



AMIG Summer Meeting 2019

5–6 September 2019
University of Birmingham, Birmingham, UK

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Organised by the Atomic and Molecular Interactions Group



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Session 1

(Invited) In Silico photochemistry using ab initio nonadiabatic molecular dynamics

B Curchod

Durham University, UK

What happens to a molecule once it has absorbed UV or visible light? How does the molecule release or convert the extra-energy it just received? Answering these questions clearly goes beyond a pure theoretical curiosity, as photochemical and photophysical processes are central for numerous domains like energy conversion and storage, radiation damages in DNA, or atmospheric chemistry, to name a few. Ab initio multiple spawning (AIMS) is a theoretical tool that aims at an accurate yet efficient in silico description of photochemical and photophysical processes in molecules.

In this talk, I intend to survey some recent developments and applications of the AIMS technique. A significant feature of the AIMS framework – besides its controlled approximations – is its adaptability, which permits the addition of critical physical processes for a realistic simulation of photochemical processes. For example, we recently included spin-orbit coupling in AIMS and the effect of an external time-dependent electric field. We also proposed a simple yet rational approximation to AIMS termed Stochastic-Selection AIMS (SSAIMS), which allows decreasing the computational cost of an AIMS dynamics substantially.

We also interfaced AIMS with the GPU-based electronic structure code TeraChem to study the excited-state dynamics of large molecular systems. Combining the accuracy of AIMS with the efficiency of GPU-accelerated electronic structure calculations (LR-TDDFT or SA-CASSCF) allows indeed for a significant step forward in the simulation of nonadiabatic events, as it pushes the boundaries of the well-known compromise between efficiency and accuracy imposed by the computational cost of such dynamics.

Quantum bridges in phase space: Interference and nonclassicality in strong-field enhanced ionisation

H Chomet, D Sarkar, and C Figueira De Morisson Faria

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We perform a phase-space analysis of strong-field enhanced ionisation in molecules, with emphasis on quantum-interference effects. Using Wigner quasi-probability distributions and the quantum Liouville equation, we show that the momentum gates reported in a previous publication [N. Takemoto and A. Becker, Phys. Rev. A, 023401 (2011)] may occur for static driving fields, and even for no external field at all. Their primary cause is an interference-induced bridging mechanism that occurs if both wells in the molecule are populated. In the phase-space regions for which quantum bridges occur, the Wigner functions perform a clockwise rotation whose period is intrinsic to the molecule. This evolution is essentially non-classical and non-adiabatic, as it does not follow equienergy curves or field gradients. Quasi-probability transfer via quantum bridges is favoured if the electron's initial state is either spatially delocalised, or situated at the upfield molecular well. Enhanced ionisation results from the interplay of this cyclic motion, adiabatic tunnel ionisation and population trapping. Optimal conditions require minimising population trapping and using the bridging mechanism to feed into ionisation pathways along the field gradient.



Ions from PF₃: Formation, collisions and reactions

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Many electron-transport codes include ionisation cross sections, but they often do not account for multiple-ionisation events[1]. Multiply ionised species, particularly gas-phase dications, are highly reactive. Bimolecular dication-neutral collisions, such as those involving PF₃²⁺, can result in fascinating intermediates and products[2] via electron transfer or bond formation. Additionally, these reactions are of relevance to both astrochemistry and the chemistry of planetary ionospheres[3].

We have performed coincidence mass spectrometry experiments detecting the cations produced following electron-molecule collisions with PF₃. Analysis of these coincidence data yields precursor-specific ionisation cross-sections - revealing the contribution to each partial cross section from single, double and triple ionization of the parent molecule. Here we report such an experimental dataset for electron ionization of PF₃, with total cross sections normalised to a Born-Encounter-Bethe ionisation calculation. Using a Monte Carlo approach to interpret the form of the coincidence signals reveals the dissociation pathways of the PF₃²⁺ dication and their dynamics. In addition we present recent experimental results studying the bimolecular collisional chemistry involving PF₃²⁺ and common neutral targets such as Ar and CO. Comparisons of competing reaction pathways at various collision energies indicate the rich landscape of possible reactions available to dications under ionospheric conditions.

