Low Energy Super-Elastic Scattering
from Laser Excited Calcium

A thesis
submitted to The University of Manchester
for the degree of
doctor of philosophy (PhD)
in the faculty of Engineering and Physical Sciences

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School of Physics and Astronomy
2012
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ACP atomic collision parameter. 39–43, 62, 189, 199, 209, 216, 217, 220, 234, 237

BSR R-matrix using B-splines. 30, 223, 226, 227, 230, 234

CCC convergent close-coupling. 28–30, 223, 225–227, 229, 230, 234, 239

CCO coupled-channel optical. 28

CEM channel electron multiplier. 80–83, 211, 214

CFD constant fraction discriminator. 83, 84

DAC digital to analogue converter. 125, 138–140, 143, 144, 146, 155, 157, 158, 160, 162–169, 175

DAQ data acquisition. 171, 172

DIP dual inline package. 138

DPSS diode-pumped solid state. 104

DWBA distorted-wave Born approximation. 23, 29

DWBA2 second-order distorted-wave Born approximation. 27, 28

EOM electro-optic modulator. 110–112, 238

FBA first Born approximation. 21–23

FOMBT first-order many-body theory. 29

HT high tension. 82
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<td>lithium triborate</td>
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<td>LCD</td>
<td>liquid crystal display</td>
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<td>LED</td>
<td>light emitting diode</td>
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<td>MAC</td>
<td>magnetic angle changer</td>
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<td>MBR</td>
<td>monolithic block resonator</td>
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<td>MOSFET</td>
<td>metal oxide semiconductor field effect transistor</td>
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<td>ND:YVO₄</td>
<td>Neodymium Vanadate</td>
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<td>NIM</td>
<td>nuclear instrumentation module</td>
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<td>operational amplifier</td>
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<td>RDW</td>
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<td>RM</td>
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<td>SHG</td>
<td>second harmonic generation</td>
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<td>TTL</td>
<td>transistor-transistor logic</td>
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<td>USB</td>
<td>universal serial bus</td>
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<td>VI</td>
<td>virtual instrument</td>
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<td>VUV</td>
<td>vacuum ultra-violet</td>
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Abstract

Super-elastic scattering measurements were taken from calcium using the spectrometer described in this thesis. Calcium atoms were excited from the $4^1S_0$ ground state to the $4^1P_1$ excited state using a high resolution continuous wave laser set to a wavelength of 423 nm. A beam of electrons with a well defined energy was directed at the laser excited calcium atoms. The excited state was then described by a set of atomic collision parameters $P_{lin}$, $\gamma$ and $L_\perp$, found from measuring scattered electrons as a function of scattering angle and energy.

The scattering chamber was held at a pressure of $3 \times 10^{-7}$ mbar. A resistively heated oven operating at 800°C produced a well collimated calcium atomic beam containing the calcium atoms. The electron gun generated a beam of electrons of well defined momentum, whose energy could be changed from $\sim 5$ eV to over 100 eV. At energies less than 20 eV the rate of super-elastic electrons was very low, and so modifications were made to the spectrometer to automate data collection for long operating times without the need for user intervention.

A new digitally controlled DC voltage supply was constructed to deliver the correct potentials to the electron-optical elements in the spectrometer. An internal microcontroller enabled supply voltages to be programmed either using the front panel or via an attached computer for automatic optimisation of spectrometer voltages using a simplex algorithm.

New data was collected for the collision parameters over the full accessible angular range from 25–140°, at energies of 8, 10 and 65 eV. The data at 8 and 10 eV was taken so as to resolve differences between theoretical models at low energies. Comparisons were made with a relativistic distorted wave calculation, an R-matrix calculation, an R-matrix calculation using B-splines and a convergent close coupling theory. A 2 eV discrepancy was identified in the measured electron energy which was thought to be due to stray fields in the chamber. With this considered, convergent close coupling predictions were found to be in excellent agreement with the experimental data.
Declaration

The University of Manchester

Candidate Name: Alexander Stephen Knight-Percival

Faculty: Engineering and Physical Sciences

Thesis Title: Low Energy Super-Elastic Scattering from Laser Excited Calcium

Declaration to be completed by the candidate:

I declare that no portion of this work referred to in this thesis has been submitted in support of an application for another degree or qualification of this or any other university or other institute of learning.

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Acknowledgements

First of all I would like to gratefully acknowledge the help and support of my supervisor, Andrew J. Murray, both for his advice and direction whilst undertaking this project, and for the useful comments made whilst writing this thesis. His enthusiasm and knowledge for the work carried out in the AMLaM group has helped me on innumerable occasions.

I would also like to extend my thanks to the group members past and present. In the lab Matthew Harvey, Martyn Hussey, Sarah Jhumka and Kate Nixon were the source of many useful pieces of information, and were always willing to spend a few moments helping me to find the correct sized allen key. Their friendship in and outside of university was much appreciated.

George King is acknowledged for the friendly words of encouragement offered and for the keen interest he has taken in the experiment.

Much of these studies would not have been possible without the assistance of some truly talented technical staff. Alan Venables and Dave Coleman, both of whom retired shortly before the end of the project are thanked for the quality work that they produced and the useful discussions that were had with them.

Mike Needham is acknowledged for quickly diagnosing and repairing the various pieces of electronic equipment that (inevitably) stopped working at crucial times, and for providing valuable electronics advice that I am sure will be useful to me in the future.

Finally I would like to thank my parents Patricia Knight and Stephen Percival for their love and support; I owe them both a great deal.
List Of Publications


Chapter 1

Introduction

1.1 Motivation

The atomic wavefunction for various electronic orbitals may be obtained completely for hydrogen by solving the Schrödinger equation. This yields an expression describing the ‘shape’ of the atomic charge cloud for the various orbital states of the electron. When a quantum system is more complicated than this, predicting its behaviour becomes far more difficult.

An important tool for interrogating the structure of an atomic or a molecular target is the scattering experiment. Here, a projectile is introduced to the target in order to investigate its structure. These scattering experiments seek to glean information about the quantum state of this target from measuring any scattered products from the collision.

The addition of a projectile makes an interaction with even the simplest of atoms into a quantum mechanical many-body problem. Ab initio calculations for the outcome of the interaction then requires the construction of a Hamiltonian for the system. To accurately model the interaction, the Hamiltonian must describe the electrostatic forces acting between every constituent electron and proton making up the atom.
The interdependence of the electrostatic forces acting between each particle in the system mean that the Schrödinger equation for the atomic wavefunction is not separable. For such an equation, no analytical solution is available, and numerical methods must be used. In the quantum system describing the target, an infinite number of electronic states must be considered. To converge upon a solution to the scattering problem in a reasonable amount of time, approximation methods must be employed.

Even when using approximations, numerical solutions to scattering problems are often difficult to obtain, and calculations require large amounts of computing power. Experiments are required to investigate whether the approximations made are valid.

This thesis describes super-elastic electron scattering experiments performed on calcium, devised to test whether methods postulated to solve the many body scattering problem are accurate, and therefore whether the approximations in different models as are used to describe the interaction are valid. Once rigorously tested, the models may be relied upon to predict outcomes in situations that cannot be accessed experimentally.

The alkaline-earth metals, such as calcium, are amenable to theoretical study due to the similarities with atomic helium. As with helium, the neutral alkalineearths may be modelled as having two valence electrons located around an oppositely charged core. The models may then be refined by introducing the effects of distortions caused by interactions between the incident electron and the bound electrons.

The excitation of calcium to the $4^1P_1$ state is accessible with radiation produced by the lasers available to the group. Calcium exists in the experimental sample as 97% $^{40}$Ca [1], which has a nuclear spin $I = 0$ and so does not exhibit any hyperfine splitting. This simplifies the theoretical treatment of the laser excitation process.

A level diagram for calcium is presented in Fig. 1.1, showing only those levels
relevant to the scattering experiment. The excited $4^1P_1$ state is seen to decay to either the ground $4^1S_0$ state, emitting 423 nm blue photons, or to the $4^1D_2$ state, emitting infrared 5.6 $\mu$m photons. The transition probability is $10^5$ times smaller for the D-state. As the transition to the D-state is so unlikely, only the S-state need be considered when analysing decay from the P-state.

### 1.2 Collision Experiments

In practice, an electron-atom scattering experiment is carried out using an electron gun and an electron analyser. More sophisticated experiments may use additional equipment. The electron gun directs a beam of electrons at the target at a defined energy. The analyser detects electrons scattered from the target which enter its aperture. Some form of energy selection is usually employed in the analyser to discriminate between electrons scattered at different energies.

When an electron is incident on the target, there are three collision processes which may take place. These processes are [2]:

**Elastic scattering** where the electron is scattered with the same energy as the incident electron beam, but the momentum may change.
Inelastic scattering where the detected electron gives up some of its energy to the target and so has a lower energy than the electron beam.

Super-elastic scattering where, under the application of laser radiation to prepare the target in an excited state, the detected electron can be found with a higher energy than the incident electron beam.

The most likely result of an electron-atom collision is elastic scattering. The electron is scattered in the target region, and then detected with the same energy, but with a different momentum. The electron undergoes Coloumb interactions in the target region and is deflected. No information about the quantum state of the target is revealed by the collision in this type of interaction, as the electronic state of the target is not affected [2].

In an inelastic collision, shown for calcium in Fig. 1.2, the incident electron gives up an amount of its energy to the target atom, exciting a specific state. The scattered electron is detected with an energy lower than the incident energy, and the energy difference is equal to the energy of the atomic transition.

At a later time, the atom may decay back to the ground state via optically allowed transitions. With a photon detector added to the experiment, timing electronics can be used to detect the photon in coincidence with the scattered
electron. This type of experiment is known as an *electron-photon coincidence experiment*, and was adapted from similar techniques being developed in nuclear physics at the same time. Such an experiment was first performed in Manchester by Imhof and Read [3].

Under certain experimental conditions, an electron-photon coincidence experiment may be considered as a *complete scattering experiment* [2]. In such an experiment, a set of complex valued scattering amplitudes may be derived from the experimental measurement, which completely describe the quantum state of the system. This allows a full description of the shape and dynamics of the excited state charge cloud at the interaction to be resolved. This complete description is advantageous because it allows for direct comparison to theory.

The first coincidence experiment able to deduce atomic alignment and polarisation parameters was performed in the Stirling University group by Eminyan and co-workers [4] on helium atoms decaying from the excited $2^1P_1$ state to the $1^1S_0$ ground state. Data was taken over a range of electron scattering angles from 15° to 50°, in the low to intermediate energy range of 40 eV to 200 eV. An ultraviolet photon detector was able to rotate around the scattering plane to record rates of photon emission over the angular range 30° to 130°. These results were compared to models based on a first Born approximation (FBA). This models the radiation from the atom as if it were produced by a single radiating dipole [5], and treats the collision as a binary encounter involving only two free electrons [6]. The incoming and outgoing electrons in the scattering process were modelled as plane waves. This simple model was shown to be an inadequate description in all but small angle and high energy data.

A distorted wave calculation was also published by Madison and Shelton [7] to describe the experimental data from the Stirling group. This treatment was more accurate than FBA calculations since the electron wave function was not modelled as a plane wave but was considered to be distorted by the atomic potential. This perturbation is important since the scattering interaction occurs in a region where the atomic potential cannot be neglected. Such a calculation was shown to be an
improvement on the simple Born method.

The experiment was later extended by Standage and Kleinpoppen to measure relaxation from the $3^1\text{P}_1$ to the $2^1\text{S}_0$ state in helium [8]. This employed measurements of the polarisation of the detected photon in order to obtain a direct measurement of the orientation and alignment parameters. In this experiment a geometry was adopted where the photon detector was fixed to detect photons scattered perpendicular to the scattering plane. Again, the results from this study indicated that a simple FBA calculation was insufficient to describe the scattering process.

Tan et al. [9] obtained similar results to Eminyan and coworkers from electron-photon coincidence techniques on helium using a different experimental geometry, which required linear polarisation analysis of vacuum ultra-violet (VUV) photons from the helium de-excitation. The new data that was collected illustrated shortcomings in all available theoretical models, particularly at low energies and at large scattering angles.

In addition to helium, the scattering of electrons from a hydrogen target is less complicated to model compared to heavier targets. Both these systems are often the subject of theoretical treatments. However atomic hydrogen is difficult to study experimentally as it must be produced from H$_2$ molecules. Additionally, as with helium, the emitted photons are in the VUV portion of the spectrum, making it difficult to perform a full polarisation measurement. The first measurements of alignment and orientation which included the full polarisation measurements were performed by Williams [10].

In general, this early experimental work demonstrated discrepancies from theoretical models. There were two types of approach taken to predicting the outcome of the scattering problem. One was based on the Born approximation, often refined using a distorted wave description of the electron wavefunction, as previously described. The other class of approaches was based on the close-coupling formalism. This was first introduced by Massey and Mohr [11]. A set of coupled integro-differential equations may be formed when expanding the wavefunction
to solve the Schrödinger equations for a scattering event. The number of coupled
equations increases as the square of the number of coupled states and so the
close-coupling formalism tends to consider states which lie close to the final and
initial atomic states [12, 13].

Early close-coupling calculations were limited to considering only a small num-
ber of states, due mostly to the limited computing power available to theorists
at this time. By the 1980s, good results were being obtained with close-coupling.
As an example, McCarthy and Stelbovics were able to calculate accurate inelastic
scattering cross sections for hydrogen by considering the 1s 2s and 2p channels
in momentum space [14]. Although at the time these did not agree with experi-
mental data, further measurements performed by Yalim and coworkers [15] would
prove the calculations correct.

The early experiments using helium and hydrogen have so far been discussed.
The scattering process for these targets involves only three or four bodies and
so serves as a good starting point for theoretical calculations. In order to pro-
vide more varied data for theoreticians, and due to the experimental difficulties
encountered in working with hydrogen and helium, other more accessible atoms
may be chosen for study due to their structural similarity to these targets. In
this way, meaningful comparisons to theory may be made. The alkali and alkali-
earth metals fall into this category as they may be modelled as having one or
two valence electron above an inert core, made up of one or more closed shells of
electrons.

A sodium atom can be considered as a single electron above an inert neon
core, and is convenient to work with experimentally due to the low (290°C [16])
temperature required to form an atomic beam. An electron-photon coincidence
experiment involving sodium as the target atom was carried out by Teubner et
al. [17, 18] to resolve the full set of scattering parameters through the angular
range of 3–10° at an energy of 100 eV. FBA and distorted-wave Born approxima-
tion (DWBA) calculations were modified to make predictions for this target and
results were found to be in limited agreement.
1.3 Super-Elastic Electron Scattering

The main drawback of the coincidence experiment described in this section is that signal acquisition is slow. An electron and photon may scatter in any direction, but only events where the electron is scattered in the direction of the analyser \textit{and} the photon is scattered towards the photon detector contribute to the coincidence signal. The probability of this occurring is very low, and so individual data points may take a month or more to collect. This requires a very stable spectrometer, and even then, data at angles with low scattering cross sections may not be accessible to experiment due to drifts in the spectrometer over the time periods necessary to accumulate data. The following section describes an alternative arrangement, the \textit{super-elastic} experiment, which vastly improves on the acquisition times, as well as having other benefits which will be discussed.
In the super-elastic experiment, a laser of well defined polarisation is used to initially prepare the target atoms in an excited state. The laser takes the place of the photon detector in the corresponding coincidence experiment. Similarly, an electron gun must take the place of the electron analyser. A beam of electrons from an electron gun then interacts with the target atoms, some of which have been excited by the laser. The two incident particles, a photon and an electron, take the place of the two scattered particles in the coincidence experiment. With the incident electron and photon interacting with the target, the need for a coincidence measurement is removed. The only product scattered from the target is a single electron.

