

Institute *of* **Physics**
Atomic and Molecular Interactions Group

WINTER MEETING

THEME: Atoms, molecules, ions and their interactions

Monday 12th - Wednesday 14th January, 2004

**National Centre for Plasma Science & Technology
&
School of Physical Sciences**

**Dublin City University
Glasnevin, Dublin 9, Ireland**

- Monday 12th** **All talks in QG13, Business School**
- 12.00 – 14.00** **Registration**
- 14.00 – 14.10 Opening: Prof. Malcolm Smyth, Dean, Faculty of Science & Health
- 14.10 – 14.50 Spectroscopy of Highly Charged Ions; Sources for EUV Applications.
Gerry O'Sullivan, Univ. College Dublin
- 14.50 – 15.30 Atomic Physics with a VUV Free Electron Laser
Eugene Kennedy, Dublin City University
- 15.30 – 16.10 Molecules and Clusters in Intense Laser Fields
Daniel Dundas, The Queen's University of Belfast
- 16.10 – 16.40** **Tea/Coffee**
- 16.40 – 17.20 Advances in Two-Dimensional Photoelectron Spectroscopy using
Synchrotron Radiation
Emma Sokell, University College Dublin
- 17.20 – 18.00 Photoionization of Atomic Systems: Theory and Experiment
Brendan McLaughlin, The Queen's University of Belfast
- 20.00 – 23.00** **Dinner (Long Room, DCU)**
- Tuesday 13th** **All talks in QG13, Business School**
- 09.30 – 10.10 Towards the Complete Ionization Experiment
Albert Crowe, University of Newcastle upon Tyne
- 10.10 – 10.30 A New Experiment for Studies of Fragmentation of Clusters
Elaine Duffy, NUI-Maynooth
- 10.30 – 11.00** **Tea/Coffee**
- 11.00 – 11.50 Observations of Slow Antihydrogen
Gerald Gabrielse, Harvard University
- 11.50 – 12.30 Production and Scattering of a Positronium Beam
Simon Armitage, University College London

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| 12.30 – 14.00 | Lunch |
| 14.00 – 14.40 | Laser and Electron Interactions with Calcium - from Excitation through to Ionization <i>Andrew Murray, University of Manchester</i> |
| 14.40 – 15.20 | Multi-Photon UV Excitation of Naphthalene-Gas Mixtures: A New Gas-Phase Oscillatory System <i>Andy Ruth, University College Cork</i> |
| 15.20 – 15.40 | Pade Approximant in the Application of Signal Processing <i>Liz O'Sullivan, Queens University of Belfast</i> |
| 15.40 – 16.00 | Entanglement and Decoherence <i>Helen McAneney, Queens University of Belfast</i> |
| 16.00 – 16.30 | Tea/Coffee |
| 16.30 – 17.10 | Slow Coulomb Explosions <i>Tom Field, The Queen's University of Belfast</i> |
| 17.10 – 17.50 | Photodetachment Microscopy <i>Christophe Blondel, Lab. Aime Cotton, Univ. Paris Sud</i> |
| 17.50 – 18.30 | AGM (All Welcome) |
| 18.30 – 20.00 | Reception (Level 1 Lab, Gnd Floor, Physics Building, Block II) |
| Wednesday 14th | Workshops - Experimental and Theoretical/ Computational Techniques in At. and Mol. Physics |
| 9.00 – 10.30 | Workshop 1 - Practical aspects of the design and construction of electron spectrometers - (QG13) <i>Workshop Leader: George King, University of Manchester</i> |
| 10.30 – 11.00 | Tea/Coffee (Level 2 Laboratory) |
| 11.00 – 13.00 | Workshop 2– The calculation of oscillator strengths and electron-ion collisional cross sections <u>(Linux Lab., Room N222, 2nd Floor, Physics Building, Block II)</u> <i>Workshop Leaders: Alan Hibbert/Penny Scott, Queens's Univ. Belfast</i> |
| 13.00 | Meeting Ends |

Monday 12th – Session 1, 14.00 – 16.00

**Spectroscopy of Highly Charged Ions:
Sources for EUV Applications.**

Gerry O'Sullivan,

Department of Experimental Physics, University College Dublin, Belfield, Dublin 4, Ireland

Knowledge of the electronic structure of moderately to highly charged ions is with a few exceptions, limited to the lowest configurations of the first few ion stages of each element [1]. Such knowledge is essential for developing astrophysical models, fusion research, testing atomic theory and for a number of technological applications. Sources of ions for spectroscopic investigation include vacuum sparks, ion gas collisions and laser produced plasmas. The radiation produced may consist of lines, recombination and bremsstrahlung depending on the source type. In some cases, where complex configurations are involved, many thousands of lines may fall within narrow energy ranges to yield unresolved transition arrays (UTA) which are best described statistically. For $\delta n = 0$ transitions UTA in adjacent stages tend to overlap to yield extremely intense emission features [2].