- [1] A. Muñoz, D. Almeida, F. Ferreira da Silva, P. Limão-Vieira, M.C. Fuss, A.G. Sanz, and G. García, *Eur. Phys. J. D* **67**, (2013).
- [2] S.D. Price, J.D. Fletcher, F.E. Gossan, and M.A. Parkes, *Int. Rev. Phys. Chem.* **36**, 145 (2017).
- [3] W.D. Geppert and M. Larsson, *Chem. Rev.* **113**, 8872 (2013).

Photoionization of H₂ and H₂O using the molecular "R-Matrix With Time" approach

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In our contribution we study one- and multi-photon photoionization of the H₂ and H₂O molecules by laser pulses using the recent extension of the originally atomic-only R-matrix with time dependence (RMT) method to molecules. The molecular RMT combines the accuracy of the time propagation provided by RMT and the ab initio target description by the stationary molecular R-matrix package UKRmol+, enabling correct description of multi-electron effects and electron correlation in the response of the target to the external field.

The RMT approach is very general and allows the study of a range of processes from the perturbative to highly non-linear regimes. Detailed understanding of the molecular RMT models for multi-photon ionization is a prerequisite for its application to processes such as strong-field ionization and high-harmonic generation.

This work validates the UKRmol+/RMT combination on several processes well studied in the past. The generalized multi-photon cross sections for photoionization of H₂ by a weak, linearly polarized field obtained using the UKRmol+/RMT suites are compared to results from the Floquet R-matrix method, to those of a direct solution of the Schrödinger equation in DVR basis with ECS boundary conditions, as well as to other approaches. Furthermore, we



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study multi-photon photoionization yields of H₂O in ultra-short strong laser pulses.

Session 2

(Invited) Generating a controllable beam of radicals for ion-neutral reaction studies

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Generating a controllable and pure source of molecular free-radicals or open-shell atoms has been one of the primary barriers hindering the detailed study of radical processes in the laboratory. A novel magnetic guide is described, for the generation of a pure beam of velocity-selected radicals. This magnetic guide will enable the study of radical interactions with exceptional control over the properties of the radical species. Only radicals with a selected velocity are transmitted through the guide; all other components of the incoming beam (radical species travelling at other velocities, precursor molecules and seed gas) are removed. The guide is composed of four Halbach arrays – hexapolar focusing elements – and two skimming blades. The relative positions of these components can be adjusted to tune the properties of the resulting beam and to optimise transmission for a given velocity. Experimental measurements of Zeeman-decelerated H atoms transmitted through the guide, combined with extensive simulations, show that the magnetic guide removes 99% of H-atoms travelling outside the narrow target velocity range[1,2]. I will also present our designs for a combined Zeeman decelerator-ion trap apparatus, and discuss progress to date.

[1] J. Toscano, C. J. Rennick, T. P. Softley and B. R. Heazlewood, *J. Chem. Phys.* **149**, 174201, (2018).

[2] J. Toscano, M. Hejduk, H. G. McGhee and B. R. Heazlewood, *Rev. Sci. Instrum.* **90**, 033201, (2019).

Sticky collisions of ultracold RbCs molecules

M Frye, P D Gregory, J A Blackmore, E M Bridge, R Sawant, J M Hutson, and S L Cornish

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Understanding and controlling collisions is crucial to the burgeoning field of ultracold molecules. All experiments so far have observed fast loss of molecules from the trap. However, the dominant mechanism for collisional loss is not well understood when there are no allowed 2-body loss processes. Here we investigate collisional losses of nonreactive ultracold ⁸⁷Rb¹³³Cs molecules, and compare our findings with the sticky collision hypothesis that pairs of molecules form long-lived collision complexes. We demonstrate that the loss of molecules in their absolute ground state is best described by second-order rate equations, consistent with the expectation for complex-mediated collisions. We model the losses with a simple single-channel model that uses an absorbing boundary condition to take account of short-range loss, and find a significant difference between the measured loss rates and those expected in the universal limit, in which all two-body collisions that reach short range lead to loss.