This super-elastically scattered electron takes the place of the incident electron in the coincidence experiment, and so these super-elastically scattered electrons must have a higher energy than the incident electrons from the gun. The energy gain is equal to the energy of the transition that is being excited. The scattered electrons are detected by the electron analyser, which takes the place of the electron gun in the coincidence experiment. To discriminate the super-elastic signal from signals due to other processes, the analyser is set to detect electrons only at a higher energy than produced from the gun. The equivalent energy is defined to be the energy that the incident electron would have had in the corresponding coincidence experiment, which is the energy of the scattered electron in this experiment.

The three stages involved in the super-elastic scattering process are shown in Fig. 1.4. The main advantage of the super-elastic technique is that the acquisition rates are much higher. This is because there is no longer any requirement to detect two particles in coincidence; the correlation of the electron and photon is inherent to the experimental setup.

Another experimental advantage of the super-elastic technique is the high state resolution that is possible. In a conventional coincidence experiment, the electron beam energy spread is limited to a minimum of \( \sim 10 \text{ meV} \). However for the high resolution lasers used in the experiment, the laser linewidth may be
as narrow as 30 kHz, corresponding to an energy spread of $\sim 0.1 \text{neV}$, a $10^8$ fold improvement on the resolution that is achievable with electron spectrometers [20]. The laser may be used to pick out close-lying states, or even to select specific magnetic sublevels by supplying radiation with the correct polarisation.

The advantages of high acquisition rates and high state resolution make the super-elastic technique attractive. However, its use is limited to atoms that have transitions that may be excited with wavelengths accessible from available laser technology. To accurately and efficiently excite a proportion of the target atoms to the excited state, the laser must be a high stability continuous-wave system capable of delivering a power in the range of hundreds of milliwatts. These types of laser systems are currently expensive and have a limited range of wavelengths.

The super-elastic scattering technique was pioneered by Hertel and Stoll using sodium as the target atom [21]. These authors describe energy loss spectra measured from target atoms prepared in the laser excited $3^2P$ state. The spectra demonstrated the detection of scattered electrons which had gained an energy of 2.1 eV, the same as the energy of the transition. The detection of these super- elastically scattered electrons demonstrated the viability of the technique.

The following work by Hermann et al. [22] used circularly polarised laser ra-
diation to make measurements of the atomic orientation induced by the collision. In further experiments on sodium, alignment and transferred angular momentum were reported [23]. Predictions for this data were made using either the Born approximation, or using the close-coupling formalism involving a limited number of states [24].

The theoretical work to model the effect of the laser excited scattering process was carried out by Macek and Hertel [25]. This established that the relationship between the super-elastic and coincidence measurements could be expressed in terms of optical pumping parameters, which manifest as a multiplicative constant in the polarisation measurements. Farrell and coworkers [26] showed that careful consideration of the optical pumping parameters is important to correctly establish the experimental results.

The close-coupling calculations for sodium were improved upon by Mitroy et al. [27], where the calculations were extended to cover a larger energy range between 10 and 217 eV. Discrepancies between the different sets of experimental data which were available made a meaningful comparison with this theoretical work difficult.

Further super elastic-scattering from laser excited sodium atoms was reported by the Griffith group [28, 29, 30]. Teubner et al. [28] also measured the full set of scattering parameters through an angular range of 5–110°, a far greater range than experimentally achievable using the coincidence technique. Data was taken at an equivalent energy of 20 eV, and good agreement was found with the work of Mitroy [27]. The work of Scholten et al. [29] extended this work to cover an equivalent energy of 10 eV. Consideration of the optical pumping terms for sodium was presented in [31]; these are important for establishing equivalence with the corresponding coincidence experiment.

Work on sodium in the Griffith group was reviewed by Sang et al. [30], where data was presented over a range of energies from 10 to 30 eV and over the angular range 5–25° to facilitate comparison to earlier work. Comparisons were made with two different theoretical calculations. The second-order distorted-wave Born
approximation (DWBA2) calculation of Madison et al. [32, 33] is an enhanced distorted wave calculation incorporating second order Born series terms. The coupled-channel optical (CCO) calculation of Bray et al. [34] was an improved method of solving the close-coupling equations in momentum-space. Fair to good agreement was found with both models.

The CCO method of solving the close-coupling equations was further refined, resulting in the convergent close-coupling (CCC) method of modelling the scattering interaction, where treatment of the continuum is achieved by approximating it using a number of pseudo-states. This method is described fully in the review articles by Bray and coworkers [35, 36].

The CCC model was first proposed by Bray and Stelbovics [37] for simple electron-hydrogen scattering, and was soon extended to describe the alkali metals [38], specifically sodium, where the CCC model compared well to the experimentally measured data. In a hydrogen-like atom such as sodium, the atom is modelled as a single electron above an inert, frozen core, where the wavefunction of the core is derived using the Hartree-Fock approximation [38].

In a comprehensive study by Shurgalin et al. [19] atomic collision parameters for both the 3S–3P and 4S–3P transitions in sodium were investigated. This showed the CCC and DWBA2 models to be in good agreement, although each model showed some disagreement in the 4S–3P transition.

Advances in the CCC model allowed it to be applied to helium [39], with two valence electrons, and then extended to handle any quasi-two-electron atoms [40]. This allowed predictions from the CCC model to be applied to scattering experiments from calcium.

The first super-elastic scattering studies to be performed on calcium were carried out by Law and Teubner [41] at Flinders University in order to determine the angular momentum transferred in the $^4\text{1S}$ to $^4\text{1P}$ state transition. These were subsequently followed by measurements of the atomic alignment parameter [42]. The experiments were carried out at energies of 45 eV and 25.7 eV, and showed
some significant deviation from results predicted by the contemporary scattering theories. These predictions were carried out using a first-order many-body theory (FOMBT) calculation by Clark et al. [43], a DWBA calculation also performed by Clark [42], and a relativistic distorted wave (RDW) calculation performed by Srivastava et al. [44].

At the Flinders University group, further super-elastic data were collected for a subset of the alkaline metals. Karaganov et al. report the orientation and alignment parameters for lithium [45, 46]. The CCC calculations were introduced for electron-hydrogen scattering by Bray and Stelbovics [37], but some discrepancies were found. Super-elastic studies were undertaken on lithium to address this difference, as lithium with its single valence electron is structured similarly to hydrogen. Comparison of the CCC model predictions and the data for lithium showed good agreement. The electron-hydrogen data were subsequently remeasured [15], and found to be in agreement with the CCC predictions.

Further super-elastic work on the alkaline metals was continued in the Flinders group by Stockman et al. on potassium [47, 48, 49], and more recently by Slaughter et al. [50] on cesium. These continued to show the utility of the CCC approach. The data did not demonstrate significant deviations from the CCC predictions for the higher atomic number, indicating that the onset of relativistic effects was not observed.

Further measurements on calcium were reported by Chwirot et al. [51] at an energy of 100 eV, over the range 10–45°. As with the measurements performed by El-Fayoumi and coworkers [52], these were electron-photon coincidence experiments. The results were compared to an RDW model and were found to be in general agreement, although with some discrepancies.

Early super-elastic scattering work at Manchester was carried out in the (e,2e) spectrometer by Murray and Cvejanovic [53] on calcium. Results for the full set of collision parameters were published at energies of 20 eV, 25 eV and 35 eV. The data was compared to an RDW calculations provided by Stauffer and colleagues. Generally good agreement was found at the higher energies, but as lower energies
were approached the model no longer compared well with the data.

Following the completion of these studies, further calculations to determine the outcome of low energy electron scattering from calcium were made. An R-Matrix method was developed by Kawazoe et al. [54] to predict the cross-sections and collision parameters at 10, 20 and 25 eV. In an R-Matrix method, the collision is divided into two distinct regions. An internal region is defined by a sphere around the nucleus where the interaction with the atom may be treated in more detail. Beyond this internal region, the interaction may be modelled more simply. A review of the R-Matrix method is given by Bartschat [55]. A related R-matrix model produced by Zatsarinny et al. [56], called the R-matrix using B-splines (BSR) method, uses B-spline functions to approximate parts of the wavefunction in the internal region.

Additionally, distorted wave calculations were produced for calcium by Chauhan and colleagues, which take relativistic effects into account [57]. This distorted wave model is expected to be more accurate at higher energies. A CCC calculation was produced by Fursa and Bray [58], which was expected to be accurate over the entire energy range.

Success with the super-elastic experiments carried out in the (e,2e) scattering chamber led to the construction of a dedicated super-elastic spectrometer by Hussey et al. [59]. Measurements carried out using the new spectrometer confirmed the collision parameters at 45 and 55 eV and were the first to measure data over the full angular range using a magnetic angle changer (MAC) device [59, 60].

This thesis describes how the new super-elastic spectrometer at Manchester was modified to work at the very lower limit of its energy range, so as to collect data at 8 eV and 10 eV equivalent incident energy [61]. This data is compared to state-of-the-art theoretical models to determine their suitability to predict the outcome of the scattering experiments at these energies.
1.4 Outline of Thesis

This introduction has described the super-elastic scattering experiment and has presented a short overview of relevant work in this area. The remainder of the thesis is laid out as follows.

In Chapter 2, the theoretical background required to justify the experiment and explain the results is presented. The theory relevant to the scattering process is given, and an appropriate framework for describing the experimental data introduced. Calculations to model the laser interaction with calcium are shown.

The equipment used to run the experiments is presented in Chapter 3. Details for the vacuum system which houses the spectrometer, and the equipment used to take measurements is given. Furthermore, the external electronics and laser system are detailed.

Chapter 4 describes the computer controlled parts of the experiment and the associated control software. This included a new digital power supply, which is described in detail.

In the penultimate chapter, the results obtained from the spectrometer are presented and discussed along with theoretical predictions. This includes work undertaken to determine the energy calibration of the spectrometer, and the alignment and orientation parameters recorded at equivalent energies of 65, 10 and 8 eV.

The concluding chapter of the thesis contains a summary of the work carried out, and presents suggestions for further study. These include technical improvements to the spectrometer, and further super-elastic scattering investigations.
Chapter 2

Theory

2.1 Introduction

This chapter is divided into two sections. In the first, an overview of the scattering theory relevant to a complete scattering experiment is presented. Specifically, an S- to P-state transition is analysed for a light target in which spin exchange processes need not be considered. This is the case for the calcium target considered in this work.

The now standard framework for experimental work, based around a ‘natural’ coordinate frame is introduced. This was first presented by Hermann and Hertel [62], and summarised in detail in a review by Andersen, Gallagher and Hertel [63].

The excitation of an ensemble of atoms is considered using the density matrix formalism, which describes the state of this quantum system. Parameters which describe the excited P-state are shown and related to the density matrix.

As is conventional in the literature, this discussion of scattering theory is based around analysis of an inelastic scattering event. The equivalence of the inelastic and super-elastic approaches under time reversal means that the analysis may also be applied to a super-elastic experiment. Some considerations due to
optical pumping are discussed, although they do not apply to the experiment with calcium since this target has no hyperfine structure.

In the second part of this chapter, the effect of laser excitation on the calcium atoms is examined. The interaction process is modelled using quantum-electrodynamic (QED) theory, which offers the most complete description of the behaviour of the atom in a laser field by using a fully quantum mechanical approach for both the atom and the field.

These QED calculations are described, and the results allow the effect of Rabi oscillations to be investigated, and the steady state excited populations to be derived. Under typical experimental conditions, the Rabi oscillations are seen to die away over a short timescale on the order of tens of nanoseconds, allowing their effects to be neglected. Furthermore it is shown that the laser is able to excite a population of almost one half of the atoms in the interaction region to the upper state, making the laser excitation process very efficient.

2.2 Electron Atom Collisions

The physical process under investigation in the experiments is the interaction of an electronic projectile with a calcium atomic target. This section will examine how scattering measurements taken using the super-elastic spectrometer relate to the alignment and orientation of the excited atom, and how these measurements then relate to the predictions made by scattering theory.

In the treatment that follows, the excitation of the calcium target is investigated by limiting the analysis to the consideration of a single valence electron. This allows meaningful parameters to be derived to describe the excited state.

Before the super-elastic experiment is considered, an inelastic collision where the atom is excited by electron impact is analysed. This is the usual approach taken in the literature, as it allows ready comparison between the super-elastic and coincidence experiments. The results from a super-elastic experiment are
then expressed in the same way as for the equivalent coincidence experiment.

2.2.1 Electron-Photon Coincidence Experiments

The geometry adopted for a coincidence experiment as described in this section is shown in Fig. 2.1. Four main pieces of equipment are used. An atomic beam source, such as an oven or a gas jet, provides the atomic target. A beam of electrons is supplied by an electron gun at a well defined energy. Scattered electrons are detected by an analyser, which is also energy selective. As atoms relax to the ground state, the photons which are emitted are detected by a photon detector, which is able to detect the polarization properties of the radiation.

The location where the electron beam and atomic beam collide is called the interaction region. Both the analyser and photon detector are focussed onto this point. The momenta of the incident and outgoing electrons are shown in the diagram, and are denoted by $k_{\text{in}}$ and $k_{\text{out}}$ respectively. These two vectors define a plane, which is known as the scattering plane. The electron analyser or the gun may be repositioned to access different scattering angles $\theta_e$ around the scattering plane. The photon detector is positioned to detect photons scattered perpendicular to this plane.

2.2.2 Overview of Collision Theory

The wavefunction of an atomic system $\Psi$ may be written as a linear superposition of orthonormal basis states [63],

$$|\Psi\rangle = \sum_{J,m_j} a_{J,m_j} |J,m_j\rangle$$

where $J$ and $m_j$ are the angular momentum and magnetic quantum numbers of the electrons. Each basis state contribution is weighted by complex coefficients $a_{J,m_j}$. 
Figure 2.1: An electron-photon coincidence experiment, showing the electron gun, the electron analyser and the photon detector, set up to resolve the $P_3$ Stokes parameter. A linear polarisation measurement can be made by removing the quarter wave plate and rotating the linear polariser.
To model an electron collision with an atom, the scattering process is characterised through a number of complex scattering amplitudes [2]. For an experiment to be considered complete, such as the coincidence experiment described here, all independent scattering amplitudes must be determined through measurement.

The scattering amplitude at an angle $\theta_e$ may be defined as

$$f_{\psi,\psi}(\theta_e) = \langle J, m_j | \mathcal{T} | J', m'_j \rangle$$

(2.2)

where the transition operator $\mathcal{T}$ describes the transition from the initial state $| J', m'_j \rangle$ to the final state $| J, m_j \rangle$.

The transition operator $\mathcal{T}$ for an electronic collision is very difficult to calculate due to the electronic potentials associated with the atom. This is where the complexity lies in predicting scattering interactions from first principles.

As the scattering amplitudes contain angular momentum components, they must be defined with reference to a quantisation axis. This necessitates the definition of a coordinate frame for the experimental system. The natural frame [62] will be used to describe the collisions throughout this thesis, and is used extensively in the literature. The collision frame is an alternative coordinate frame which is often used in theoretical work. The collision frame sets the quantisation axis along the incident beam direction, and will not be discussed further.

A diagram illustrating the natural frame is shown in Fig. 2.2. The natural frame defines the direction of the $z$-axis to be perpendicular to the scattering plane. This axis is used as the quantisation axis. The $x$-axis is then defined to be in the direction of the incident electron, congruent with $\mathbf{k}_{\text{in}}$.

Using equation (2.1), the wavefunction of an excited P-state may then be written

$$|\psi\rangle^P = \sum_{m_j} a_{m_j} |1, m_j\rangle$$

(2.3)

$$= a_{+1} |1, 1\rangle + a_0 |1, 0\rangle + a_{-1} |1, -1\rangle$$
where the $J$ subscript on the $a$ coefficient has been dropped for brevity. The $a$ coefficients may be directly related to the scattering amplitudes $f$ as indicated in the literature [64].

