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Recent results from the Oxford EBIT

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Abstract. Here we summarise the present status of the experimental programme of the Oxford electron beam ion trap. Most notably this research has recently culminated in the successful measurement of the $2s_{1/2} - 2p_{3/2}$ transition in hydrogenlike nitrogen by a laser resonance method. We also introduce preliminary results from some computational investigations of both electron beam transport and the trapped ion ensemble. In particular, we show that the contribution of the magnetic field to ion confinement has a potentially measurable effect on the ion phase space distribution.

EXPERIMENTAL RESULTS

The Oxford electron beam ion trap [1] has been operating now for over ten years. The goal of much of this experimental programme has been to realise sufficiently accurate measurements of the structure of very simple highly ionized atomic systems in order to make tests of fundamental theory, in particular the contributions made by QED and relativistic effects.

Laser spectroscopy

Methods of spectroscopy based on various laser induced resonance techniques are capable of achieving exquisite levels of precision. To this end we have implemented a relatively straightforward laser induced fluorescence experiment on the Oxford EBIT. A $^{14}\text{C}^{16}\text{O}_2$ laser is used to drive the $2s_{1/2} - 2p_{3/2}$ (fine structure–Lamb shift) transition in hydrogenlike nitrogen which is created and excited to the $2s_{1/2}$ state within the trap. The resulting modification to the $1s_{1/2} - 2s_{1/2}$ and $1s_{1/2} - 2p_{3/2}$ radiative intensities is then observed via energy dispersive spectroscopy using a Si(Li) detector. By measuring the modification of x-ray emission as a function of driving laser wavelength (in particular, the enhancement of the $1s_{1/2} - 2p_{3/2}$ transition) a resonance profile may be obtained and thus the transition energy may be measured. This experiment is described in detail in a recent article [2].

The present result from the laser resonance experiment is $835.0 \pm 0.5 \text{ cm}^{-1}$ and is in agreement with QED theory. However, in order to make what might be described as an interesting test of fundamental theory it is necessary for an experimental result to be sensitive to the theoretical effects of interest. With respect to the hydrogenlike
system the so-called two-loop self-energy corrections have received a great deal of recent attention [3, 4, 5]. For the \( n = 2 \) Lamb shift the two-loop self-energy contribution is of order \( 0.01 \text{ cm}^{-1} \) (to a total Lamb shift of \( 45.41 \text{ cm}^{-1} \)). In order to be sensitive to this contribution demands a measurement uncertainty of less than 10 ppm in the \( 2s_{1/2} - 2p_{3/2} \) transition, approximately 50 times more accurate than the current experiment.

The present experimental result is limited by the statistical quality of the data, and so considerable improvements may be achieved by simply by increasing the number of photons collected. We have already carefully optimized the operating parameters of EBIT and have increased the operating current at a 1.5 keV electron beam energy from 30 mA, as used for the result in [2], to 100 mA. The concomitant increase in x-ray count rates completely saturates the current detector system, but at least an order of magnitude improvement is anticipated. A factor of six improvement may be obtained by exploiting the full solid angle made available by the trap design. Further improvements may also come by increasing the laser power, careful optimization of the laser-ion interaction region, and simply increasing the total observation time. Therefore, it seems that sufficient experimental statistics can be achieved with quite reasonable improvements to the experiment design. However, a high precision result will also be sensitive to a great many systematic effects, such as for example changes in the trapped ion distributions, or variations of the responsivity of the laser power-meter. Preliminary results suggest that although these issues present a considerable challenge no show-stoppers have yet been identified.

**X-ray emission spectroscopy**

In hydrogenlike ions, the ground state \( (n = 1) \) Lamb shift is approximately eight times greater than the \( n = 2 \) shift. In principle a sufficiently accurate measurement of transitions to the ground state, such as \( 1s_{1/2} - 2p_{1/2,3/2} \) Lyman–\( \alpha \) radiation, should be able to test QED contributions to this state. Rapid energy scaling of atomic structure with atomic number, \( Z \), means that in highly charged ions such transitions will lie at x-ray wavelengths. Furthermore, hydrogenlike systems of intermediate atomic number \( (Z \simeq 18 \sim 36) \) represent an interesting theoretical challenge for QED theory, lying in-between the low–\( Z \) regime where series expansion in \( Z \alpha \) methods are employed [3] and the high–\( Z \) regime where numerical calculations to all orders are used [6].

Using a Johann-geometry crystal spectrometer\(^\dagger\) the \( 1s_{1/2} - 2p_{1/2,3/2} \) transitions in hydrogenlike titanium have been measured with a statistical precision approaching 1 ppm [8]. However, the non-trivial complications of calibrating instruments at x-ray wavelengths, due to the nature of so-called standard sources, limits the overall accuracy that can be obtained to much worse than this [8, 9].