The inbetweeners – orbits beyond born type scattering

A Bray, A Maxwell, and C Figueira De Morisson Faria

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Similarly, to light holography, ultrafast photoelectron holography makes use of a probe and a reference wave to reconstruct a target using phase differences. This makes use of the fact that different pathways for an electron in a strong laser field may be associated with specific interference patterns. Typically, the reference is a direct pathway and the probe is associated to a laser-induced rescattering process. If traditional orbit-based approaches are employed, such as the strong-field approximation, for linearly polarized fields rescattering will occur near and on the polarization axis. This will make it detrimental for probing targets whose geometry is oriented perpendicular to the field. In the present contribution, we employ a novel approach which goes beyond that and takes into account the residual binding potential and the external laser field on equal footing: The Coulomb Quantum Orbit Strong-Field Approximation (CQSFA).

By studying a variety of atomic species prepared in excited states of different geometries, we show that, due to the presence of the Coulomb potential, rescattering will no longer be confined to this axis, which makes it possible to probe orbitals whose polarization is perpendicular to that of the field. We also identify the main types of orbits responsible for a non-vanishing photoelectron signal within the CQSFA and initial momentum distributions of the instances of tunnelling and re-scattering. We further probe the interplay between the driving field and the binding potential by modifying parameters such as the field intensity and the binding energy.

Session 3

(Invited) Exploring quantum interference in strong-field ionization and attosecond imaging

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An electron recolliding with its parent ion is a widely used physical picture describing intense-field laser-matter interaction. As, quantum mechanically, there is more than one pathway that the electron may follow, the associated transition amplitudes will interfere. Thus, quantum interference may be explored to probe the ultrafast dynamics of matter. In this talk, I will exemplify this using the work by my group at UCL on two topics: ultrafast photoelectron holography and below-threshold nonsequential double ionization.

In photoelectron holography, different types of interfering orbits are used as a “probe” and “reference” in order to reconstruct a specific target. Most models interpreting the patterns obtained, however, are oversimplified and neglect the residual potentials. By developing a novel semi-analytic approach that fully accounts for the laser field and of the binding potential, we not only explained in far more detail well-known holographic structures, but also unveiled a myriad of previously overlooked patterns, that only now are being identified experimentally.

Laser-induced nonsequential double ionization (NSDI) is the quintessential example of a correlated strong-field process. For over two decades, it was widely believed that this correlation is essentially classical. We call this assumption into question in the below-threshold regime, in which the returning electron excites a second electron, by showing that quantum interference is more robust than anticipated. We identify two interference types,



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associated with electron exchange and different excitation channels, and show that it survives focal averaging and integration over several degrees of freedom. Our work is compared with experimental findings.

Positron binding, scattering, and annihilation with molecules

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The positron is the antiparticle of the electron. Calculations in the late 1990s showed that it is possible for a positron to bind to certain atomic species, as a result of polarization of the electron cloud and other short-range attractive correlation effects; however, experimentalists have so far been unable to detect the existence of such bound states for atoms. Conversely, calculations of positron binding to molecules have proven to be very difficult, but experimentalists have measured positron binding energies for around 80 molecules, as the positron is captured into a characteristic vibrational Feshbach resonance. Here, we use a model-potential method to calculate positron-molecule binding energies for the alkanes. We obtain excellent agreement with experiment. By calculating the overlap of the positron density with the molecular electron density, we also calculate the expected lifetime of these states before annihilation, which is found to scale inversely with the square root of the binding energy. This opens the way to calculating positron binding energies and lifetimes for the vast majority of molecules for which experimental data is available. We will also be able to compute the annihilation gamma-ray spectra, for which experimental data is available but awaits theoretical analysis. Finally, we use the model to calculate elastic scattering of a positron by a range of atomic and small molecular targets, namely, Be, Mg, He, Ar, H₂, N₂, Cl₂, and CH₄. We also calculate the rates of annihilation from the positron continuum for these species, obtaining excellent agreement with experiment.

Rydberg-Stark deceleration and trapping of NO molecules

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An atom or molecule in a Rydberg state can have an extremely large electric dipole moment, upon which an inhomogeneous electric field will exert considerable force. Previous experiments have exploited this effect to decelerate and trap H₂. The trapped molecules were subsequently used to study slow decay processes and ion-molecule reactions at low temperatures. The principle upon which Rydberg-Stark deceleration is based applies to any species that can be excited to long-lived high-*n* states.