Due to the choice of natural frame quantisation axis, a transition $m'_j = 0 \rightarrow m_j = 0$ would imply that the electronic projectile had imparted some momentum out of the scattering plane. As reflection symmetry is conserved in the scattering geometry that is being considered, this would imply that the electron had changed its spin during the interaction. It is assumed here that this process does not occur [2].

The consequence of this assumption is that the scattering amplitude $a_0$ must be zero, and so the term may be dropped from (2.3), leaving

$$|\psi\rangle^P = a_{+1}|1, 1\rangle + a_{-1}|1, -1\rangle$$

(2.4)

This shows that in the natural frame, the excited P-state may be represented as a superposition of only the two magnetic substates with $m_j = +1, -1$ as illustrated in Fig. 2.3.

The complex coefficients $a_{m_j}$ may be represented as:

$$a_{+1} = |a_{+1}|e^{i\phi_{+1}}$$

(2.5a)

$$a_{-1} = |a_{-1}|e^{i\phi_{-1}}$$

(2.5b)
This gives four independent real parameters; $|a_{+1}|$, $|a_{-1}|$, $\phi_{+1}$ and $\phi_{-1}$. Quantum mechanics does not allow measurement of the absolute phases $\phi_{+1}$ and $\phi_{-1}$, and so only the relative phase between them,

$$\delta = \phi_{-1} - \phi_{+1}$$

(2.6)

can be measured. This leaves three independent real parameters; $|a_{+1}|$, $|a_{-1}|$ and $\delta$, to be determined by experiment in order to fully characterise the P-state.

### 2.2.3 The Density Matrix

For a pure state, the density operator $\rho$ is defined as the outer product of a wavefunction $\Psi$ [65],

$$\rho = |\Psi\rangle \langle \Psi|$$

(2.7)

With an appropriate choice of coordinate frame, the density matrix may be defined. The elements of the density matrix are then given by:

$$\rho_{ij} = \langle i | \rho | j \rangle$$

(2.8a)

$$\Rightarrow \rho_{ij} = \langle i | \Psi \rangle \langle \Psi | j \rangle$$

(2.8b)

Hence the density matrix for the excited state can be derived from the wave-
function $|\psi|^P$ (2.4).

$$
\rho_{ij} = \begin{pmatrix}
|a_1|^2 & 0 & a_1a_{-1}^* \\
0 & 0 & 0 \\
a_{-1}a_1^* & 0 & |a_{-1}|^2
\end{pmatrix} = \begin{pmatrix}
\rho_{11} & 0 & \rho_{1-1} \\
0 & 0 & 0 \\
\rho_{1-1}^* & 0 & \rho_{-1-1}
\end{pmatrix}
$$

(2.9)

The elements along the diagonal are real quantities, and are directly related to the population of the states. Therefore the elements $\rho_{11}$ and $\rho_{-1-1}$ are both real and correspond to the probability amplitudes for the corresponding magnetic sublevels [64].

As can be seen from the formation of the density matrix in equation (2.9), the density matrix must be Hermitian, ie.

$$
\rho_{ij} = \rho_{ji}^*
$$

(2.10)

This means that the quantity $\rho_{-11} = \rho_{1-1}^*$. The off-diagonal elements in the density matrix measure the coherences between the various magnetic substates since these carry information on the relative phase $\delta$. As the population in the $m_j = 0$ level is zero, the corresponding coherences with this state are also zero [64].

An advantage of the natural frame is that a density matrix of the form (2.9) may be parameterised in terms of alignment and orientation parameters. These parameters were suggested by Fano and Macek [66]. The density matrix may then be rewritten in the following form, as given by Andersen and coworkers [63]:

$$
\rho_{ij} = \frac{1}{2} \begin{pmatrix}
1 + L_\perp & 0 & -P_{\text{lin}}e^{-2i\gamma} \\
0 & 0 & 0 \\
-P_{\text{lin}}e^{2i\gamma} & 0 & 1 - L_\perp
\end{pmatrix}
$$

(2.11)

The parameters $P_{\text{lin}}$, $\gamma$ and $L_\perp$ are defined as the atomic collision parameters (ACPs). They describe the alignment and orientation of the P-state, and will be discussed further in the next section.
2.2.4 Relationship Between Measurements and the Density Matrix

By obtaining values for the ACPs, the density matrix elements may be calculated. In a coincidence experiment, the number of coincidence events are measured for a given scattering angle as a function of photon polarisation. This may be denoted \( I(\theta_{pol}) \), where \( \theta_{pol} \) denotes the type of polarisation measurement made.

For linearly polarised radiation, as detected perpendicular to the scattering plane, the relationship between the ACPs and the measured scattering intensities, is given by [67]

\[
I(\theta_{pol}) = C \left[ 1 + P_{\text{lin}} \cos 2(\theta_{pol} - \gamma) \right]
\] (2.12)

where the coefficient \( C \) represents constant multiplicative factors that affect the measurement [67]. This coefficient is unity for an atom that has no hyperfine structure. The angle of the linear photon polarisation, \( \theta_{pol} \) is measured from the electron beam axis.

The linear polarisation of the P-state, \( P_{\text{lin}} \) describes the relative difference between the length \( l \), and width \( w \) of the charge cloud, as shown in Fig. 2.4 [68],

\[
P_{\text{lin}} = \frac{l - w}{l + w}.
\] (2.13)

In equation (2.12), the angle that the charge cloud makes to the polarisation vector of the radiation is represented by \( \gamma \), which is related to the relative phase \( \delta \) as follows [2]:

\[
\delta = 2\gamma \pm \pi
\] (2.14)

The parameter \( \gamma \) is the charge cloud alignment angle. When \( \theta_{pol} = \gamma \), the polarisation vector is aligned with the maximum of the charge cloud density.

The populations \( \rho_{11} \) and \( \rho_{-1-1} \) can be determined directly from the number of coincidence events for circularly polarised light. The \( P_3 \) stokes parameter may
then be determined from these coincidence measurements as follows [64, 68]:

\[ P_3 = \frac{I(\text{RHC}) - I(\text{LHC})}{I(\text{RHC}) + I(\text{LHC})} \]  

(2.15)

By conservation of angular momentum, the \( L_\perp \) parameter, which defines the orientation of the charge cloud is then given by

\[ L_\perp = -P_3 \]  

(2.16)

This quantity is a measure of the angular momentum transferred to the atom during the interaction.

Hence in summary the ACPs are given by \( P_{\text{lin}}, \gamma \) and \( L_\perp \) which can then be directly related back to the scattering amplitudes that are calculated by theory through the density matrix.
2.2.5 Application to Super-Elastic Measurements

In the super-elastic experiment, introduced in Section 1.3, a laser is used to prepare the atom in a excited state. An electron scattered from the excited atom carries away the energy of the excitation. The atom is de-excited by the scattering interaction and so the scattered electron also carries away information about the excited state. The same set of ACPs are used to describe the P-state as were used in the coincidence experiment.

In the general case, the expressions for calculating the ACPs in the coincidence experiment cannot be used directly for the super-elastic measurements. In atoms with hyperfine structure the laser radiation works to dephase the optical transitions. Populations are transferred into other hyperfine levels which affects the results of the super-elastic measurement. This may be described by a set of optical pumping parameters, which are multiplicative constants that are applied to the polarisation measurements [69]. This is seen for measurements on the alkali atoms such as sodium, potassium and rubidium [31, 47, 70].

For calcium, with no hyperfine splitting, the optical pumping parameters all evaluate to unity [53]. Therefore the constant $C$ in equation (2.12) may be neglected and the linear polarisation measurement is given by:

$$S(\theta_{pol}) = 1 + P_{lin} \cos 2(\theta_{pol} - \gamma)$$

(2.17)

where $S$ is now the number of super-elastic electron counts resolved as a function of scattering angle. This expression is sufficient to calculate $P_{lin}$ and $\gamma$.

Laser photons transfer their angular momentum to the charge cloud when they excite the atom. This means that the laser acts to set the orientation parameter $L_\perp$. The relationship to the circular polarisation of the incoming photons, $P_3^S$ is simply

$$L_\perp = P_3^S$$

(2.18)

again, with the optical pumping term set to be unity.
The relationships presented in this section are used in Chapter 5 to calculate the ACPs for the super-elastic scattering experiments described in this thesis.

2.3 Atoms in a Laser Field

In this section the effect of incident laser radiation on the calcium atoms in the interaction region will be considered, using a full QED approach. To describe the quantum mechanical behaviour of the atomic system, the equation of motion for the atomic operator in the Heisenberg representation is solved. The method followed in this section is similar to that used by Farrell [69], Murray [71] and Harvey [72], and these works may be referred to for additional detail.

The density matrix formalism is used again in this section, to describe the laser excited transition between the ground and excited atomic states. By solving the equations of motion, a set of general equations are found for the density matrix elements.

These general equation are then applied specifically to calcium atoms. When calcium is excited from the ground state to the $4^1P_1$ state by a laser beam of well-defined polarisation, a two level system is created between the ground and excited states. The resulting reduced $2 \times 2$ reduced density matrix then fully describes the time evolution of the two level system. This is then used to model the transient behaviour and steady state solutions of the atomic system as the laser radiation is applied.

2.3.1 The General Equations of Motion

The state of the atom is described by the atomic operator, $\hat{\sigma}$. The operator $\hat{\sigma}$ is created from the outer product of states $i$ and $j$,

$$\hat{\sigma}_{ji} = |j\rangle \langle i|.$$  \hspace{1cm} (2.19)
This operator represents the coherences between two atomic states $|i\rangle$ and $|j\rangle$. If $i = j$, the population of the state can be ascertained.

The Hamiltonian for an atom in a laser field can be represented by the following expression:

$$H = H_A + H_F + H_I$$

(2.20)

where $H_A$ is the unperturbed atomic Hamiltonian for an atom in free space, and $H_F$ is the Hamiltonian for the electromagnetic field. The interaction between the field and the atom is described by the interaction Hamiltonian $H_I$.

The expression for the atomic Hamiltonian can be written as follows [73],

$$H_A = \sum_i \hbar \omega_i |i\rangle \langle i|$$

(2.21)

where $i$ represents all the possible normalised orthogonal basis states of the system. The summation is therefore carried out over all states of the target. The quantity $\hbar \omega_i$ is the energy of the state with respect to an arbitrary level, where $\omega_i$ specifies the transition frequency.

The free field Hamiltonian, $H_F$, represents the electromagnetic field due to the laser beam in the interaction region. It is described in terms of the annihilation and creation operators for the field, written $a_\lambda$ and $a_\lambda^\dagger$ [74], so that

$$H_F = \hbar \sum_\lambda \omega_\lambda a_\lambda^\dagger a_\lambda$$

(2.22)

and is a sum over all the field modes $\lambda$, where $\lambda$ defines the properties of the field; the laser wavelength, polarisation and propagation vector $k$. As the laser field is assumed to be along a single axis, the vector quantity $k$ simplifies to a scalar quantity $k$.

The interaction Hamiltonian may be expressed as follows [73]:

$$H_I = \hbar \sum_{\lambda'} \sum_{e'} \sum_{g'} \left( g_{e'g'}^X \hat{\sigma}_{e'g'} a_{\lambda'} e^{ik_{\lambda'}z} + g_{e'g'}^{Xs} a_{\lambda'}^\dagger e^{-ik_{\lambda'}z} \hat{\sigma}_{g' e'} \right)$$

(2.23)
The $\lambda'$, $e'$ and $g'$ terms represent sums over possible field modes, excited states, and ground states, respectively. The $g_{\lambda'g'}$ terms represent the coupling coefficient between the field mode $\lambda'$ and the excited and ground states, $|e'\rangle$ and $|g'\rangle$. The expression is derived from taking the dot product of the electric field from the laser with the electric dipole operator of the atom. For a detailed derivation see for example Loudon [73]. The terms inside the summation are expressed in normal ordering. In this scheme the creation operators for the field are placed to the left of the atomic operators, and the annihilation operators to the right. It is valid to reorder the terms at this point since the quantities commute, however approximations made later in this derivation will depend on the ordering of terms, as they then break the commutation relation.

The field operators $a$ and $a^\dagger$, as seen in the expressions for $H_F$ (2.22) and $H_I$ (2.23) are the annihilation and creation operators. They operate on the system to remove or add one discrete quantum of energy to the system, and are calculated as follows [73]:

$$a_{\lambda'}(t) = a_{\lambda'}(0) e^{-i\omega_{\lambda'}t} - i \sum_{e''} \sum_{g''} g_{e''g''}^{\lambda'} e^{-ik_{\lambda'}z} \int_0^t \hat{\sigma}_{e''g''} (t') e^{-i\omega_{\lambda'}(t-t')} dt'$$  \hspace{1cm} (2.24) $$a_{\lambda'}^\dagger(t) = a_{\lambda'}^\dagger(0) e^{+i\omega_{\lambda'}t} + i \sum_{e''} \sum_{g''} g_{e''g''}^{\lambda'} e^{ik_{\lambda'}z} \int_0^t \hat{\sigma}_{e''g''} (t') e^{+i\omega_{\lambda'}(t-t')} dt'$$  \hspace{1cm} (2.25)

The properties of the field mode $\lambda'$ are given by the frequency, $\omega_{\lambda'}$, and the wavenumber $k_{\lambda'}$. The distance $z$ is specified along the direction of the laser beam from the atomic nucleus.

The general equations of motion for the atomic operator will be found in the Heisenberg picture. In this representation of quantum mechanics, the state vectors are time independent, and the operators may vary with time. Therefore the atomic states $|i\rangle$ do not evolve with time, and the atomic operator $\hat{\sigma}_{eg}$ is time dependent. The equation of motion for the atomic system is then given by

$$\frac{d\hat{\sigma}_{eg}}{dt} = -i \frac{\hbar}{\hbar} [\hat{\sigma}_{eg}, H] = -i \frac{\hbar}{\hbar} [\hat{\sigma}_{eg}, H_A + H_F + H_I]$$  \hspace{1cm} (2.26)
where the substitution (2.20) has been made. Evaluating the commutator $[\hat{\sigma}_{eg}, H_F]$ yields zero since these quantities commute with one another. This removes the $H_F$ term from (2.26), leaving two separable terms:

$$\frac{d\hat{\sigma}_{eg}}{dt} = -\frac{i}{\hbar} [\hat{\sigma}_{eg}, H_A + H_I] = -\frac{i}{\hbar} [\hat{\sigma}_{eg}, H_A] - \frac{i}{\hbar} [\hat{\sigma}_{eg}, H_I]$$

(2.27)

The full equation of motion will then be found by analysing these two terms.