The two loop contribution to the \( n = 1 \) Lamb shift in \( \text{Ar}^{17+} \) is of order 0.4 meV, compared to a total transition energy of \( \sim 3320 \text{ eV} \) for the \( 1s_{1/2} - 2p_{1/2,3/2} \) transitions (of which \( \sim 1.14 \text{ eV} \) is due to the total \( n = 1 \) Lamb shift). A very demanding measurement

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\(^\dagger\) see [7] for a general discussion of the instrument
uncertainty of <0.1 ppm is therefore required to be sensitive to this effect, although this will increase somewhat for higher-Z systems, due to rapid Z-scaling.

Improvements in absolutely calibrated measurements may be realised by observing hydrogen-like systems for which more accurately measured calibration data are available, such as the measurements presented in [10]. Alternatively, one may employ techniques which rely on direct measurement of Bragg angles and use externally measured crystal lattice spacings. However this approach will potentially run into statistical problems given the low efficiency of such methods and the relatively weak nature of the EBIT source. Such statistical problems may be avoided by creating a transfer standard. An intense source of x-rays may be generated inside the EBIT by use of a metal wire inserted into the path of the electron beam (see e.g. [8]). These x-rays may then be measured simultaneously by both a high precision instrument and a high efficiency instrument.

Thus, one may transfer the absolute calibration of a high precision instrument to a high efficiency instrument, which may then be used to make measurements of x-rays generated by trapped highly charged ions.

Such a range of wavelength calibrated x-ray experiments are being investigated on the Oxford EBIT. However, achieving measurement errors below the 1 ppm level will be exceedingly difficult. For this reason we are also pursuing experiments which instead aim to measure differences in QED contributions between ions of similar atomic number. This intercomparison approach [12] avoids the calibration difficulties suggested above and so in principle may allow more sensitive measurements of theoretical effects, although observing the caveat that a difference in effects between different systems is now being measured. Figure 1 shows early data from such an intercomparison experiment based on measuring the $1s_{1/2} - 3p_{1/2,3/2}$ transitions in $V^{22+}$ against the $1s_{1/2} - 2p_{1/2,3/2}$ transitions in $Mn^{24+}$. The results of this ongoing intercomparison work will be the subject of a future publication.

DEVELOPMENT OF EBIT MODELLING

The electron beam ion trap has proved to be a versatile and capable instrument for studying the physics of highly charged ions. However, certain classes of measurement, such as absolute measurements of cross-sections have been hampered by uncertainties arising due to the exact population and distribution of ions contained within a given trapped ensemble. Furthermore, whilst the modelling code of Penetrante [13] and its derivatives [14, 15, 16] have served well, a new code, featuring extensions beyond more accurate cross-sections and refined treatment of so-called overlap factors would be highly advantageous. Indeed, further motivation for such work is provided by the excellent possibilities presented by developments of x-ray microcalorimeters [17, 18], which are now capable of producing extremely high quality, broad spectrum x-ray data on EBITs [19, 20, 21]. Described here are the results of some preliminary efforts to

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2 such as a suitably constructed flat crystal spectrometer or more novel approaches [11]
3 such as a curved crystal spectrometer
FIGURE 1. Preliminary results for the $^{22+} V_{1/2} - 3p_{1/2,3/2}$ vs. $^{24+} Mn_{1/2} - 2p_{1/2,3/2}$ intercomparison experiment.

help develop an improved quantitative understanding of highly charged ion production in electron beam ion traps.

**Electron beam transport**

Using the OPERA 3D software package\(^4\) a three-dimensional model of the Oxford EBIT has been constructed, based directly on the AutoCAD design files. The electrostatic and magnetostatic problems may then be solved by use of the TOSCA module within the OPERA 3D package, which employs the finite element method and can handle non-linear magnetic problems, as is required to properly calculate the magnetic field environment of the electron gun.

The purpose of this model is two fold: first to provide a platform for considering design modifications to and optimization of the Oxford EBIT, and in this respect the work is very similar to previous efforts performed for many other EBITs. The second motivation is to generate accurate quantitative results regarding the electron beam phase space distribution which may insist in interpreting experimental measurements. For example, atomic structure measurements that make use of radiative recombination must accurately account for the energy of the free electrons [22], and this information should be provided by a sufficiently capable model (although exactly how best to use any simulated data requires careful consideration). Alternatively, the fraction of electron kinetic energy in the cyclotron mode\(^5\) can be extracted from simulated data, and may

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\(^4\) [http://www.vectorfields.co.uk](http://www.vectorfields.co.uk)

\(^5\) i.e. motion in the plane orthogonal to the trap axis
help resolve a disagreement in the literature[23, 24]. For such applications to be realised it is essential that the simulation takes a proper and realistic account of the thermal distribution of electron trajectories as generated at the cathode of the electron gun. As demonstrated by Hermann’s theory of electron beam transport [25], such finite temperature considerations can have an extremely important role in determining the resulting electron beam distribution.

