the PENGEOM [2] sub-tool and consisted of a 3D hemispherical detector, which is used to detect the X-rays backscattered from different materials at different depths. The model was validated with the theoretical NIST database [3]. The incident X-rays are mono-directional to the idealised target at energies up to 200 keV. A 'phase-space' file [4] is generated from the simulation, which contains information about the interaction of the X-rays within the concealed object. Using an analysis programme written in MATLAB, the 'phase-space' data allows each object to be studied from different angles and depths in terms of the X-ray interactions.

The model and subsequent analysis reveals the fundamental scattering information needed to select the right conditions for good brightness and contrast in X-ray backscatter imaging. The required information is not as simple as considering Compton, elastic, fluorescent, and attenuation cross sections, mass and atomic densities all individually. It is only the combination that will define the quality of an image and how the combination changes between materials with depth and energy. Firstly, the work demonstrates a way to efficiently gather the relevant data through the application of simulation to a novel hemispheric detector model. Secondly, we interpret the data to guide the selection of experimental conditions such as incident X-ray energy and relative camera angle to achieve good X-ray backscatter imaging of structures involving carbon, aluminium, copper and lead.

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Electron-impact Ionisation of Mo and Mo+ using the R-matrix with Pseudostates method

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Neutral and singly ionised molybdenum (Mo) continues to be of interest within the magnetically-confined plasma community, as a candidate for plasma facing components due to their favourable physical properties. The National Spherical Torus Experiment Upgrade (NSTX-U) currently employs a molybdenum lining for its PFCs [1], and experiments with molybdenum probes are currently being conducted at the Compact Toroidal Hybrid (CTH) at Auburn University, and the DIII-D tokamak at General Atomics, San Diego. Although molybdenum can withstand the high temperatures within a reactor, loss of plasma energy due to sputtering and radiation still needs to be characterised. Plasma parameters such as ionisation fraction, impurity influx and radiative transport are underpinned by the quality of the available atomic data. Our focus is on the ionisation of neutral and singly ionised molybdenum for which the R-matrix with pseudo-states (RMPS) method [2,3] is well suited.

Fundamentally, it is known that perturbative distorted wave methods for neutral and low-charge systems may overestimate electron-impact ionisation cross sections, in particular for higher n shell. Currently the two calculations that exist within the literature by Badnell et al. [4] and Kwon et al. [5] exhibit differences in ionisation cross sections of almost a factor of two, albeit using simple models in both cases. We address this discrepancy through the implementation of large scale RMPS ground-state and metastable ionisation calculations. A modified version of the RMPS codes has been employed to determine ionisation rates for both neutral and singly-ionised molybdenum, requiring the inclusion of over 11,000 terms in the close-coupling expansion for the neutral system. Ionisation from the ^{7}S ground state of Mo and the ^{6}S and ^{6}D ground and metastable states of Mo^{+} shall be compared with other theoretical methods and experiment where available. In conjunction with updated electron-impact excitation data, a better theoretical impurity influx parameter shall be derived.

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