In order to analyse the first term, the expression for the atomic operator given in (2.19) is introduced. The operator is defined between states $e$ and $g$, representing the excited and ground states of the atom.

$$-\frac{i}{\hbar} [\hat{\sigma}_{eg}, H_A] = -\frac{i}{\hbar} (\hat{\sigma}_{eg} H_A - H_A \hat{\sigma}_{eg})$$

$$= -\frac{i}{\hbar} (|e\rangle \langle g| H_A - H_A |e\rangle \langle g|)$$

(2.28)

Then using the expression for the atomic Hamiltonian (2.21) in the above equation, the following is obtained:

$$-\frac{i}{\hbar} [\hat{\sigma}_{eg}, H_A] = -\sum_i \delta_{eg} |i\rangle \langle i| + \sum_i \delta_{ie} |i\rangle \langle i|$$

(2.29)

The inner product $\langle g|i \rangle$ between two orthogonal basis states $i$ and $j$ is defined by the Kronecker delta function $\delta_{ij}$, which evaluates to unity when $i = j$ and zero otherwise. This removes all terms from the first summation where $i \neq g$ and removes from the second summation the terms where $i \neq e$. Both summations therefore disappear leaving

$$\frac{i}{\hbar} [\hat{\sigma}_{eg}, H_A] = -i(\omega_g - \omega_e)\hat{\sigma}_{eg}$$

(2.30)

as the expression for the commutator involving the atomic Hamiltonian, where the remaining inner product has been rewritten as the atomic operator. The calculation for the second term in (2.27), which represents the interaction, is more involved and will be the subject of the remainder of this section. The
commutator involving the interaction Hamiltonian may be expanded as before to give:

\[
-\frac{i}{\hbar} [\hat{\sigma}_{eg}, H_I] = -\frac{i}{\hbar} (\hat{\sigma}_{eg} H_I - H_I \hat{\sigma}_{eg}) = -\frac{i}{\hbar} |e\rangle \langle H_I | e\rangle + \frac{i}{\hbar} H_I |e\rangle \langle g| \tag{2.31}
\]

The interaction Hamiltonian $H_I$ was specified in (2.23). Using this, the preceding expression for the commutator now becomes:

\[
-\frac{i}{\hbar} [\hat{\sigma}_{eg}, H_I] = -i \sum_{\lambda'} \sum_{e'} \sum_{g'} \left( g_{eg'}^{X'} |e\rangle \langle g'| a_{\lambda} e^{i k_{\lambda x} z} + g_{eg'}^{X'} a_{\lambda}^{\dagger} e^{-i k_{\lambda x} z} |e\rangle \langle g'| \langle e'| \langle e| \right) \right.
+ \left. i \sum_{\lambda'} \sum_{e'} \sum_{g'} \left( g_{eg'}^{X'} |e\rangle \langle g'| a_{\lambda} e^{i k_{\lambda x} z} + g_{eg'}^{X'} a_{\lambda}^{\dagger} e^{-i k_{\lambda x} z} |g'| \langle e'| \langle e| \right) \right.
\]

\[
\] 

(2.32)

The terms containing $\langle g|e'\rangle$ and $\langle g'|e\rangle$ evaluate to zero since the ground and excited states are orthogonal. This removes the terms containing the annihilation operator. This is to be expected as this is an expression describing an excited to ground state transition where a photon would be created, not annihilated. With these terms removed the expression reduces to:

\[
-\frac{i}{\hbar} [\hat{\sigma}_{eg}, H_I] = -i \sum_{\lambda'} \sum_{e'} \sum_{g'} \left( g_{eg'}^{X'} a_{\lambda}^{\dagger} e^{i k_{\lambda x} z} \frac{|e\rangle \langle g'|}{\delta_{gg'}} \right)
+ \left. i \sum_{\lambda'} \sum_{e'} \sum_{g'} \left( g_{eg'}^{X'} a_{\lambda}^{\dagger} e^{-i k_{\lambda x} z} \frac{|g'| \langle e'| \langle e|}{\delta_{ee'}} \right) \right.
\]

\[
\] 

(2.33)

When summing over the $\delta_{gg'}$ and $\delta_{ee'}$ terms, the only nonzero terms are those where either $g = g'$ or $e = e'$. This eliminates the summation involving $g'$ from the first triple summation, and eliminates the $e'$ summation from the second triple sum. Additionally, this fixes one of the subscripts on each of the $g^{X'}$ coupling
coefficients. This leads to the expression:

$$\frac{-i}{\hbar} [\hat{\sigma}_{eg}, H_I] = -i \sum_{\lambda'} \sum_{e'} \left( g^{\lambda'\lambda}_{e'g} a^{\dagger}_{\lambda'} e^{-ik_{\lambda'}z} \hat{\sigma}_{ee'} \right)$$

$$+ i \sum_{\lambda'} \sum_{g'} \left( g^{\lambda'\lambda}_{eg} a^{\dagger}_{\lambda'} e^{-ik_{\lambda'}z} \hat{\sigma}_{gg'} \right)$$

(2.34)

where the atomic operator expression (2.19), was used to replace the remaining outer products.

The expressions for the field operators were defined earlier. Substituting the creation operator (2.25) into the previous expression gives the following result:

$$\frac{-i}{\hbar} [\hat{\sigma}_{eg}, H_I] = -i \sum_{\lambda'} \sum_{e'} \left( g^{\lambda'\lambda}_{e'g} a^{\dagger}_{\lambda'} (0) e^{+i(\omega_{\lambda'}t - k_{\lambda'}z)} \hat{\sigma}_{ee'} \right)$$

$$+ \sum_{\lambda'} \sum_{e'} \left( \sum_{e''} \sum_{g''} g^{\lambda'\lambda}_{e'g} g^{\lambda'}_{e''g''} \int_0^t \hat{\sigma}_{ee''} (t') e^{+i\omega_{\lambda'}(t-t')} dt' \right) \hat{\sigma}_{ee'}$$

$$+ i \sum_{\lambda'} \sum_{g'} \left( g^{\lambda'\lambda}_{eg} a^{\dagger}_{\lambda'} (0) e^{+i(\omega_{\lambda'}t - k_{\lambda'}z)} \hat{\sigma}_{gg'} \right)$$

$$- \sum_{\lambda'} \sum_{g'} \left( \sum_{e''} \sum_{g''} g^{\lambda'\lambda}_{eg} g^{\lambda'}_{e''g''} \int_0^t \hat{\sigma}_{ee''} (t') e^{+i\omega_{\lambda'}(t-t')} dt' \right) \hat{\sigma}_{gg'}$$

(2.35)

The application of normal ordering now becomes significant. Although the field operator $a^{\dagger}$ and the atomic operator commute with one another, this relation is no longer guaranteed to hold once the symbol for the field operator has been substituted by its full expression; the atomic operator does not commute with the constituent parts of the field operator, only the operator as a whole.

The integrals over $t'$ in (2.35) can be solved by taking the atomic operator (which is a function of $t'$) outside of the integral. In order to do this the harmonic approximation [75] is introduced. This approximation states that the integral will only contribute to the sum over the modes when $t \approx t'$. This is due to the rapidly oscillating field modes which quickly cancel each other out through destructive
interference as \( t \) and \( t' \) diverge. Therefore \( \hat{\sigma}(t') \) may be taken outside the integral, since this term only contributes when \( t \approx t' \).

Using the harmonic approximation, the equation of motion (2.27) may be used to form an expression for the atomic operator to be used inside the summation of the previous expression. This is an approximation which neglects the coupling of the atomic operator to the laser field, it is treated as if evolving freely. Therefore for the free atom, (2.27) may be rewritten:

\[
\frac{d\sigma_{eg}}{dt} = -\frac{i}{\hbar} [\sigma_{eg}, H_A]
\] (2.36)

The expression for the time evolution of the atomic Hamiltonian previously derived in (2.30), may be applied to the preceding equation:

\[
\frac{d\sigma_{eg}}{dt} = -i (\omega_g - \omega_e) \sigma_{eg}
\] (2.37)

This differential equation may be solved using the standard methods:

\[
\int_t^{t'} \frac{d\sigma_{eg}}{\sigma_{eg}} = -i (\omega_g - \omega_e) \int_{t'}^t dt
\]

\[
\ln (\sigma_{eg} (t')) - \ln (\sigma_{eg} (t)) = +i (\omega_g - \omega_e) (t - t')
\]

\[
\sigma_{eg} (t') = \sigma_{eg} (t) e^{i(\omega_g - \omega_e)(t-t')}
\] (2.38)

This is an equation which describes the coherences between the excited and ground state as the atomic operator evolves with time. As the harmonic approximation has been made, this does not consider the effect of the interaction Hamiltonian, \( H_I \). This expression includes an exponential term that implies the atom freely oscillates cosinusoidally between the ground and excited states, with a frequency \( \Delta \omega = (\omega_g - \omega_e) \). This oscillation is not measurable since taking the expectation value of the operator would the remove the exponential term from the expression.

A similar expression can be derived which describes the coherences between
the ground and excited states:

\[
\sigma_{ge}(t') = \sigma_{ge}(t) e^{i(\omega_e - \omega_g)(t-t')}
\]  

(2.39)

By using the result from the freely evolving atomic operator (2.38) and substituting this back into (2.35):

\[
-\frac{i}{\hbar} [\hat{\sigma}_{eg}, H_I] = -i \sum_{\lambda'} \sum_{e'} g_{e'g}^{\lambda'*} a_{\lambda'}^\dagger(0) e^{+i(\omega_{\lambda'}-k_{\lambda'}z)(t-t')} \hat{\sigma}_{ee'}
\]

\[
+ \sum_{\lambda'} \sum_{e'} \left( \sum_{\lambda''} \sum_{e''} g_{e'g}^{\lambda'*} g_{e''g}^{\lambda''*} \hat{\sigma}_{e'e''} \int_0^t e^{+i(\omega_{\lambda'}-\omega_{e''}+\omega_{g''})(t-t')} dt' \right) \hat{\sigma}_{ee'}
\]

\[
+ i \sum_{\lambda'} \sum_{g'} g_{eg}^{\lambda'*} a_{\lambda'}^\dagger(0) e^{+i(\omega_{\lambda'}-k_{\lambda'}z)(t-t')} \hat{\sigma}_{g'g}
\]

\[
- \sum_{\lambda'} \sum_{g'} \left( \sum_{e''} \sum_{g''} g_{eg}^{\lambda'*} g_{e''g''}^{\lambda''*} \hat{\sigma}_{e'e''} \int_0^t e^{i(\omega_{\lambda'}-\omega_{e''}+\omega_{g''})(t-t')} dt' \right) \hat{\sigma}_{g'g}
\]  

(2.40)

The two integral terms in the expression are identical. With the atomic operator taken outside the integration, the term may be evaluated:

\[
\int_0^t e^{+i(\omega_{\lambda'}-\omega_{e''}+\omega_{g''})(t-t')} dt' = e^{+i(\omega_{\lambda'}-\omega_{e''}+\omega_{g''})t} \int_0^t e^{-i(\omega_{\lambda'}-\omega_{e''}+\omega_{g''})t'} dt' = e^{+i(\omega_{\lambda'}-\omega_{e''}+\omega_{g''})t} \left[ e^{-i(\omega_{\lambda'}-\omega_{e''}+\omega_{g''})t'} \right]^t_0
\]

\[
= e^{+i(\omega_{\lambda'}-\omega_{e''}+\omega_{g''})t} - e^{i(\omega_{\lambda'}-\omega_{e''}+\omega_{g''})t} = \frac{1 - e^{+i(\omega_{\lambda'}-\omega_{e''}+\omega_{g''})t}}{(\omega_{\lambda'} - \omega_{e''} + \omega_{g''})}
\]

(2.41)

Then re-expressing \( e \) in terms of the trigonometric functions yields the following
expression for the integral term.

\[
\int_0^t e^{i(\omega_\lambda - \omega_e + \omega_g)(t-t')} dt' = \frac{\sin \left( (\omega_\lambda - \omega_e + \omega_g) t \right)}{(\omega_\lambda - \omega_e + \omega_g)} + \frac{1 - \cos \left( (\omega_\lambda - \omega_e + \omega_g) t \right)}{(\omega_\lambda - \omega_e + \omega_g)}
\]

This expression can be simplified by considering only what happens at large \(t\), that is, in the steady state once the transient behaviour has died away. This implies that the expression should be evaluated in the limit where \(t \to \infty\). As the laser frequency \(\omega_\lambda\) is resonant with the transition, additionally the term \((\omega_\lambda - \omega_e + \omega_g) \to 0\). In the limit \(t \to \infty\), the term in (2.42) involving cosine vanishes:

\[
\lim_{t \to \infty} \frac{1 - \cos \left( (\omega_\lambda - \omega_e + \omega_g) t \right)}{(\omega_\lambda - \omega_e + \omega_g)} \to 0
\]

The term involving sine can be simplified to

\[
\lim_{t \to \infty} \frac{\sin \left( (\omega_\lambda - \omega_e + \omega_g) t \right)}{(\omega_\lambda - \omega_e + \omega_g)} = \frac{\pi}{(\omega_\lambda - \omega_e + \omega_g)} \delta (\omega_\lambda - \omega_e + \omega_g)
\]

where the delta function \(\delta(x)\) is defined to be unity at \(x = 0\) and zero everywhere else. The integral from (2.40) therefore evaluates to the following as \(t\) tends to infinity:

\[
\int_0^t e^{i(\omega_\lambda - \omega_e + \omega_g)(t-t')} dt' \to \pi \delta (\omega_\lambda - \omega_e + \omega_g)
\]

This expression may then be used in the expression for the commutator in (2.40). With both of the terms from (2.27) now evaluated, the full equation of
motion for the atomic operator can be expressed as:

\[
\frac{d\hat{\sigma}_{eg}}{dt} = -i(\omega_g - \omega_e) \hat{\sigma}_{eg} - i \sum_{\lambda'} \sum_{e'} g_{e'g}^{\lambda'} a_{\lambda'}(0) e^{+i(\omega_{\lambda'}t - k_{\lambda'}z)} \hat{\sigma}_{ee'} + i \sum_{\lambda'} \sum_{g''} g_{e'g}^{\lambda'} a_{\lambda'} (0) e^{+i(\omega_{\lambda'}t - k_{\lambda'}z)} \hat{\sigma}_{g'g} - \sum_{\lambda'} \sum_{g''} \sum_{e'} g_{e'g}^{\lambda'} g_{e'g}^{\lambda'} \hat{\sigma}_{ee'} \pi \delta (\omega_{\lambda'} - \omega_{e'} + \omega_{g'}) \tag{2.46}
\]

2.3.2 Transformation to Slowly Varying Operators

The expression for the atomic operator (2.46) contains exponential terms which oscillate at the optical frequency of the transition. These oscillations are too rapid to be measured by the experiment and can be eliminated from the operator equations by transforming to slowly varying operators, denoted by \(\chi\), using the transforms:

\[
\sigma_{eg} = \chi_{eg} e^{i(\omega_L t - k_L z)} \\
\sigma_{gg'} = \chi_{gg'} \\
\sigma_{ee'} = \chi_{ee'} \tag{2.47}
\]

The addition of the exponential term, oscillating at a frequency \(\omega_L\) will cancel with the rapidly oscillating terms in the equation of motion. Differentiating the expression for \(\chi_{eg}\) gives:

\[
\frac{d\sigma_{eg}}{dt} = \frac{d\chi_{eg}}{dt} e^{i(\omega_L t - k_L z)} + i\omega_L \chi_{eg} e^{i(\omega_L t - k_L z)} - ik_L \frac{dz}{dt} \chi_{eg} e^{i(\omega_L t - k_L z)} - i k_L v_z \chi_{eg} e^{i(\omega_L t - k_L z)} \tag{2.48}
\]

where the quantity \(v_z = \frac{dz}{dt}\).