I will describe a compact chip-based Rydberg-Stark decelerator comprised of a 100 mm long linear array of electrodes. And I will present the results of recent experiments in which this device was employed to decelerate and trap laser-excited Rydberg NO molecules. The molecules were observed to have an average lifetime of approximately 300 μs in the 30 K cryogenic environment of the trap. The cold, trapped NO molecules prepared in this work are of interest for studying low-temperature inelastic scattering processes in which long-range interactions play an important role.



Controlling chaos in the quantum regime using adaptive measurements

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The emergence of the classical limit from the quantum theory is well understood for regular dynamics. But what happens to the quantum system when the classical limit is chaotic? Quantum chaos is the study of such quantum systems. The emergence of chaos for dissipative systems is interesting because of the breakdown time between the classical and quantum systems. How can we reconcile this breakdown with the classical chaotic dynamics that we observe in nature?

By considering an open quantum system with interaction with an environment, we can see the emergence of dissipative chaos from the underlying quantum system. Going further, by continuously monitoring a quantum system whose dynamics are chaotic in the classical limit, we are able to observe the emergence of chaos for single quantum trajectories. But the choice of measurement strategy itself can determine the degree of chaos that we observe. Here I address the effect that continuous measurement has on the emergence of chaos and offer a real time feedback scheme that uses the measurement as a control knob in order to control the degree of chaos in the system. This answer's the questions posed about the emergence of chaos in dissipative systems but also poses some new ones. Is the measurement effect dependent on one particular system or is there a general explanation that can be used for all chaotic systems?

Session 4

(Invited) Vacuum ultraviolet laser induced breakdown spectroscopy (VUV – LIBS) for the analysis of pharmaceuticals

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As Laser Induced Breakdown Spectroscopy (LIBS) matures as an analytical technique, particularly with the expansion beyond elemental characterisation provided by advanced chemometric techniques, the range of potential applications has grown steadily. One such area where the ease of measurement, robustness and accuracy of LIBS can have a significant impact is in the analysis, development and production of pharmaceutical and nutraceutical products.

This presentation will introduce Vacuum Ultraviolet LIBS (VUV-LIBS), utilising emission from 35–120 nm range, and its usefulness in meeting the off-line requirements at the design stage. VUV-LIBS has a number of advantages, such as increased access to resonance transitions, higher ion stages, less complex spectra, reduction of plasma interference effects etc.

In addition to traditional spectral analysis, the information rich spectra are interrogated with more complex chemometric techniques, such as Principal Component Analysis (PCA), Convolutional Neural Networks (CNN), Self-Organizing Maps (SOM) and Support Vector Machines (SVM). This leads to enhanced performance in the identification and classification of the LIBS spectra, allowing improvements in the correct separation of the pharmaceutical samples.



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Modelling density effects on carbon ion populations in the solar transition region

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University of Cambridge, UK,

Higher densities and lower temperatures in the solar chromosphere and transition region mean the most common assumptions used for modelling ion populations in the solar atmosphere (the zero density, ionization equilibrium approximation) no longer hold. The presence of metastable levels in the lower charge states will increase the ionization rates once higher densities begin to populate the levels. Recombination rates reduce as density increases, and the combined effect is to lower the formation temperatures of charge states in these conditions. Using carbon as a test case, new ionization rates for metastable levels have been calculated and other processes added to determine the ion populations. Significant changes with the zero density models are found. Such changes can alter values for plasma parameters derived from ion populations, such as temperature, density and elemental abundances. Modelling the line intensities of C III and C IV using the new ion populations shows improved agreement with observations, when compared to zero density modelling.

Benchmark calculations of electron impact electronic excitation of the hydrogen molecule

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Using the latest UKRMol+ R-Matrix codes, we have calculated accurate electron impact cross-sections for highly excited states of molecular hydrogen. Both differential and integrated cross-sections have been calculated. These are compared with current state-of-the-art calculations using the Convergent Close-Coupling method and recent experiment. Good agreement is found between both the existing theory and experimental measurements.