In general there is a tendency for levels to regroup according to principle quantum number with increasing ionisation, so systems become more hydrogenic in character. This is evident in inner-shell photoabsorption spectra, where continuum resonances gradually disappear and intensity anomalies along Rydberg series vanish also. More striking is the effect of level crossing, especially in the lanthanides where in the lower stages the 4f electrons are less tightly bound than either the 5s or 5p, but more tightly bound past the 14th or 15th stage. In the crossing region the electronic structure becomes so complex that it has essentially the same properties as compound nuclear states and the level and spectral distributions obey the same statistics [3]. The spectra are so complex that no individual lines are observed as there are essentially as many possible transitions as there are ions in a given source. Such line free continua have been exploited as table top sources for EUV emission and can be a substitute for synchrotron sources if absolute flux and polarisation are not an issue [4]. More recently the UTA emission has become the focus of activities requiring narrow band sources. In particular the 4-4 UTA emission in ionised tin matches closely the reflectance curves for MoSi multilayer mirrors being developed for lithography at 13,5 nm [5]. Much of the current research of the UCD group is aimed at optimising this emission and understanding the underlying physics.

References:

1. G. O'Sullivan, Comments in Atomic and Molecular Physics, **28**,143-178 (1992).
2. G.O'Sullivan and P. K. Carroll, J. Opt. Soc. Am.**71**, 227-230 (1981)
3. D Kilbane, A Cummings, C McGuinness, N Murphy and G O'Sullivan, *J. Phys. B: At. Mol. Opt. Phys.* **35**, 309-321 (2002)
4. J. T. Costello, J. P. Mosnier, E. T. Kennedy, P. K. Carroll and G. O'Sullivan, Phys. Scr. **T34**, 77-92 (1991)
5. G. O'Sullivan and R. Faulkner Opt. Eng. **33**, 3978-3983 (1994)

Acknowledgement:

Support from Science Foundation Ireland under the National Development Plan, Enterprise Ireland, IRCSET and Intel (Ireland) is gratefully acknowledged.

Atomic Physics with a VUV Free Electron Laser

Eugene Kennedy

*National Centre for Plasma Science and Technology & School of Physical Sciences,
Dublin City University, Dublin 9, Ireland.*

Attainment of the long sought after goal of tunable laser-like radiation in the VUV and EUV spectral regions is now becoming a reality with the construction of single-pass Free Electron Lasers (FELs) based on the principle of Self Amplified Spontaneous Emission (SASE). VUV FELs will provide uniquely intense, polarised, short pulse (~ 100 fs) and tunable coherent radiation.

A full-scale VUV-FEL facility at DESY Hamburg, including a new experimental hall and infrastructure to direct the FEL beam into different beamlines, is expected to become operational as a user facility in late 2004. The FEL accelerator will be capable of reaching 1GeV and will produce photon wavelengths ranging down to 6 nm. Ultimately the average values of brilliance and photon flux will be more than three orders of magnitude higher than those provided by the current most advanced third generation storage rings e.g. achievable by BESSY II (Berlin) or the Advanced Light Source (Berkeley) synchrotron storage rings; the peak values are expected to be more than nine orders of magnitude higher!! *Such FEL lasers will constitute scientific investigative tools of dramatically new capability.*

The talk will introduce some of the reasons for the interest in brighter, short pulse duration, short wavelength sources for atomic physics, outline how the FEL produces its intense photon beams and will provide an overview of some of the early experiments on atoms planned for the DESY FEL.

Molecules and Clusters in Intense Laser Fields

Daniel Dundas

*Department of Applied Mathematics and Theoretical Physics,
Queen's University Belfast, Belfast BT7 1NN, UK.*

The advent of high-intensity ($> 10^{15}$ W/cm²), short-duration (< 100 femtoseconds) laser pulses has provided theorists and experimentalists with a unique opportunity to manipulate atoms, molecules and clusters with controlled, intense time-dependent forces. Understanding the physical mechanisms that underlie the results obtained in laboratory measurement requires theoretical approaches that model real systems and make as few approximations as possible. This is a non-trivial task, since the systems under investigation range from single-electron systems to large clusters comprising hundreds of complex atoms.