Equating this result with the expression for the atomic operator (2.46), and using the substitutions (2.47) gives the equation of motion in terms of the slowly
varying operator:

\[
\frac{d\chi_{eg}}{dt} = -i (\omega_L - k_L v_z - \omega_{eg}) \chi_{eg}
- i \sum_{\lambda} \sum_{e'} g^\lambda_{e'g} a^+_\lambda (0) e^{+i((\omega_{\lambda} - \omega_{L})t - (k_{\lambda} - k_L)z)} \chi_{ee'}
+ i \sum_{\lambda} \sum_{g'} g^\lambda_{eg'} a^+_\lambda (0) e^{+i((\omega_{\lambda} - \omega_{L})t - (k_{\lambda} - k_L)z)} \chi_{g'g}
- \sum_{\lambda} \sum_{g'} \sum_{e'} g^\lambda_{eg'} g^\lambda_{e'g'} \chi_{ee'} \pi \delta (\omega_{\lambda} - \omega_{e'} + \omega_{g'})
\]

(2.49)

The laser operates on a single mode with \( \lambda = L \). The Doppler detuning \( \Delta_{L,eg} \) is separated out in the first term of the expression and is proportional to the velocity \( v_z \) when the laser is on resonance:

\[
\Delta_{L,eg} = \omega_L - k_L v_z - \omega_{eg}
\]

(2.50)

To obtain a measurable quantity of the system, the expectation value of the slowly varying operator equation of motion (2.49) must be taken. The expectation value of an operator is formed by ‘sandwiching’ the slowly varying operator between the bra and ket for the wavefunction, and is denoted by an angle bracket around the operators. The equation (2.49) may be written in terms of expectation values as:

\[
\langle \dot{\chi}_{eg} \rangle = -i \Delta_{L,eg} \langle \chi_{eg} \rangle - i \sum_{L} \sum_{e'} \Omega^L_{ee'} \langle \chi_{ee'} \rangle + i \sum_{L} \sum_{g'} \Omega^L_{eg'} \langle \chi_{g'g} \rangle
- \sum_{\lambda} \sum_{g'} \sum_{e'} g^\lambda_{eg'} g^\lambda_{e'g'} \langle \chi_{ee'} \rangle \pi \delta (\omega_{\lambda} - \omega_{e'} + \omega_{g'})
\]

(2.51)

where \( \Omega_L \) is the half-Rabi frequency, given by:

\[
\Omega^L_{eg} = g^L_{eg} \langle a^\dagger_L (0) \rangle = g^L_{eg} \langle a_L (0) \rangle
\]

(2.52)
The expectation values may be re-expressed as follows:

\[
\langle \chi_{eg} \rangle = \langle \Psi | \chi_{eg} | \Psi \rangle
\]
\[
= \langle \Psi | \sigma_{eg} | \Psi \rangle
\]
\[
= \langle \Psi | e \rangle \langle g | \Psi \rangle
\]
\[
= (\langle e | \Psi \rangle \langle \Psi | g \rangle)^* \tag{2.53}
\]

where the exponential term from (2.47) has been dropped for the part of the expression containing \(\sigma_{eg}\) as taking the expectation value causes the exponential term to vanish. On the final line the conjugate has been taken which swaps the ordering of the bra-kets to form an outer product. The density operator \(\rho\) is formed from the outer product as shown in equation (2.7), and so the expectation value can be directly related to the density matrix element:

\[
\langle \chi_{eg} \rangle = (\langle e | \Psi \rangle \langle \Psi | g \rangle)^* = \rho_{eg}^* = \rho_{ge} \tag{2.54}
\]

Hence a rate equation is found for the coherences between the upper and lower state, given by:

\[
\dot{\rho}_{ge} = -i\Delta_{eg}\rho_{ge} - i \sum_L \sum_{e'} \Omega^L_{e'g}\rho_{e'e} + i \sum_L \sum_{g'} \Omega^L_{eg'}\rho_{gg'} + i \sum_{\lambda} \sum_{g'} \sum_{e'} \rho_{ge'} G_{eg'}^\lambda G_{g'e'}^\lambda \pi \delta (\omega_{e'} - \Delta_{e'g'}) \tag{2.55}
\]

where \(\Delta_{eg} = \omega_e - \omega_g\). This gives the time evolution of the two off-diagonal elements of the density matrix for the two level system, since \(\dot{\rho}_{eg}\) is simply the complex conjugate of \(\dot{\rho}_{ge}\).

To find the diagonal elements in the density matrix, the process outlined in this and the previous section to formulate an expression for \(\rho_{eg}\) was repeated for
\[ \dot{\rho}_{gg}^{''} = -i (\omega_g - \omega_g^{''}) \rho_{gg}^{''} + i \sum L \sum e \Omega_{eg}^{L} \rho_{ge}^{''} - i \sum L \sum e \Omega_{eg}^{L} \rho_{eg}^{''} \]
\[ + \sum \lambda \sum e' \sum e'' g_{e'g}^{\lambda} g_{e''g}^{\lambda} \pi \delta (\Delta_{e'g}^{''} - \omega_{\lambda}) \rho_{e'g}^{''} \]
\[ + \sum \lambda \sum e' \sum e'' g_{e'g}^{\lambda} g_{e''g}^{\lambda} \pi \delta (\omega_{\lambda} - \Delta_{e''g}^{''}) \rho_{e''g}^{''} \]
\[ \dot{\rho}_{ee}^{''} = -i (\omega_e - \omega_e^{''}) \rho_{ee}^{''} + i \sum L \sum g \Omega_{eg}^{L} \rho_{ge}^{''} - i \sum L \sum g \Omega_{eg}^{L} \rho_{eg}^{''} \]
\[ - \sum \lambda \sum g' \sum e' g_{e'g}^{\lambda} g_{e''g}^{\lambda*} \pi \delta (\Delta_{e'g}^{''} - \omega_{\lambda}) \rho_{e'g}^{''} \]
\[ - \sum \lambda \sum g' \sum e' g_{e'g}^{\lambda} g_{e''g}^{\lambda*} \pi \delta (\omega_{\lambda} - \Delta_{e''g}^{''}) \rho_{e''g}^{''} \]

In these equations, the terms containing \( \Omega^{L} \) correspond to stimulated emission and absorption. The \( g^{\lambda} \) terms are spontaneous emission. Hence equations (2.55), (2.56), and (2.57) form a set of coupled differential equations that describe the time evolution of the system under study.

\subsection*{2.3.3 The Two-Level System in Calcium}

Figure 2.5 is a schematic diagram of the relevant states for excitation to the \( 4^1P_1 \) level in calcium. The excited state is given by three degenerate magnetic substates. There is only one ground state \(|1\rangle\). The three excited substates corresponding to \( m_j = -1, 0, +1 \) are labelled \(|2\rangle, |3\rangle \) and \(|4\rangle \) respectively.

The density matrix was introduced for the P-state in Section 2.2.3. The \( 4^1P_1 \) state has three substates and so can be fully represented by a \( 3 \times 3 \) density matrix. To represent the 4 level system, which includes the \( 4^1S_0 \) state, a \( 4 \times 4 \) density
The 3 × 3 submatrix at the bottom right is the density matrix for the P-state, where states $|−1\rangle$, $|0\rangle$ and $|+1\rangle$ have been renamed $|2\rangle$, $|3\rangle$ and $|4\rangle$. The submatrix $ρ_{11}$ defines the ground state. As before the elements along the diagonal represent the populations in each state. The remaining elements represent the optical coherences between the S- and P-states.

The two-level system in calcium is formed between the ground state $|1\rangle$ and one of the excited state magnetic sublevels $|2\rangle$, $|3\rangle$ or $|4\rangle$. Optical selection rules limit the level which may be excited; a $σ^−$ polarised photon may only excite the $|2\rangle$ sublevel, where $m_L = −1$, and similarly the $|3\rangle$ and $|4\rangle$ levels may only be excited by $π$ or $σ^+$ polarised radiation. The excited state may then decay back to the ground state $|1\rangle$, emitting a photon of the same polarisation in this system.

For the case of $σ^−$ excitation, the populations in levels $|3\rangle$ and $|4\rangle$ are assumed to be zero since transitions to these states are never made. The reduced density
matrix is then written as

\[
\rho = \begin{pmatrix}
\rho_{11} & \rho_{12} & 0 & 0 \\
\rho_{21} & \rho_{22} & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{pmatrix} = \begin{pmatrix}
\rho_{11} \\
\rho_{12} \\
\rho_{21} \\
\rho_{22}
\end{pmatrix}
\] (2.59)

where the states that are not involved in the transition have been omitted for clarity.

Before finding the expressions for the density matrix elements \(\rho_{ij}\), the equation for the generalised decay constants [76] is introduced, as this parameter appears in the rate equations:

\[
\Gamma_{ege'} = \sum_{\lambda} \left[ g_{e'g}^{\lambda} g_{eg}^{\lambda*} \pi \delta (\omega_{\lambda} - \Delta_{e'g}) + g_{e'g}^{\lambda} g_{eg}^{\lambda*} \pi \delta (\omega_{\lambda} - \Delta_{eg}) \right]
\] (2.60)

When there is only one excited and one ground state involved in the transition, this term reduces to:

\[
\Gamma_{e} = \sum_{\lambda} \Gamma_{e\lambda} = 2 \sum_{\lambda} \left| g_{e\lambda} \right|^2 \pi \delta (\omega_{\lambda} - \Delta_{e\lambda})
\]

\[
\Rightarrow \Gamma_{e} = \sum_{g} \Gamma_{e\lambda} = 2 \sum_{g} \sum_{\lambda} \left| g_{eg}^{\lambda*} \right|^2 \pi \delta (\omega_{\lambda} - \Delta_{eg})
\] (2.61)

The inverse of the decay constant, \(\Gamma_{e}^{-1}\), represents the lifetime of the excited state, which is 4.6 ns.

The general equations derived for the density matrix elements \(\rho_{ij}\) may now be used to calculate the evolution of the atomic states for the specific case of \(\sigma^-\) excitation. This occurs between the ground state \(|1\rangle\) and the excited state \(|2\rangle\).

Four separate equations are required to describe the time evolution of the system. These correspond to the four entries in the reduced density matrix (2.59). To begin with, the \(\rho_{11}\) term in the density matrix is evaluated. The equation for \(\rho_{gg'}\) (2.56) describes the time evolution of the ground states. In this case there
is only one ground state and so \( g = g'' = 1 \). Hence from equation (2.56):

\[
\dot{\rho}_{11} = -i (\omega_1 - \omega_1) \rho_{11} + i \sum_L \sum_e \Omega^L_{e_1} \rho_{1e} - i \sum_L \sum_e \Omega^L_{e_1} \rho_{e1} \\
+ \sum_\lambda \sum_{e'} \sum_{e''} g_{e'1}^e g_{e''1}^e \pi \delta (\Delta_{e''1} - \omega_\lambda) \rho_{e''e'} \\
+ \sum_\lambda \sum_{e'} \sum_{e''} g_{e''1}^e g_{e'1}^e \pi \delta (\omega_\lambda - \Delta_{e'1}) \rho_{e'e''}
\]

(2.62)

In the above equation, the first term evaluates to zero. Each of the double sum terms act to sum over only a single excited state \( e = 1 \), and a single field mode \( L(\sigma^-) = -1 \). In a similar manner, the triple summations also collapse to a single term each. The reduced density matrix element can then be rewritten:

\[
\dot{\rho}_{11} = i \Omega^{-1}_{21} (\rho_{12} - \rho_{21}) + 2 |g_{21}^{-1}|^2 \pi \delta (\Delta_{21} - \omega_{-1}) \rho_{22} \\
= i \Omega^{-1}_{21} (\rho_{12} - \rho_{21}) + \Gamma_{21} \rho_{22}
\]

(2.63)

where the expression for the generalised decay constant (2.61) has been used.

Similarly for the \( \rho_{22} \) term, equation (2.57) is used to calculate the density matrix element:

\[
\dot{\rho}_{22} = i \Omega^{-1}_{21} (\rho_{22} - \rho_{21}) - 2 |g_{21}^{-1}|^2 \pi \delta (\Delta_{21} - \omega_{-1}) \rho_{22} \\
\Rightarrow \dot{\rho}_{22} = i \Omega^{-1}_{21} (\rho_{22} - \rho_{21}) - \Gamma_{21} \rho_{22}
\]

(2.64)

To find the \( \rho_{12} \) term equation (2.55) is used:

\[
\dot{\rho}_{12} = i \Omega^{-1}_{21} (\rho_{11} - \rho_{22}) - \left[ \frac{\Gamma_{21}}{2} + i \Delta_{L,21} \right] \rho_{12}
\]

(2.65)

As the density matrix is Hermitian, \( \rho_{21} \) can be found by taking the complex conjugate of the equation above, which gives the final density matrix element:

\[
\dot{\rho}_{21} = i \Omega^{-1}_{21} (\rho_{22} - \rho_{11}) - \left[ \frac{\Gamma_{21}}{2} - i \Delta_{L,21} \right] \rho_{21}
\]

(2.66)

In summary, the four rate equations which specify the elements of the reduced
density matrix representing the two-level system for $\sigma^-$ excitation are given by:

$$
\dot{\rho}_{11} = i\Omega_{21}^{-1} (\rho_{12} - \rho_{21}) + \Gamma_{21}\rho_{22}
$$

$$
\dot{\rho}_{22} = i\Omega_{21}^{-1} (\rho_{21} - \rho_{12}) - \Gamma_{21}\rho_{22}
$$

$$
\dot{\rho}_{12} = i\Omega_{21}^{-1} (\rho_{11} - \rho_{22}) - \left[ \frac{\Gamma_{21}}{2} + i\Delta_{L,21} \right] \rho_{12}
$$

$$
\dot{\rho}_{21} = i\Omega_{21}^{-1} (\rho_{22} - \rho_{11}) + \left[ \frac{\Gamma_{21}}{2} - i\Delta_{L,21} \right] \rho_{21}
$$

(2.67)

In order to evaluate the transient behaviour of the system, these four rate equations were recast as a single matrix equation,

$$
\dot{y} = Ay
$$

(2.68)

where $y$ is a column vector which represents the four density matrix elements in an arbitrary order, and $A$ is a matrix of complex coefficients. Rewriting the above matrix equation in full then gives:

$$
\begin{pmatrix}
\dot{\rho}_{11} \\
\dot{\rho}_{22} \\
\dot{\rho}_{12} \\
\dot{\rho}_{21}
\end{pmatrix} =
\begin{pmatrix}
0 & +\Gamma_{21} & +i\Omega_{21}^{-1} & -i\Omega_{21}^{-1} \\
0 & -\Gamma_{21} & -i\Omega_{21}^{-1} & +i\Omega_{21}^{-1} \\
+i\Omega_{21}^{-1} & -i\Omega_{21}^{-1} & \frac{\Gamma_{21}}{2} + i\Delta_{L,21} & 0 \\
-i\Omega_{21}^{-1} & +i\Omega_{21}^{-1} & 0 & -\frac{\Gamma_{21}}{2} - i\Delta_{L,21}
\end{pmatrix}
\begin{pmatrix}
\rho_{11} \\
\rho_{22} \\
\rho_{12} \\
\rho_{21}
\end{pmatrix}
$$

(2.69)

A computer program, MATLAB [77], was used to find a numerical solution for this system of linear differential equations. The values from Table 2.1 were used to calculate the values for the matrix elements. The results are shown in Fig. 2.6 for a 50 ns period starting at the point where the atom is initially excited by the laser.

The atom is seen to exhibit Rabi oscillations, which are rapidly damped within the 50 ns time period shown on the graph. This damping is caused by spontaneous emission from the atom in the upper state, which acts to dephase the transition from the coherent laser excitation.
Figure 2.6: Time evolution of the state populations in calcium, illustrating Rabi oscillations. The probability of finding an atom in either state is shown on the vertical axis, time is represented on the horizontal axis.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Value</th>
<th>Units</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$I$</td>
<td>25</td>
<td>mW/mm²</td>
<td>Laser intensity</td>
</tr>
<tr>
<td>$\Omega_{21}^{-1}$</td>
<td>$9.95 \times 10^7 \times \sqrt{I}$</td>
<td>rad s⁻¹</td>
<td>Rabi frequency</td>
</tr>
<tr>
<td>$\Gamma_{21}$</td>
<td>$2.2 \times 10^8$</td>
<td>rad s⁻¹</td>
<td>Decay constant</td>
</tr>
<tr>
<td>$\Delta_{21}$</td>
<td>0</td>
<td>rad s⁻¹</td>
<td>Laser detuning parameter</td>
</tr>
</tbody>
</table>

Table 2.1: Values used for numerical calculation of Rabi oscillations for $\sigma^-$ excitation shown in Fig. 2.6. The laser intensity is a typical value for the super-elastic experiment. The Rabi frequency is quoted from the calculation by Murray and Cvejanovic [53], and the decay constant is taken from the NIST database [78]. The laser is modelled to be on resonance and so the detuning parameter is zero.
The steady state populations can be found by solving the rate equations (2.67) with all time derivatives set to zero. This gives the excited steady state population, \( \rho_{22}^{ss} \) as:

\[
\rho_{22}^{ss} = \frac{2 \left( \Omega_{21}^{-1} \right)^2}{\Gamma^2 + 4 \Delta_{21}^2 + 8 \left( \Omega_{21}^{-1} \right)^2} = 0.49
\]  

(2.70)

and so in this example, almost half of the atoms in this model are in the excited state, with the remainder in the ground state.