In this presentation I will discuss the latest developments to the UKRMol+ code that have allowed us to carry out such calculations. The most significant of which has been the possibility to use B-splines to describe the continuum.

This work has pushed previous limits of electron-molecule scattering using the R-matrix method. For example we have increased our R-matrix radii by a factor of 10 with the latest work using a radii of 100 atomic units. Using a bigger radius is imperative because we need to contain the charge density of the molecule. Highly excited electronic states are Rydberg-like and therefore occupy a larger volume.

We propose that these two well established theories provide reliable method of obtaining accurate electron-impact cross-sections for both elastic and inelastic processes.



Poster Session

(P1) Positron Accelerator for Positronium - Cold Ion Scattering Experiments

R Clayton, C Baker, W Bertsche, M Charlton, S Eriksson, H Evans, A Isaac and Dirk van der Werf

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Positron trajectories through an accelerator, designed for positronium (Ps) production via implantation into mesoporous silica (SiO₂), were simulated in preparation for scattering experiments involving Ps and laser cooled ions in an RF-trap^[1]. This would allow for high implantation depths into the SiO₂ sample with a low local electric field. The design consists of a single electrode to which an electric potential is applied, while positrons from a two-stage positron accumulator^[2] are within the device.

Simulations (run on Simion 8.0.8) used a positron cloud of 10⁴ particles with a Gaussian energy distribution of 26.68 eV with standard deviation 0.18 eV and three-dimensional Gaussian spatial distribution corresponding to 11 ns length and 1.5 mm radius to match obtained experimental data. The simulated positron cloud is accelerated by an electrode of length, inner diameter and outer diameter of 130 mm, 26 mm and 28 mm respectively, to which a potential of -2.0 kV is applied with a 20 ns rise time. Characterisation of the simulated particle cloud will be discussed with respect to trigger delay time of accelerator electrode. At optimum efficiency 93.21 ± 0.01 % of positrons were accelerated to 2021.4 ± 0.3 eV with a similar time width to the input (11.18 ± 0.19 ns). Progress towards experimental realisation of the proposal in^[1] will be discussed.

[1] A. Bertsche *et al.*, *New Jour. Phys*, **19**, (2017), 053020.

[2] Clarke *et al.*, *Rev. Sci. Instrum.*, **77**, (2006), 0663302.

(P2) A quantum model for the attoclock: studying non-adiabaticity and interference effects

G Kim, A S Maxwell, and C Figueira de Morisson Faria

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The attoclock scheme is very important in strong-field physics because it can relate angular offsets in photoelectron angular momentum distributions (PADs) to tunnel ionization times and the influence of the residual Coulomb potential. It uses elliptically or circularly polarized laser fields in order to control this offset. However, the majority of theoretical models used to describe the attoclock is based on classical trajectories and quasi-static tunneling rates. This leaves no room for investigating quantum interference or non-adiabatic effects, which may be important in this case. The Coulomb-Quantum orbit strong-field approximation (CQSFA) is a newly developed approach in which both effects are taken into consideration, and in which the Coulomb potential and the external laser field are treated in equal footing. This makes it a powerful tool for investigating the attoclock, which is the topic of the present contribution.

Using the plain, Coulomb-free Strong-Field Approximation, we find four types of orbits in the attoclock scenario, whose transition amplitudes interfere. Each split orbit by ellipticity shows different aspects. One has a minimum imaginary part of ionization-time, while the other now has two symmetric minimum points along with a parallel component of the momentum. They are taken as the starting point to investigate non-adiabaticity and quantum



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interference using the CQSFA. We expect these studies to provide powerful insights into how this method applies to more sophisticated types of tailored fields.

(P3) Time-independent Approximations for Time-dependent Optical Potentials

R Tenney, and A Fring

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The Lewis-Riesenfeld method of invariants is a widely used approach for finding the exact solution to time-dependent quantum mechanical systems. The initial step in the method involves the construction of an invariant which results in a solvable time-independent eigenvalue problem. We propose using approximate methods at the second step for when the time-independent eigenvalue problem is not exactly solvable, such as time-independent perturbation theory or the WKB approximation, and use the resulting expressions to find an approximate time-dependent solution. To illustrate the effectiveness of the method we consider a time-dependent perturbation to the Stark Hamiltonian, and compute the eigenvalues, wave functions and expectation values of the observables for the system using the proposed approximations and compare with the exact result. We find that while time-independent perturbation theory can give highly accurate results provided that the perturbation is small, the WKB approximation results in the exact eigenvalues independent of any of the parameters, and the accuracy is improved for increasing quantum number n , for both the wave function and expectation values.