The fundamental equation governing these systems is the many-body Schrödinger equation, established in the 1920s. It is only in the last few years that computer technology and methodologies have advanced sufficiently for solutions of the full time-dependent Schrödinger equation (TDSE) describing fundamental three- and four-body, time-dependent, systems to be both constructed and explored [1–3]. For large aggregates of atoms, the explicit solution of the Schrödinger

odinger equation is not feasible and a many-body theory such as time-dependent density functional theory (TDDFT) is required [4]. In this talk I will present a numerical grid-based approach which can be applied to the solution of both the full-dimensional TDSE for few-electron diatomic molecules and the time-dependent Kohn-Sham equations of TDDFT for complex atoms, molecules and clusters.

Results from the solution of these two equations including ionization rates, harmonic generation spectra and movie animations of both ionizing and dissociating wavepackets will be presented.

References

- [1] Parker J S, Taylor K T, Clark C W and Blodgett-Ford S, *J Phys B: At Mol Opt Phys*, 29:L33 (1996)
- [2] Dundas D, *Phys Rev A*, 65:023408, (2002)
- [3] Dundas D, Meharg K J, McCann J F and Taylor K T, *Euro Phys J: D*, 26:51, (2003)
- [4] Runge E and Gross E K U, *Phys Rev Lett*, 52:997, (1984)

Monday 12th – Session 2, 14.30 – 17.50

Advances in two-dimensional photoelectron spectroscopy using synchrotron radiation

Emma Sokell

Dept. of Physics, University College Dublin, Belfield, Dublin 4

The use of photoelectron spectroscopy in conjunction with synchrotron radiation to study photoionisation processes is well established. However, the technological advances of third generation synchrotrons have enabled new phenomena to be investigated with relatively simple experimental techniques. Angle-resolved two-dimensional photoelectron spectroscopy, in which spectra are recorded as a function of both photon and electron kinetic energy, is such a method and its high sensitivity has revealed new features in photoelectron spectra of systems that have often been studied in detail before. Specific examples of new discoveries in the rare gases and diatomic molecules will be presented and the photoionisation processes responsible for these new spectral features explained.

A new experiment for studies of fragmentation of clusters

Elaine Duffy

NUI-Maynooth, Maynooth, Co. Kildare, Ireland

A new experiment has been constructed at NUI Maynooth for study of electron and photon impact fragmentation of clusters. Pure rare-gas clusters and metal-embedded rare-gas clusters ($M \cdot R_n$ clusters with $M = \text{Hg, Na, K}$, and $R = \text{Ar, Kr, Xe}$) are generated in a supersonic expansion. The clusters are probed with energy-resolved electron impact and with photo-excitation and ionisation, and fragmentation into ions and long-lived neutral metastable species will be investigated. A reflectron time-of-flight mass spectrometer is used for detection of ionized fragments. Time-of-flight detectors for neutral metastable fragments are being developed. Detection of neutral metastable fragments has been applied with great success in electron and photon impact dissociation of many different molecules, but has only recently been applied in fragmentation studies of rare-gas clusters. An overview will be given of the apparatus and the data acquisition, and plans for the future will be discussed.

Tuesday 13th – Session 2, 11.00 – 12.30

Observations of Slow Antihydrogen

Gerald Gabrielse

Spokesperson for the ATRAP Collaboration & Leverett Professor of Physics

Harvard University

The positron cooling of antiprotons in a nested Penning trap produces slow antihydrogen atoms. This has been confirmed by two different detection techniques. The distribution of antihydrogen states can be measured with ATRAP's field ionization method, and antihydrogen velocity distributions have been measured. Finally, a second method for the production of slow antihydrogen using resonant charge exchange collisions has just been demonstrated.

Production and Scattering of a Positronium Beam.

S. Armitage, J. Beale, D. E. Leslie and G. Laricchia.

Department of Physics and Astronomy, University College London, London WC1E 6BT, UK

Recent progress is reviewed concerning the production and scattering of a positronium beam. The efficiency of the conversion of a positron- into a positronium-beam has been investigated for simple atomic and molecular targets [1-3]. From these measurements, estimates of the positronium total cross-section may be extracted [2,3]. Total cross-sections for positronium scattering have also been measured directly for a number of atoms and molecules [4-6]. Recently, the first measurement of the fragmentation cross-section for positronium atoms in collision with He atoms has been reported [7]. The longitudinal energy distributions of the residual positrons from positronium fragmentation has also been measured and found to be peaked around half of the residual energy, suggesting the occurrence of electron-loss-to-the-continuum.