So far in this section, the two-level system formed by \( \sigma^- \) laser excitation from the \( |1\rangle \) ground state to the \( |2\rangle \) excited state has been discussed. Excitation with \( \pi \) or \( \sigma^+ \) radiation also forms a two-level system, with states \( |3\rangle \) or \( |4\rangle \). The process of deriving the rate equations is very similar to the process already described, so this shall be omitted and the results displayed directly below for \( \pi \) excitation:

\[
\dot{\rho}_{11} = i \Omega_{31}^0 (\rho_{13} - \rho_{31}) + \Gamma_{31} \rho_{33} \\
\dot{\rho}_{33} = i \Omega_{31}^0 (\rho_{31} - \rho_{13}) - \Gamma_{31} \rho_{33} \\
\dot{\rho}_{13} = i \Omega_{31}^0 (\rho_{11} - \rho_{33}) - \left[ \frac{\Gamma_{31}}{2} + i \Delta_{L,31} \right] \rho_{13} \\
\dot{\rho}_{31} = i \Omega_{31}^0 (\rho_{33} - \rho_{11}) - \left[ \frac{\Gamma_{31}}{2} - i \Delta_{L,31} \right] \rho_{31}
\]  

(2.71)

Finally the rate equations for \( \sigma^+ \) excitation are:

\[
\dot{\rho}_{11} = i \Omega_{41}^{+1} (\rho_{14} - \rho_{41}) + \Gamma_{41} \rho_{44} \\
\dot{\rho}_{44} = i \Omega_{41}^{+1} (\rho_{41} - \rho_{14}) - \Gamma_{41} \rho_{44} \\
\dot{\rho}_{14} = i \Omega_{41}^{+1} (\rho_{11} - \rho_{44}) - \left[ \frac{\Gamma_{41}}{2} + i \Delta_{L,41} \right] \rho_{14} \\
\dot{\rho}_{41} = i \Omega_{41}^{+1} (\rho_{44} - \rho_{11}) - \left[ \frac{\Gamma_{41}}{2} - i \Delta_{L,41} \right] \rho_{41}
\]  

(2.72)

It should be noted that the choice of polarisation axis for \( \pi \) polarised radiation used in the above derivation is parallel to the polarisation axis of the beam. For \( \sigma \) polarised radiation, the choice of polarisation axis is parallel to the propagation direction of the laser beam. The density matrix for \( \pi \) excitation can be transformed to one where the quantisation axis is in the natural frame by using
a coordinate transformation. This process is detailed by Murray, MacGillivray and Hussey [79].

The preceding sets of rate equations may be solved in a similar manner to predict the time evolution of the atomic system. This provides identical results as for the $\sigma^{-}$ excitation due to symmetry arguments.

### 2.4 Summary

In this chapter, the theory relating to a super-elastic electron scattering experiment from the $4^1P_1$ state of calcium was presented and discussed. This discussion began with the theoretical formalism used to describe the results of the electron scattering experiment. This was presented in terms of an equivalent coincidence experiment, where an inelastically scattered electron is detected together with a scattered photon.

For such an interaction, a discussion of the ACPs was presented. These were shown to describe the alignment and orientation of a laser excited P-state. These parameters are also related to the values of the density matrix elements for the excited atomic system in the natural frame. The density matrix elements can be related back to the theoretical scattering amplitudes, which are predicted by theoretical models of the scattering interaction. The results of such calculations are shown in Chapter 5.

In the remainder of the chapter, a QED model for laser excitation of the calcium atoms was presented. The derivation of the general equations of motion for the atomic operator was shown and these were used to find the elements of the atomic density matrix.

It was then shown that the transition between the $4^1S_0$ and $4^1P_1$ levels in calcium can be considered to form a two-level system and the expressions for the corresponding $2 \times 2$ density matrix were generated from the general equations of motion.
Using these QED calculations, it was shown that the populations of the system would oscillate between the ground and excited state on the application of laser radiation. These Rabi oscillations decay within $\sim 50\,\text{ns}$ as the system becomes dephased due to spontaneous radiative emission in the upper state. This time is short compared to the interaction time of the atoms in the laser field ($\sim 2\,\mu\text{s}$), and so to a good approximation the steady state solutions can be used to calculate the populations and coherences for the experiment.
Chapter 3

Experimental Apparatus

3.1 Overview

The electron scattering experiments are carried out in the scattering chamber. This is a vacuum sealed tank which is held at a low pressure of $3 \times 10^{-7}$ mbar. An oven inside the chamber emits calcium atoms which are the atomic target for these experiments. The calcium atoms are excited from the $4^1S_0$ ground state to the $4^1P_1$ state by a laser beam at $\sim 432$ nm which enters via a window in the top of the scattering chamber. An electron gun provides a source of electrons with a well defined momentum, and an electron analyser detects electrons of well defined momentum scattered from the atomic target.

The scattering experiment is controlled and measured by the equipment shown in Fig. 3.1. This is the block diagram for the spectrometer. All of the major connections between its component parts are shown. Table 3.1 presents a short description of all of the labels in the diagram, and lists the section where it is described in more detail.

This chapter covers the equipment that makes up the spectrometer, with the exception of the electron-optical power supplies and the controlling computer. These are described in Chapter 4.
Figure 3.1: System block diagram showing major connections between the equipment that makes up the spectrometer. See Table 3.1 for a description of the labels.
<table>
<thead>
<tr>
<th>Label</th>
<th>Description</th>
<th>Section</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>Vacuum chamber.</td>
<td>3.2</td>
</tr>
<tr>
<td>W1, W2</td>
<td>Windows.</td>
<td>—</td>
</tr>
<tr>
<td>FT1, FT2</td>
<td>Electrical feedthroughs.</td>
<td>—</td>
</tr>
<tr>
<td>ER</td>
<td>Equipment rack.</td>
<td>—</td>
</tr>
<tr>
<td>IG</td>
<td>Ion gauge.</td>
<td>3.2</td>
</tr>
<tr>
<td>IG CTL</td>
<td>Ion gauge controller.</td>
<td>3.2</td>
</tr>
<tr>
<td>G</td>
<td>Electron gun.</td>
<td>3.3.1</td>
</tr>
<tr>
<td>G Fil. PSU</td>
<td>Gun filament power supply.</td>
<td>3.3.1</td>
</tr>
<tr>
<td>FC</td>
<td>Faraday cup.</td>
<td>3.3.1</td>
</tr>
<tr>
<td>Electrom.</td>
<td>Electrometer.</td>
<td>3.3.1</td>
</tr>
<tr>
<td>A1</td>
<td>Electron energy analyser.</td>
<td>3.3.2</td>
</tr>
<tr>
<td>CEM HT</td>
<td>CEM high voltage supply.</td>
<td>3.3.3</td>
</tr>
<tr>
<td>CEM CFD</td>
<td>Electron counting electronics.</td>
<td>3.3.3</td>
</tr>
<tr>
<td>AS</td>
<td>Analyser stepper motor assembly.</td>
<td>3.3.4</td>
</tr>
<tr>
<td>A1 Driver</td>
<td>Analyser stepper motor driver.</td>
<td>3.3.4</td>
</tr>
<tr>
<td>OV</td>
<td>Atomic beam source.</td>
<td>3.4</td>
</tr>
<tr>
<td>Oven TA</td>
<td>Oven thermocouple amplifier.</td>
<td>3.4.4</td>
</tr>
<tr>
<td>Oven PSU</td>
<td>Oven current supply.</td>
<td>3.4.4</td>
</tr>
<tr>
<td>TR</td>
<td>Trace laser.</td>
<td>3.5</td>
</tr>
<tr>
<td>LDC</td>
<td>Laser diode controller.</td>
<td>3.5</td>
</tr>
<tr>
<td>Laser</td>
<td>Laser system including wavemeter.</td>
<td>3.6</td>
</tr>
<tr>
<td>WS</td>
<td>Wave-plate stepper motor.</td>
<td>3.7.2</td>
</tr>
<tr>
<td>WS Driver</td>
<td>Wave-plate stepper motor driver.</td>
<td>3.7.2</td>
</tr>
<tr>
<td>QPD</td>
<td>Quadrant photodiode.</td>
<td>3.7.5</td>
</tr>
<tr>
<td>QPD Lock</td>
<td>Laser locking controller.</td>
<td>3.7.5</td>
</tr>
<tr>
<td>EO PSUs</td>
<td>Electron-optics power supplies.</td>
<td>4.1 / 4.2</td>
</tr>
<tr>
<td>DAQ</td>
<td>Data acquisition card.</td>
<td>4.5.2</td>
</tr>
<tr>
<td>PC</td>
<td>Controlling PC.</td>
<td>4.5</td>
</tr>
</tbody>
</table>

**Table 3.1:** Explanation of labels from the block diagram in Fig. 3.1.
3.2 The Scattering Chamber

3.2.1 Introduction

The experimental apparatus, pictured in Fig. 3.2, sits inside a cylindrical tank. This is shielded with $\mu$-metal to cancel the effects of external magnetic fields to less than 3 mG.

A vacuum flange entirely covers the top of the tank, and the addition of an O-ring forms an airtight seal. Most of the equipment inside the spectrometer is mounted on a baseplate which is secured to the top flange with three long metal posts. The Faraday cup and the cold trap are mounted directly to the side of the vacuum chamber. A vacuum pumping system maintains a pressure of $3 \times 10^{-7}$ mbar, which is low enough to perform electron scattering experiments inside the chamber.

All of the materials used in the chamber are non-magnetic, and are selected to have minimal outgassing. The system is baked out when the oven heater and electron gun filament are heated. With the oven at full temperature, $\sim 800^\circ$C, the temperature measured by thermocouples on the baseplate reaches $\sim 60^\circ$C.

3.2.2 Vacuum System

The layout of the vacuum chamber and pumping system is shown in Fig. 3.3. When the spectrometer is operating, it is kept under vacuum by a 360 ls$^{-1}$ turbomolecular pump (T). This pump is a Leybold Turbvac 360, operated via a control unit, a Leybold Turbotronic NT 150/360 [80]. The baseline pressure for the chamber is $3 \times 10^{-7}$ mbar.

The turbopump is backed by a roughing pump, a BOC Edwards E1M18 single-stage direct drive rotary pump. A foreline trap FT1 installed on the pump inlet prevents oil vapour migrating into the chamber. Valve V1 is the vacuum system isolation valve. While the turbopump was operating this valve was open and the
Figure 3.2: Arrangement of the gun, analyser and oven inside the spectrometer. The gun and oven are fixed to the baseplate. The path of calcium atoms from the oven crosses the electron beam at the interaction region, where it may be excited by the laser beam. The analyser is attached to the turntable, which allows it to be rotated around the interaction region to detect scattered electrons over a large range of scattering angles.
Figure 3.3: The vacuum system.

R1, R2 – Rotary pumps.
V1-V4 – Valves.
TF – Top flange.
FT – Foreline trap.
T – Turbopump.
SS – Splinter shield.
RG – Regulator.
FC – Flexible coupler.
C – Chamber.
GL – Gas line.
GB – Gas bottle.
GJ – Gas jet nozzle.
CT – Cold trap.
LN – Liquid nitrogen.
DW – Dewar.
EX – Nitrogen exhaust pipe.
rotary pump was running. Additionally, before the turbopump is switched on, the rotary pump was used to bring the pressure down to at least $10^{-2}$ mbar. This prevents excessive strain on the turbopump as it spins up.

The roughing pump inlet connects to the turbopump exhaust via a flexible coupler FC. This reduces (but does not eliminate) the level of vibration from the roughing pump coupled into the chamber.

The pressure inside the chamber is measured by a Leybold ITR 90 Hot Ion Combi Gauge. This unit combines an ion gauge and a Pirani gauge to measure pressures from atmospheric down to $10^{-10}$ mbar [81]. A control box supplies power for the ion gauge, and exposes the pressure output from the ITR 90 head unit via a BNC analogue voltage output which connects to the controlling computer.

The pressure is continuously monitored while the oven is being heated and while the spectrometer is gathering data. If a failure occurs in the vacuum system, this allows the precise time of the failure to be to be obtained.

When the spectrometer was not in use, it was kept under vacuum to prevent contamination of the instruments in the spectrometer. When it needed to be opened for maintenance or examination, the chamber was vented to nitrogen via valve V4. Venting to nitrogen is preferable to venting to atmosphere since water vapour in the air can coat the surfaces in the spectrometer.

### 3.2.3 Gas Jet and Gas Delivery System

To calibrate the spectrometer, it was useful to be able to inject gas into the interaction region. To do this, a gas jet nozzle (GJ) was used. A screw connection at the rear connects to a flexible hose which was brought out to a feedthrough on the top flange. At this point a connection was made to the gas line GL via a needle valve V3.

The gas line (GL) was evacuated using the rotary pump R2. This is a BOC Edwards E2M8 two-stage direct drive rotary pump, with a maximum displace-
ment of $9.5 \text{ m}^3\text{h}^{-1}$ and an ultimate pressure of $2.5 \times 10^{-4} \text{ mbar}$ [82]. The gas line was evacuated by opening valve V2 while the rotary pump is running.

A gas bottle containing the target gas was connected to the gas line via regulator RG. The gas line was filled by first opening V2 to evacuate it, then closing V2 and opening the regulator to fill the line with the target gas. This process was repeated several times to flush the line. Then needle valve V3 was opened to allow gas into the interaction region.

### 3.2.4 Liquid Nitrogen Cold Trap and Refiller

The cold trap is located on the opposite side of the chamber from the atomic beam source. Atoms from the beam travel through the interaction region and are then deposited onto the cold trap. A gravity fed liquid nitrogen line holds the cold trap at a temperature of $\sim -200^\circ\text{C}$, and the calcium incident on the trap condenses at this surface. A brief discussion of the cold trap and its refilling apparatus follows, for a more complete description consult reference [83].

While running the spectrometer, it is undesirable for calcium vapour to be present outside of the atomic beam. For this reason the atomic beam source, described in Section 3.4, emits a well collimated beam into the chamber. The cold trap acts as a beam dump, preventing the calcium from escaping into the rest of the chamber where it may degrade the instruments or influence any measurements being taken.

The cold trap also helps to maintain a better vacuum inside the chamber as other gases present in the chamber will condense onto the cold trap or the liquid nitrogen pipes.

Two photographs of the cold trap are presented in Fig. 3.4. In Fig. 3.3 the trap is shown diagrammatically with the rest of the vacuum system, and is labelled CT. The trap is gravity fed from a dewar (DW) via thin walled stainless steel tubing. The reservoir of liquid nitrogen in the dewar is located above the trap,
so the liquid will fill the length of tubing below the fill level. Heat radiated from
the chamber heats the nitrogen and causes some of it to boil. This nitrogen gas
escapes via the exhaust pipe (EX). The pipe leaves the dewar enclosure at the
top and then bends back around into the dewar. This arrangement preserves low
temperature gas in the enclosure.