Charged beam transport is simulated within OPERA 3D via the SCALA module. Space charge effects are included via an iterated approach: a set of test trajectories (beamlets) emitted from some surface are propagated through the current electromagnetic environment; the electrostatic potential generated by this beam is then calculated and used to update the electrostatic potential of the environment including the electron beam; a new set of beamlets are then traced through the updated environment. The procedure repeats until convergence to a user-defined tolerance is achieved. Thermal effects may be included in a straightforward fashion by simply ensuring that the initial beamlets are distributed according to a Maxwellian velocity distribution.  

For these simulations an initial current density was calculated by assuming the validity of Child’s law for space-charge current limited beams, and which gives results for the total current in good agreement with that obtained in general operation of the gun.  
Initial electron beam trajectories are then generated by randomly generating different points in (position, velocity) phase-space on the cathode surface and where the velocity distribution is Maxwellian. For these simulations a total of 2000 beamlets were used, at a temperature of 1300 K. This was found to be sufficient to ensure an acceptable level of model ergodicity, whilst maintaining a reasonable level of computational tractability and file size.

As a simple test and preliminary optimization, simulations were run for a variety of different magnetic field conditions at the electron gun surface. This was achieved by altering the simulated current density in the bucking coil electromagnet and so closely mirrors an easily performed experimental adjustment. By fitting a Gaussian distribution to the resulting radial profiles a measurement of the effective “Hermann radius” of a given electron beam profile may be made. By extracting the magnetic field on the cathode surface from simulation a calculation of the expected Hermann radius may be made, as defined by

\[
\begin{align*}
    r_{\text{Hermann}} &= \frac{1}{2} + \frac{1}{2} \left[ 1 + 4 \left( \frac{8m_e kT_c r_c^2}{e^2 B^2 r_B^4} + \frac{B_c^2 r_c^4}{B^2 r_B^4} \right) \right]^{1/2}.
\end{align*}
\]

(1)

Where \( r_c \) is the cathode radius, \( r_B \) is the Brillouin radius [27], and \( B_c \) and \( kT_c \) are the magnetic field and electron energy at the cathode respectively.

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6 such an approach is described in [26].

7 Ideally a great many initial trajectories should be generated according to the Richardson-Dushmann law for thermionic emission and the resulting space-charge limited beam allowed to form naturally following the production of a virtual cathode located close to, but not on the gun cathode. However, this approach was not possible with the limited mesh resolution available in the finite element model of the apparatus. A too coarse mesh will not be able to accurately reproduce the virtual cathode, and this was the case here.
FIGURE 2. Results for electron beam transport simulations, an 8.0 keV, 50 mA beam is simulated from a 1300 K cathode. The graph on the left shows a comparison of simulated characteristic beam radii against the predictions made by Hermann theory. The graph on the right shows three different electron beam profiles taken at an optimal (close to zero) magnetic field at the gun cathode (achieved by a bucking coil current density of 6.0 A/cm²), a significant positive axial magnetic field (5.6 A/cm²) and a significant negative axial magnetic field (6.4 A/cm²). The creation of a hollow profile for this last case is clearly shown.

As shown in figure 2, reasonable agreement between calculation and simulation appears to be achieved. However, on closer inspection a significant difference in the electron beam profile generated for positive or negative axial magnetic fields on the cathode surface (where the positive direction is chosen to be that of the magnetic field generated at the trap center). Electron beams which pass through a reversal of axial magnetic field acquire a large amount of angular momentum and subsequently generate a hollow electron beam profile. This asymmetry with respect to optimal conditions may explain results observed on the NIST EBIT, wherein the x-ray intensity is much greater for positive current biases in the bucking coil and with respect to optimal conditions⁸ as compared to negative biases[28]. However, further work both experimental and numerical is required in order to conclude whether this is the case. Further work is also required to determine whether there is any use for a hollow or 'halo' beam as simulated here, should it prove to be a real phenomenon.