(P4) Many-body theory calculations of positron binding, scattering and annihilation in magnesium and zinc group atoms

D Waide, D Green, and G Gribakin

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Following the prediction of positron-atom bound states by many-body theory calculations it is now known that positrons can bind to many atoms. Positron-atom bound states are supported by the strong electron-positron and positron-atom correlation effects, i.e., atomic polarization and virtual positronium formation. They make the calculation of the positron-atom system a challenging theoretical problem.

We use many-body theory to calculate positron binding energies for Be, Mg, Zn, Cd and Hg. The positron-atom interaction is described via the Dyson equation which relates the positron (quasiparticle) wavefunction to a zeroth-order Hamiltonian, taken in the Hartree-Fock approximation, and a non-local energy-dependent correlation potential.

We calculate the correlation potential diagrammatically including diagrams up to third order in the Coulomb interaction, taking account of the polarisation of the atom by the positron and screening of the electron-positron interaction by the atomic electrons, and an infinite diagrammatic series which describes the important virtual-Ps contribution. The latter is found by solving an integral equation, thus improving on the earlier calculations.

We use the many-body framework previously successfully used for positron interaction with noble-gas atoms and halogen negative ions to calculate the annihilation rate in the bound states, the total and differential scattering cross sections and the normalised annihilation rates for energies below the first inelastic threshold, i.e. the Ps-



formation threshold. This will include any resonant features. This represents the first time that a highly-accurate method is used to predict both binding and scattering.

(P5) Positron Cloud Characterisation

H T Evans, C J Baker, M Charlton, and C A Isaac

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Low energy positron clouds from a two-stage buffer gas accumulator [1] have been characterised with the aim of implementing resistive cooling. Resistive cooling can be described by a Stokes's viscous drag term, which offers a more correct test of the independent particle compression model [2]. The lifetime, energy distribution, magnetron frequency and axial bounce frequency have all been determined using destructive diagnostic methods. Without the use of rotating wall electric fields, positron clouds have been held in a deep, harmonic potential well within a '3rd stage' Penning-Malmberg trap for more than 100 s.

[1] J. Clarke *et al.*, *Rev. Sci. Instrum.*, **77**, (2006), 063302.

[2] C. A. Isaac *et al.*, *Phys. Rev. Lett.*, **107**, (2011), 033201.

(P6) R-matrix calculations of the resonances contributing to symmetry breaking during dissociative electron attachment to the H₂ molecule.

P Bingham, and J Gorfinkiel

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Recent velocity slice imaging experiments (Nat. Phys. 14 (2017) 149) looking at dissociative electron attachment (DEA) to the hydrogen molecule have revealed in the angular distributions of the dissociated hydrogen ions (around 14.5eV) a loss of symmetry from what would be expected when the dissociation is via a single completely symmetric resonant state. This asymmetry has been proposed to arise from the attachment of the scattering electron to two resonant states of opposite parities, which are close enough in energy for their widths to overlap. Under these conditions, the DEA takes place via a coherent superposition of the two resonances. These resonances have so far not been well characterized.

We present results of calculations using the ab initio R-matrix method aiming at accurately describing the resonances involved. This technique divides configuration space into an internal region, where the electron-molecule interaction is complex and an external region, where it is typically much simpler. Scattering quantities are obtained by matching the internal and external solutions at the boundary between the two regions and then propagating them to an asymptotic region.

We used the d-aug-cc-pVTZ basis set, 29 target states (in D_{2h} symmetry), full configuration interaction and a continuum modelled using B-splines. An internal region radius of 40 bohr was used with propagation to 200 bohr sufficient for most bondlengths. The resonances involved in the DEA process around 14.5 eV have been identified and their behaviour as a function of bondlength studied. We will discuss the experimental results in light of our findings.

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