The dewar is a double walled container which holds the liquid nitrogen. The
space between the two walls is evacuated by the pumping system in the main
chamber. This minimises thermal conduction into the nitrogen. When filled
completely, and with the oven emitting, the nitrogen in the dewar can last for up
to 6 hours before it has all boiled away.

To keep the cold trap at low temperatures when the spectrometer is left unatt-
tended for longer than this, an automatic refiller was designed as reported in [84].
This controls a pump to fill the dewar from an external reservoir when the liquid
nitrogen fill level is low.

The fill level inside the dewar is detected by two green light emitting diodes
(LEDs). The voltage drop over the LEDs changes non-linearly with temperature,
and when they are immersed in the liquid nitrogen the voltage drop reduces substantially. They are each suspended from the top of the dewar; one near the top, at the maximum fill level; and one near the bottom, at the minimum fill level.

When the level of nitrogen in the dewar falls below the lower LED, the controller detects this and engages a cryopump to pump liquid nitrogen in from the external reservoir. This nitrogen is fed into the dewar through the entry at the top until the level of the liquid nitrogen is at the maximum fill level. The controller detects the change in the top LED voltage and disengages the pump to stop the filling process. By using such a system, the cold trap can remain operational until the external reservoir is exhausted, while ensuring that the cold trap in the chamber remains filled with liquid nitrogen.

The controller also provides current for a length of heater wire which is wrapped around the vacuum seal at the top of the dewar. This keeps the O-ring temperature raised to prevent a failure of the seal. A sudden inrush of atmosphere can cause damage to the electron source and would contaminate the calcium, so this is prevented by ensuring the seal is at a temperature above 0°C.

3.3 Electron Source and Detector

3.3.1 Electron Gun

To run the spectrometer, a beam of electrons is required with a well defined energy. This is aimed at the target atoms in the interaction region. Ideally the beam should be well collimated. For an electron beam, this is measured by the pencil angle, \( \alpha_0 \). The beam angle \( \theta_B \) of the beam should also be small. These conditions ensure that the beam is hitting the atomic target efficiently, and minimises the number of electrons making unwanted contact with other parts of the spectrometer. The electron gun has been designed to produce this type of high quality beam, and is described in this section.
The electrons which leave the gun are collected on the opposite wall of the chamber by a Faraday cup. This is connected to a sensitive electrometer and provides a good measure of the beam current. The electrometer is connected to the controlling computer which allows the beam current to be monitored and logged.

Figure 3.5 shows a schematic of the inside of the electron gun, described in detail in [85]. The gun is cylindrical in shape and is shown in cross-section. The power supplies for each element of the gun are shown as rectangles, with the name of the supply written inside in capitals, and a typical voltage written beside it. For example, the anode is held at ANODE potential, which is around 70 V. The power supplies themselves are discussed in Chapter 4.

The electrons are emitted from the cathode, which is a tungsten filament electrically heated by an Instek PC-3030 power supply set in constant current mode. At approximately 1.95 A, the filament is hot enough to produce electrons through thermionic emission. The rest of the elements in the gun form these electrons into a beam. A current of 1.95 A at the filament will produce a beam current of a few hundred nanoamps measured at the Faraday cup. By increasing the filament current to a maximum of 2.25 A, beam currents in excess of 10 µA are measured.

The gun is not energy selected, and so the resolution is determined by the emission width of the filament. For the tungsten filament, this is measured to be 0.6 eV.

Conceptually, the gun can be considered to be a series of lenses chosen to focus the beam of electrons to produce an image of the final 1 mm aperture at the interaction region. These electrostatic lenses are similar to thick optical lenses, albeit with higher aberration coefficients. Figure 3.6 is a computer simulation of the electron trajectories from the filament, as calculated by the computer package SIMION [86]. It shows how the beam of electrons is affected by the two lenses GL1 and GL2. These are the two triple-element aperture lenses which make up the electron gun, the properties of which are discussed in [87].
Figure 3.5: Internal layout of the elements of the electron gun. The gun is cylindrical and is drawn in cross section. Deflectors perpendicular to the $y$-axis are not shown for clarity. Deflectors D1, D2 and D3 are each made from four deflector plates, which are electrically isolated from the rest of the gun. Apertures before and after each set of deflectors shield the potential on the plates.
Figure 3.6: The electron gun as simulated in SIMION 7 [86]. The path of the electrons from the filament is shown in black, going across the page from left to right. Field lines of constant potential due to the electrostatic lens elements are drawn in red. The deflectors are omitted in the simulation as there are no mechanical misalignments in the computer model. Voltages and values are as labelled in Fig. 3.5. The gun brings the electron beam to a tight focus at the interaction region. Space charge effects are not simulated and are assumed to be negligible.
The first lens is formed from three potentials; ANODE, GL1B and GL1C. The second lens is formed from GL1C, GL2B and the final aperture of the gun, which is held at earth potential. Each lens is made from three lens apertures held at each of the lens potentials. This allow the gun to be constructed in a shorter length than would otherwise be possible.

The energy of the outgoing electron is selected by varying the gun energy (GUNE) potential. The filament is held at this potential, and the other power supplies are referenced to this supply. The final section of the gun is held at earth potential, and so electrons should leave the gun with a potential equal to $-V_{\text{GUNE}}$. In practice the electron work function at the tungsten filament means that the measured energy of the electrons will differ from this by up to 1.5 eV. This was measured periodically, see Section 5.2.1 for a full discussion.

The gun is constructed from several 310 grade stainless steel hollow cylinders, stacked end-to-end, and insulated from one another with PTFE spacers. The electrons leaving the filament are first shaped by the grid, which is a Pierce electrode, and are then accelerated into a beam by the anode. The two electrostatic lenses then shape the beam further.

At the points illustrated in Fig. 3.5, circular sheets of molybdenum with 1 mm holes at the centre form defining apertures through which the electron beam must pass. The lens apertures were constructed in a similar manner, with a larger hole size, and were also made from molybdenum.

To correct for any mechanical misalignment inside the gun, the first two sets of deflectors D1 and D2 help to steer the beam through the first and second defining apertures. The final set of deflectors D3 can be used to steer the output beam direction. Each deflector is made from two pairs of parallel plates. Each pair is in either the $x$- or $y$-plane (note that the figure only shows one of the pairs of plates for each deflector). The plates are held at symmetrically opposite voltages.

The gun is designed to produce an electron beam with zero beam angle and
a pencil angle of $\sim 2^\circ$ over a range of energies from $\sim 20\text{ eV}$ to $300\text{ eV}$.

### 3.3.2 Electron Energy Analyser

The analyser is built to detect electrons scattered from the interaction region. The design is similar to the analyser described in [88]. The analyser is capable of discriminating between electrons of different energies and scattering angles. Figure 3.7 presents a diagram of the analyser. Voltages to each of the electron-optical elements are controlled from a bank of power supplies.

The analyser is mounted on the edge of a turntable inside the scattering chamber. It is oriented such that it always points at the interaction region. The turntable can be rotated by turning a mechanical feedthrough on the top flange of the spectrometer. This rotates the analyser around the interaction region and so discriminates between electrons for a range of different scattering angles.

The scattering angles $\theta_e$ that can be accessed directly by the analyser lie in the scattering plane and run from $\theta_e = +145^\circ$ where it meets the electron gun, to $\theta_e = -97^\circ$ where the gas jet nozzle is situated. There are also limitations on some of the forward angles that can be accessed. A very high flux of electrons into the analyser can damage the instrument, so it must not be angled to face the gun ($-20^\circ < \theta_e < +20^\circ$), since this would be in the path of the forward scattered electrons. The analyser should also not be placed in front of the gas jet nozzle or the calcium beam.

A full range of scattering angles from $0^\circ$ to $180^\circ$ can be accessed if needed, using the MAC [59]. This consists of two electromagnets placed above and below the interaction region which apply a magnetic field that twists the path of incoming and outgoing electrons, allowing those scattered electrons which would otherwise be inaccessible to reach the detector. This was not used in the current experiments.

Electrons enter through an aperture in the cone at the front of the analyser.
Figure 3.7: The inside of the analyser, drawn in cross-section. Typical voltages are shown for each element so as to pass electrons to the cone with an energy of 40 eV. The A1IH voltage supply is electrically connected to the inner hemisphere (connection not shown in diagram). The entrance aperture is 6 mm across and defines a 5° angular resolution. A cylindrical lens stack with an inner diameter of 15 mm focuses the electron beam into the hemispherical energy selector. Electrons at the residual energy (A1RSE) are detected by the CEM.
They are then focussed by a triple-element cylindrical lens formed by the inside of the cone, which is connected to earth, A1L1B and A1AM. A set of deflectors placed after the lens correct for any mechanical misalignment so that the beam is aligned to pass through the first aperture. The design of the deflectors is the same as in the electron gun, with a pair of parallel plates in both the $x$– and $y$–planes.

A hemispherical energy selector, as first proposed in [89], discriminates between electrons at different energies. Electrons enter a region between two concentric hemispheres. The potential on the inner and outer hemispheres is controlled by the two power supplies A1IH and A1OH, respectively.

The analyser power supplies are referenced to the analyser residual energy, A1RSE. When an electron enters the analyser with an energy equal to the residual energy, its energy at the entrance to the hemisphere will be equal to the *pass energy* for the hemispherical selector. This pass energy is set by the analyser mean voltage, A1AM. The electric field causes the electron to follow a curved path around the hemisphere, illustrated by the dotted line on the diagram (Fig. 3.7). This leads it through the second aperture, where it is detected by the channel electron multiplier (CEM).

Electrons which do not enter the analyser at the residual energy will not be at the pass energy when they encounter the entrance to the selector. The path taken will curve either too much or too little, depending on whether the electron has an energy above or below the pass energy set by A1AM. The trajectory of such an electron will not take it through the second defining aperture, and so it will not be detected by the CEM.

The resolution of the analyser can be adjusted by changing the voltage, $V_0$ on A1AM and then adjusting A1IH and A1OH accordingly. The required formulae for calculating the hemisphere voltages $V_1$ and $V_2$ on the inner and outer
hemispheres are reproduced here from [90]:

\[ \begin{align*}
V_1 &= V_0(2R_0/R_2 - 1) \\
V_2 &= V_0(2R_0/R_2 - 1)
\end{align*} \]

The radii of the inner and outer hemispheres are \( R_1 \) and \( R_2 \) respectively. The radius \( R_0 \) is the radius between the two hemispheres and is defined as:

\[ R_0 = (R_1 + R_2)/2 \]

Smaller field gradients increase the resolution of the analyser, at the expense of lower count rates. With the analyser mean energy set to \( E_0 \), a good approximation to the resolution is given in [91] as

\[ \Delta E_s = E_0 \left[ 0.43 \frac{d}{R_0} + 0.25\alpha_0^2 \right] \]

where \( \alpha_0 \) is the pencil angle of the electron beam and \( d \) is the diameter of the hemisphere’s apertures. With the hemispheres set to the voltages shown in Fig. 3.7, this gives a resolution \( \Delta E_s \approx 0.02E_0 \) eV. This value was chosen to be similar to the gun resolution.

Electrons which reach the CEM are therefore energy selected. With an appropriate high voltage supply, and amplifying and counting electronics, individual electron events can be counted, each resolved at a specific angle and energy.

### 3.3.3 Detecting Electrons with a Channel Electron Multiplier

The CEM, pictured in Fig. 3.8, is a sensitive charged particle detector. It is used in the spectrometer to detect electrons which have scattered from target atoms in the interaction region. It is situated inside the analyser, as was shown in Fig. 3.7. The X719BL CEM used here is shaped as a hollow spiral, closed at one end and with an open cone at the other to allow electrons to enter. It is also
referred to as a *channeltron* in some literature.

Figure 3.9 shows how the CEM is configured to detect negatively charged particles. A high tension (HT) supply is used to apply a voltage of between +2.7 and +3.2 kV to the inside end of the spiral. A small bias voltage equal to A1AM is applied to the cone end so that it sits at the correct potential between the two hemispheres.

Electrons which enter the cone at the front of the detector are accelerated and will collide with the inside wall. This releases several more electrons, which are in turn accelerated and are then involved with more collisions with the detector wall. This creates an avalanche effect, whereby the initial interaction of a single electron at the cone end creates a measurable current at the other.
With the CEM configured in this way, it is possibly to detect and count single electrons reaching the detector. Each detection event causes a characteristic pulse, which is preamplified by a wideband amplifier, a Phillips 6954 B50. To reduce noise, the preamplifier is connected as close to the electrical feedthrough as is possible, using a short length of 50 Ω coaxial cable. The amplifier increases the pulse height from tens of millivolts up to around two volts. The output from the amplifier is fed into a constant fraction discriminator (CFD), an Ortec 584, which outputs a digital pulse for each of these detection events, suitable for input into counting electronics. Using a CFD here ensures that the timing of the pulse is independent of the pulse height, which may be important in any future experiments which rely on coincidence techniques.

Output from the CFD is taken to the computer, where electron counting is combined with control of other equipment. This allows the data to be recorded,
and is described in more detail in Section 4.5.

The CFD output is also split off into three different counting devices, housed inside the nuclear instrumentation module (NIM) crate with the CFD. These can be useful when manually tuning the device and for troubleshooting. A ratemeter, the Ortec 449-2, gives a quick visual indication of the count rate at the detector. It is also able to output an audible tone, with a higher pitch indicating a higher count rate, which is useful when the display is obscured. The second is a digital counter, the Ortec 771. It displays a count which shows how many detection events have occurred since it was last reset. An Ortec 871 is used as a timer to gate the Ortec 771, and this allows counts to be gathered over a predefined period of time.

3.3.4 Analyser Stepper Motor

The analyser is mounted on a turntable to allow it to rotate around the interaction region. The turntable is pictured in Fig. 3.10, and sits on top of a number of ruby balls arranged into a radial groove cut into the baseplate. When the turntable is rotated, the ruby balls roll along the groove, allowing the turntable to move freely.

A mechanical rotary feedthrough on the top flange drives a 30 tooth spur gear via a long connecting rod. The gear is positioned to mesh with the outer edge of the turntable, which has 360 teeth cut into it. Rotating the feedthrough will rotate the turntable. The ratio between the gears is 1:12, so for example a rotation of sixty degrees on the feedthrough will rotate the turntable by five degrees in the opposite direction.

By manually turning the rotary feedthrough, the analyser angle can be changed. In addition to this, the angle can be set under computer control by driving the analyser using a stepper motor.

The stepper motor was fitted to the rotary feedthrough, and turns the drive
Experimental Apparatus

Figure 3.10: A side-on view of the turntable sitting on top of the ruby balls. These allow it to rotate smoothly on top of the baseplate.

Sensing the potentiometer position provides a means to detect the position of the analyser. The controller provides a 5 V reference voltage across the potentiometer and the rotation of the analyser can be inferred by monitoring the voltage on the wiper terminal.

The ten-turn range on the potentiometer maps to a range of $300^\circ$ on the turntable. This is adequate for the analyser as mechanical constraints limit its range of movement to under $250^\circ$.

The stepper motor controller is built with an integrated interlock system to stop the analyser from running into the electron analyser or gas jet. The system is a failsafe, and the software controlling the analyser angle should never attempt to drive it outside of the angular limits which have been configured. Nevertheless, if the software were to fail for some reason, or if communication between the stepper controller and the computer were corrupted, it is important that the controller
can act to stop the analyser drive motor and prevent damage to the spectrometer.