Trapped Ion Distributions

A proper understanding of the trapped ion distribution in \((\text{position}, \text{velocity}) = (r, v)\) is essential to accurately simulate the evolution of the trap contents. In the absence of collisions ion motion is dictated by a combination of the electrostatic potential generated by the electron beam space-charge, ion space-charge, and the drift-tube potentials, as well as the magnetic field generated by the superconducting Helmholtz coils. Furthermore, the magnetic field will contribute to the confinement of an ion cloud. However,

⁸ i.e. negative initial axial magnetic field
given that the magnetic field does no actual work, it is expected that in a fully collisional plasma, under equilibrium conditions the effects of magnetic confinement will become negligible [29, 30]. The situation inside an electron beam ion trap may well be somewhere between these extremes, in particular the lossy nature of the trap environment means that a proper Boltzmann-distributed kinetic equilibrium may not be established.

In cylindrical coordinates \((\rho, \phi, z)\) the effective potential for single ion motion is given by

\[
V_{\text{effective}} = V(\rho, z) + \frac{qeB^2}{8m_i} \rho^2 + \frac{L_i^2}{2m_i qe \rho^2}
\]

(2)

where \(m_i\) is the ion mass, \(q\) the ion charge, and \(B\) the applied magnetic field. \(V(\rho, z)\) represents the contribution due to purely electrostatic terms (space charge and drift tube potentials) and \(L_i\) is the generalized angular momentum, given by \(L_i = m_i \rho_i^2 \left( \dot{\phi}_i + \frac{qeB}{2m_e} \right)\), and is conserved between collisions.

It is the last term in equation (2) that has potentially the most significant effect. This is because it introduces terms which depend on both position and velocity. Without this term the total ion energy is formally separable into a part which depends only on velocity (the kinetic energy) and a part which depends only on position (the potential energy). As such the anticipated Boltzmann-equilibrium phase space distribution (supposing it exists) will consist of a Maxwellian velocity distribution and an independent spatial distribution determined by the ion potential. However, the last term of (2) removes this independence and so one would expect a change in the ion phase space distribution. This modification may lead to, for example, an overall Doppler shift for different transverse slices through an ion cloud.

In order to qualitatively examine the effect of the magnetic contribution to ion confinement a procedure similar to that used to simulate the electron beam transport has been employed. Here a set of test Boltzmann-distributed trajectories are generated

\[
f(\mathbf{r}, \mathbf{v}) d^3r d^3v = n_0 \exp \left( -\frac{m_i v^2}{2kT} \right) \exp \left( -\frac{qV(\mathbf{r}, \mathbf{v})}{kT} \right) d^3r d^3v
\]

(3)

where \(V = V(\rho, z)\) or \(V_{\text{effective}}\) as appropriate. Some 10 000 to 100 000 ions have been used to generate the results presented here, although a self-consistent solution for the electrostatic potential has not yet been implemented and so these results are only valid in the limit of very weak injection. By numerically integrating the motions it is also possible to generate predicted radiative profiles for the ion cloud. This is important in order to properly interpret the results of ion cloud imaging experiments [31, 32]. These experiments attempt to either measure the ion or the electron beam distribution by respectively observing either long or short lifetime radiative transitions. A short lifetime or “fast” radiative transition is defined here as where the mean distance travelled by an ion between the moment of excitation of the moment of radiation is much smaller than the characteristic amplitude of the ion motion (or here much smaller than the electron beam radius). A long lifetime or “slow” transition corresponds to one where the ion will typically execute a number of radial oscillations before radiating. Strictly speaking there are two qualitatively distinct regimes for long lifetime transitions, as measured relative to the collision rate.
Figures 3 and 4 show results for a weakly, and strongly coupled ion clouds. The former demonstrates a very significant modification to the ion spatial distribution, whereas for the latter it is negligible. However, this modification on the actual radiative profiles is not observable. Collisions will tend to change this situation somewhat, and will probably lead to broader emission, however, it seems unlikely that a particular distinction between the cases with and without magnetic confinement will be determined. Figure 5 shows the simulated radiative profile for the different shapes of electron beam simulated above, demonstrating that a radiative method should be able to determine whether hollow beam formation is occurring or not. Finally figure 6 shows that indeed there is a small, but potentially measurable modification to the ion phase-space distribution resulting in a varying Doppler shift across the profile. Such a spatially dependent Doppler shift can be measured by employing a suitably high resolution spectrometer. For example, by combining low-photon count imaging with a scanning-mode etalon. 

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9 essentially every pixel in the detector acts like a different pinhole examining a different part of the source.
FIGURE 4. Simulated spatial distribution of ions, Xe$^{4+}$ in a 150 mA, 8.0 keV electron beam at a temperature of 500 eV. The contribution made by magnetic confinement is negligible here. It’s also interesting to note that the ion distribution is somewhat narrower than the electron beam distribution.

FIGURE 5. Expected radiative profiles for different electron beams demonstrating that it should be possible to observe the formation of a ‘halo’ beam mode of operation, should it exist.

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