- [1] D. E. Leslie, S. A. Armitage and G. Laricchia, JPB **35** (2002) 4819-4827
- [2] A. J. Garner, G. Laricchia and A. Özen, JPB **29** (1996) 5961-5968
- [3] G. Laricchia, S. Armitage and D. E. Leslie, in publication
- [4] A. J. Garner, A. Özen and G. Laricchia, NIMB **143** (1998) 155-161
- [5] A. J. Garner, A. Özen and G. Laricchia, JPB **33** (2000) 1149-1157
- [6] D. E. Leslie, J. Beale, S. Armitage, in preparation.
- [7] S. Armitage, D. E. Leslie, A. J. Garner and G. Laricchia, PRL **89** (2002) 173402-1-4

Tuesday 13th – Session 3, 14.00 – 16.00

Laser and electron interactions with calcium – from excitation through to ionization

Andrew Murray

*Schuster Laboratory, Physics and Astronomy Department, The University of Manchester,
Manchester M13 9PL, England, UK*

Recent developments in CW laser systems which produce high power tuneable radiation in the deep blue have allowed the interaction between electrons and laser excited calcium to be studied for both excitation and ionization the first time. In these experiments, calcium is excited by tuneable laser radiation prior to electron collision with the target. The electrons may undergo super-elastic scattering, leaving the interaction region with more energy than they started with, or if the incident energy is high enough, ionization may occur. Details of the process of laser interaction will be discussed, and new results on excitation and ionization of calcium will be presented.

Multi-Photon UV Excitation of Naphthalene-Gas Mixtures: A New Gas-Phase Oscillatory System

A. A. Ruth

Physics Department, NUI-University College Cork, Cork, Ireland

A new closed *gas-phase system* with oscillatory behaviour will be presented. Employing the pulsed cavity ring-down technique, the absorption at 650 nm of static naphthalene vapour buffered with a noble gas at room temperature was studied as a function of time after UV multi-photon laser photolysis at 308 nm. The absorption dynamics of the static (unstirred) system exhibits extraordinary periodic and complex oscillations with periods ranging from seconds to many minutes, persisting for up to several hours. Depending on the buffer gas pressure, several types of dynamical responses can be generated. Aspects that may lead to possible explanations of the observed phenomena will be briefly discussed.

Pade Approximant in the application of Signal Processing

Liz O'Sullivan

The Queen's University of Belfast, Belfast BT7 1NN, N. Ireland, UK

Recent progress in the field of Nuclear Magnetic Resonance spectroscopy has presented novel high resolution signal processing methods. The Decimated Pade Approximant (DPA) acts as an accurate parameter estimation technique, a high resolution spectral estimator and lends itself as a noise reduction method. We have extended the existing method to look at noise reduction in the complex plane. We demonstrate that it is possible to reliably identify signal components that cannot be resolved by existing FFT techniques. Results will be shown highlighting the difficulties and advances in obtaining signals from noisy spectra.

Entanglement and Decoherence

Helen McAneney, Jinhyoung Lee, Myungshik Kim

The Queen's University of Belfast, Belfast BT7 INN, N. Ireland, UK

Entanglement, or as Einstein described it, “a spooky action at a distance”, has now been widely accepted to exist. The reason then why we do not see these strange effects in everyday life is due to what is termed decoherence.

In this talk, I will begin by describing what entanglement actual is using examples within a 2 level spin system (i.e. qubit system), from simple 2 body entanglement to the more complicated 3 body entanglement scenarios. I will also briefly discuss how, for an arbitrary state, these entanglement properties are distinguished.

From the 2 dim spin system, I will move to the infinite dim continuous variable system, and talk about many body entanglement within optics. The decoherence process can be modelled by the interaction of a system with a reservoir in thermal equilibrium. In this scenario, it was found that the initial system entanglement is destroyed due to the existence of many body entanglement of the system and environment. Through the study of decoherence, a better understanding of the underlying properties of a system may be gained.

Tuesday 13th – Session 4, 16.30 – 17.50

Slow Coulomb Explosions

Tom Field

School of Mathematics and Physics, The Queen's University of Belfast,

Belfast BT7 INN, N. Ireland, UK

Molecular ions with two positive charges, such as $(\text{CO}_2)^{++}$, are generally thermodynamically unstable with respect to fragmentation, for example $(\text{CO}_2)^{++} \rightarrow \text{CO}^+ + \text{O}^+$, because of the release of potential energy in the separation of the two positively charged fragments. Metastable states, however, have been observed for many years in mass spectroscopy. A number of studies have been undertaken to measure the lifetimes of these metastable species. In most of these studies the initial state of the metastable ions observed was not determined.

Coincidence methods have been used in the present experimental investigation to investigate the metastability of energy selected doubly charged molecular ions. The metastability of energy selected $(\text{CO}_2)^{++}$, $(\text{C}_6\text{H}_6)^{++}$ [benzene], $(\text{C}_6\text{D}_6)^{++}$ [deuterobenzene], $(\text{C}_6\text{H}_6)^{++}$ [2,4-hexadiyne] and $(\text{C}_6\text{F}_6)^{++}$ [hexafluorobenzene] ions has been observed and lifetimes have been determined. The new information gained from energy selection of these species gives insight into the mechanism of the fragmentation of these molecular ions and clues concerning the details of their potential energy surfaces. Theoretical calculation of potential energy surfaces for the larger dications, a significant challenge with 12 atoms and 30 normal vibrational modes, would give further insight into the metastable fragmentation of these species.

Photodetachment Microscopy

Christophe Blondel

*Laboratoire Aimé-Cotton, Centre national de la recherche scientifique,
Université Paris-sud, Orsay, France*

When a negative ion undergoes detachment in the presence of an electric field, the electron that goes out at a well-defined energy may follow two trajectories to the detector. The aim of detachment microscopy is to have a direct look at the corresponding interference pattern.

Since 1996, laser photodetachment microscopy experiments have been carried out on several atomic and one molecular anion. The number of rings in the interferogram is very sensitive to the ejection energy of the electron. This gives an interferometric way of measuring the energy brought in excess to the electron affinity, and the electron affinity itself.

The free-electron approximation used to analyse the electron interference pattern has been questioned when one deals with a big atom or a molecular anion. The first molecular photodetachment microscopy experiments have been carried out on OH⁻. Surprisingly enough, the electron interference pattern is still observable, even when OH happens to be left in a high angular momentum state. Even on a quantitative basis, the electron interferogram appears very robust with respect to either internal or external perturbations.

Wednesday 14th – Session 1, 9.00 – 11.00

Workshop I - Practical aspects of the design and construction of electron spectrometers

George King

*Schuster Laboratory, Physics and Astronomy Department, The University of Manchester,
Manchester M13 9PL, England, UK*

An electron spectrometer typically consists of an energy analyser, electrostatic lenses to collect and focus the electrons and physical apertures to define the radial and angular extents of the electron beam. In an electron impact spectrometer there will also be an electron gun and an energy monochromator to produce the incident electron beam. The workshop will describe the action of these various components and how they can be designed and combined to produce a complete spectrometer. Various aspects of the mechanical construction of a spectrometer will also be covered. The workshop will mainly cover electrostatic devices and their use for electrons of energy below 1000eV. Since these devices are electrostatic in nature, however, they can also be used for any charged particle irrespective of their mass or charge.

Lecture notes on Electron Optics that are relevant to the workshop can be found at:
<http://es1.ph.man.ac.uk/george-king/gcking.html>

Wednesday 14th – Session 2, 11.00 – 13.00

(Hands-on) Workshop II - The calculation of oscillator strengths and electron-ion collisional cross sections

Alan Hibbert and Penny Scott

Queen's University Belfast, Belfast BT7 INN, UK.

This short workshop aims to introduce participants to some of the types of calculation we would undertake in our research. Two of the QUB computer codes will be available:

CIV3 which is our atomic structure package, and is used to determine oscillator strengths of transitions in a wide range of atoms or ions: it is generally also used to provide 'target state' wave functions for -

R-matrix which is a suite of programs, used to determine electron-atom/ion collisional data and photoionisation cross sections.

We will offer a number of short exemplars which participants can work through using these codes, and we will be on hand to provide advice and guidance. We suggest the following exemplars, in all of which we will use LS coupling for angular momenta (ie, no relativistic effects):

1. (a) the resonance transition in He-like ions;
(b) the resonance transition in Be-like ions;

these will demonstrate the sort of calculation needed to obtain agreement between length and velocity forms of the oscillator strengths of the transitions.

2. Cross sections of $e\text{-He}^+$ collisions.

This has the advantage of there being exact target state (He^+) wave functions available, without having to use CIV3 to generate them. We will begin with some introductory comments on the main ideas behind the codes and on what to look out for in the exemplars.

A handout with full guidance on running the codes and on how to interpret the results will be provided.