Two limit points, called \textit{endstops}, are defined by the interlock system. The stepper motor is prevented from driving the analyser beyond these limits. As the controller runs the motor it continually checks to see whether the potentiometer resistance has been driven to either of the endstop values. If so, it stops the motor and prevents any further movement in that direction. The controller also checks that the motor is turning the potentiometer at the correct rate, and in the correct direction. These additional checks are a guard against wiring or mechanical problems with the drive system.

3.4 Atomic Beam Source

3.4.1 Introduction

The design of the oven closely follows, and indeed uses many of the original parts from, the oven detailed in [92]. A previous failure of a knife edge seal caused a catastrophic calcium leak which fused the oven crucible to the heater. This forced a partial rebuild, and necessitated some small design changes.

The atomic beam source uses mechanical collimation to produce a beam of atoms with a small angular divergence. Previous oven designs [93, 94] suffered from poorly collimated beams, which led to contamination of the scattering chamber. A well defined beam is especially important in experiments involving calcium, since any surfaces inside the chamber which become coated in calcium can charge up. These charged surfaces would divert the paths of electrons, adding a source of error to the experimental data or even making it impossible to take reliable measurements.

Once the calcium atoms in the beam have left the oven and crossed the chamber, they are deposited onto a cold trap on the opposite wall of the scattering chamber. The cold trap was described in Section 3.2.4.
3.4.2 Theory of Operation

A diagram of the oven is shown in Fig. 3.11. The oven is loaded with a crucible, which is a hollow cylinder closed at one end and with a nozzle at the other. The crucible contains the material to be heated, which is calcium for the experiments described here. A coil of resistive heater wire in the oven raises the temperature of the crucible up to around 800°C. This is just below the melting point of the metal and at this temperature sublimation causes the charge to give off a large amount of calcium vapour.

The pressure inside the vessel forces the calcium vapour out of the nozzle.
Experimental Apparatus

and into an arrangement called a skimmer. This takes the crude beam from the crucible and reduces its angular divergence by mechanically trapping those atoms which do not pass through a 1 mm aperture at the exit. The skimmer is at a lower temperature than the crucible, and so some of the calcium vapour incident on the skimmer condenses and is deposited there. This keeps the vapour pressure of calcium in the skimmer lower than inside the crucible, and allows the beam to be defined by the crucible nozzle and the exit aperture.

By probing the atomic beam with a laser beam, and by measuring the size of the calcium spot deposited onto the cold trap, the angular divergence of the atomic beam was measured to be $±1.3^\circ$.

The oven heater assembly is housed inside three concentric stainless steel cylinders which act as heat shields. These are located using ceramic spacer rods which are mounted inside front and rear face plates. These hold the oven together. The oven is mounted on a baseplate which is thermally insulated from the rest of the spectrometer.

Most of the parts required to build the oven are shown in Fig. 3.12. Each part in the figure is labelled, and a short description of each part can be found in Table 3.2. Throughout the remainder of this section, a letter in brackets will refer back to the corresponding part of the oven shown in the picture, for example (N) refers to the oven crucible.

3.4.3 Refilling the Oven Crucible

The crucible (N), illustrated in Fig. 3.13, sits at the heart of the oven, it is made from grade 310 stainless steel and holds the calcium charge. It was filled either with between 1 and 2 grammes of calcium shot, or around 3 grammes of solid calcium, which was machined into a solid cylinder shape to fit inside. A titanium plug screws into the rear end of the crucible, this pushes a seal made from grade 310 stainless steel against the body of the crucible. The interface between the two surfaces is a knife edge seal. The front end of the crucible is
Figure 3.12: The parts used to construct the atomic beam source are illustrated in this photograph, with a fifty pence piece shown for scale. Table 3.2 lists the labels and descriptions for each part.

<table>
<thead>
<tr>
<th>Label</th>
<th>Description</th>
<th>Label</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Inner heat shield</td>
<td>M</td>
<td>Stainless steel spacer rods (3x)</td>
</tr>
<tr>
<td>B</td>
<td>Middle heat shield</td>
<td>N</td>
<td>Oven crucible with plug and seal inserted</td>
</tr>
<tr>
<td>C</td>
<td>Outer heat shield</td>
<td>O</td>
<td>Back cover</td>
</tr>
<tr>
<td>D</td>
<td>Defining aperture for the atomic beam</td>
<td>P</td>
<td>Thermocoax end termination block</td>
</tr>
<tr>
<td>E</td>
<td>Skimmer</td>
<td>Q</td>
<td>PTFE wire junction block</td>
</tr>
<tr>
<td>F</td>
<td>Front face plate</td>
<td>R</td>
<td>Base</td>
</tr>
<tr>
<td>G</td>
<td>Mount for front face plate</td>
<td>S</td>
<td>Assorted screws and ceramics</td>
</tr>
<tr>
<td>H</td>
<td>Rear face plate</td>
<td>T</td>
<td>Fifty pence piece (shown for scale)</td>
</tr>
<tr>
<td>I</td>
<td>Mount for rear face plate</td>
<td></td>
<td></td>
</tr>
<tr>
<td>J</td>
<td>Pre-former (unused)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>K</td>
<td>Former</td>
<td></td>
<td></td>
</tr>
<tr>
<td>L</td>
<td>Heat shield jacket</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 3.2: Descriptions of oven parts shown in Fig. 3.12. More detailed descriptions can be found in the text.
formed into a molybdenum nozzle through which the calcium vapour escapes into the skimmer.

The process of refilling the oven with calcium involves removing the crucible from the oven heater jacket, which required access to the inside of the scattering chamber. If the oven had been operating, it would be left to cool down to room temperature. This was to ensure that the calcium in the oven did not react violently with the contents of the air. The chamber would then be brought up to atmospheric pressure under an inert gas such as nitrogen. The top flange was then winched from the chamber and placed onto a stand. This allows access to the oven assembly.

The back cover (O) of the oven can then be removed to gain access to the crucible. The crucible is removed by inserting an M3 screw thread into the threaded hole on the plug at the exposed end. This gives some purchase to remove the oven crucible from the heater jacket. The crucible should then slide out of the oven when the screw thread is pulled, although usually a purpose built extraction tool was used which pushes up against the outer edge of the heater jacket to work the crucible free.

At this stage the skimmer (D, E) would also be removed for cleaning. It is unscrewed from the front of the oven by unfastening the three M2 bolts which
Figure 3.14: Equipment used to refill the oven. The picture shows a jar of calcium shot, the oven crucible with the plug and seal removed, a set of tweezers, two spanners used for unscrewing the plug from the crucible, a metal tray and a plastic bag.

hold it in place. The skimmer, crucible, back plate and screws were generally all cleaned together. Any calcium deposited on them was dissolved in tap water and then the parts were cleaned in an ultrasonic methanol bath.

Once these parts were clean and had dried, the skimmer was reattached to the front face of the oven. The crucible was then refilled inside an Atmos bag, which is a large transparent plastic bag which is airtight when sealed. It is attached to a vacuum pump and a gas line.

The Atmos bag is prepared beforehand, with the necessary equipment to refill the oven placed inside it. These are shown in Fig. 3.14. This would normally include some tweezers, a pair of pliers and a tray on which to work, as well as the calcium charge. The calcium may either be calcium shot from a jar (pictured) or machined cylindrical solid plugs of calcium.

With the crucible placed inside, the bag is filled with argon, then emptied, then filled again. This process is repeated a few times to purge the bag of air. The calcium was placed into the oven inside this protective atmosphere. This
minimised oxidation and other forms of contamination to the calcium.

Once refilling was complete, the crucible was removed from the Atmos bag and reinserted into the oven body. The back cover was reattached to complete the reassembly of the oven, and then the top flange was lowered back into the tank and the scattering chamber was then depressurised. Once the pressure had dropped to below $1 \times 10^{-4}$ mbar the oven heater was turned on. The current was increased in steps of around 100 mA until the desired temperature was reached.

### 3.4.4 The Oven Heater

The oven heater jacket consists of an outer jacket (L) and a former (K) made from a solid block of oxygen free copper. The former is heated by a coil of heater wire, wound into a spiral groove machined onto its outer surface. A photograph of a previous oven is shown in cutaway in Fig. 3.15. It was suspected that a...
The failed plug seal had caused the copper former to react with calcium vapour at high temperature. This caused the crucible to fuse in place, which necessitated this destructive method of examination.

The oven heater is shown schematically in Fig. 3.16. It is constructed from a copper bar, machined to an outer diameter of 20 mm, and hollowed out to an inner diameter of 16.1 mm up to a distance of 10 mm from the front end, where it forms an enclosure for the crucible nozzle, with an inner diameter of 4 mm and an outer diameter of 7 mm. A spiral thread of depth 1 mm and pitch 2 mm is cut onto the outside of the heater. The heater wire has a diameter of 1 mm and sits inside this spiral. The outer jacket slips tightly over the wire, which keeps it pressed against the copper to maintain good thermal contact.

The heater wire is Metreware wire from Thermocoax [95], reference 2NcNcI10. The outer shielding is made from Inconel 600 alloy, which is non-magnetic and has good outgassing properties under high vacuum. The wire has two cores made from a nickel/chromium 80/20 alloy. These two cores are insulated from one another with a mineral powder.

A length of 2.5 m of heater cable is used to heat the oven. The heater cable was wound by hand around the former (K). Cable ties were used to keep the...
heater cable positioned flush against the former during the winding process. This is illustrated in Fig. 3.17. A length of cable was left at each end to bring out of the oven assembly and to the connection blocks (P) and (Q).

The jacket heat shield (L) was then placed over the former. To do this, it was cut into two sections, shown in Fig. 3.17, of lengths 65 mm and 45 mm. This was to allow the heat shield to slide on more easily, as it was found that the entire length would get stuck due to the cumulative frictional force of each loop of heater cable pushing outwards on the inside of the heat shield.

As the heat shield was added, a type K thermocouple cable was inserted at the rear end of the former, away from the nozzle end. This was wound around it to half a turn, and aligned so both the thermocouple cable and the heater cable could exit via the slit in the jacket for the cables to feed through. This thermocouple was used to provide a measure of the oven temperature.

The heater wire is brought out of the oven at the front and rear ends. The front end makes a connection to the end termination block (P). This joins the two cores of the wire together at this point so that the current flows back along the second core of the heater cable. This cancels the magnetic field that would
otherwise be induced by the coil of heater wire. At the rear end of the oven, each core of the heater wire is brought to a terminal on the wire junction block (Q) where they make connections to a pair of PTFE coated copper wires. These wires carry current to the oven via an electrical feedthrough on the top flange of the spectrometer. The heater current is supplied from a constant current power supply with 325 V compliance, as described in [92].

The maximum temperature that the heater wire can withstand is 1000°C. The manufacturer states that the wire should be subjected to a potential difference no higher than 100 V m$^{-1}$. Around 2.5 m of cable are used in the oven, and the voltage required over the cable is around 175 V to reach the maximum temperature of 800°C.

The thermocouple connections are brought out of the chamber via an electrical feedthrough which connects to a thermocouple amplifier outside the chamber. This displays the temperature of the oven and also connects to the controlling computer to provide it with a temperature reading. The temperature of the oven was continuously monitored while oven heater current was supplied. The computer stores the temperature data indexed by time, so all spectrometer measurements can be correlated to oven temperature.

### 3.4.5 Oven Construction

The heater assembly, comprising of parts (K) and (L) and without heat shields (A), (B) and (C), was screwed into the front face plate. Four M2 bolts were used which screw into the front of the former (K). To minimise heat conduction, ceramic spacers prevented the heater from being in direct contact with the faceplate.

The skimmer assembly (the two pieces D and E) were screwed onto the front of the face plate (F). The holes for the outer ceramic rods are drilled all the way through the plate. Attaching the skimmer prevents the ceramics from falling through these holes. The face plate mounts (G) and (I) were attached to their respective face plates using M2 bolts.
Figure 3.18: Thin walled ceramic spacer rods separate the heat shields from one another. The photograph on the left shows nine new ceramics, and four used ceramics removed from the oven. The photograph on the right shows a close up of the end of one ceramic rod, which is 2 mm in diameter.

Three concentric hollow cylinders (A, B and C) act as heat shields, which maintain a large temperature gradient between the inside and outside of the oven. This protects other components in the vacuum chamber from damage due to excessive heat, and also means that less heater power is needed to heat the oven crucible compared to an oven with no heat shielding.

The heat shields are separated from one another, and from the oven heater, by the thin walled ceramic rods shown in Fig. 3.18. These are each 123 mm long, with an outer diameter of 2 mm. Each ceramic rod slots into one of the blind holes drilled into the inner side of the front face plate (F), and is held at the opposite end by a through hole drilled into the rear face plate (H). The rods are prevented from sliding out by the back cover (O), a circular disc which screws onto the rear face plate. There are three rods for each of the heat shields, making nine in total.

The three inner ceramic spacer rods were inserted into the blind holes in the face plate and the inner heat shield (A) was slid over the top, with care taken not to bend or break the cables from the heater. There is a slit on the heat shield to allow cables to pass through, and this was aligned to allow space for the cables to reach outside of the oven.
The remaining two heat shields (B) and (C) were added in a similar manner, by first placing the three ceramics into the face plate, and then sliding the heat shield over the top. Again, the slits in these shields were aligned to allow a path for the cables to exit the oven. The three stainless steel spacer rods (M) were then screwed into place on the front face plate. Finally the rear face plate (H) was attached by carefully guiding the ceramic tubes into their respective holes. The rear face plate was secured by screwing it into the stainless steel spacer rods.

The oven was mounted on a stainless steel block (R). The two face plate mounts screw into the block, and this holds the oven in place. The two electrical contact blocks (P) and (Q) were screwed into the side and this allowed the connection between the oven heater cable and the Thermocoax.

Four 3 mm diameter synthetic sapphire spheres are used for four of the six contact points between the oven and the rest of the chamber. This is to reduce heat conduction from the oven.

### 3.4.6 Oven Heating Characteristics

The oven heater was tested by assembling the spectrometer, evacuating the chamber, and then waiting for the pressure to drop below $1 \times 10^{-5}$ mbar. A second thermocouple was placed on the outer heat shield to measure the heat shield performance.

These initial tests were performed with no calcium in the oven. The oven was heated from room temperature with a current of either 200 mA or 300 mA supplied to the oven heater. The temperature of the inner and outer thermocouples were recorded as the oven was heated.

The final equilibrium temperatures were estimated by fitting an exponential curve to the final portion of the temperature curve on the graph, where it best resembles an exponential function. Figure 3.19 shows the results. At 300 mA, the highest current used in these tests, the oven heater reached a temperature of
Figure 3.19: The four graphs show oven temperature against time for heating (when a current is applied) and cooling (when an applied current is switched off) for currents of 200 mA and 300 mA. There is no crucible in the oven for these tests. The two lines in each graph show the temperature of the oven heater thermocouple, and the temperature measured by a thermocouple placed on the outer heat shield. In each case the outer heat shield temperature is lower than the oven heater.
540°C and the head shield 200°C. The heat shielding is able to maintain a good temperature differential between the inside and outside of the oven.

3.5 Alignment

3.5.1 Introduction

Correct alignment is essential in the spectrometer to reduce uncertainties in the experimental data. The gun, analyser, atomic beam source and gas jet all point at the interaction region in the centre of the chamber and all lie in the same plane; the scattering plane. The scattering plane is defined by the momenta of the incoming and outgoing electrons, $k_{\text{in}}$ and $k_{\text{out}}$. The plane in which the analyser moves is restricted to detect electrons scattered from the interaction region where

$$k_{\text{out}} \cdot r_t = 0$$

where $r_t$ is parallel to the direction of the trace laser beam. This restricts a detected electron to lie in a scattering plane perpendicular to $r_t$.

The normal to the scattering plane is defined by the trace laser, which points vertically upwards from underneath the turntable. The point where the trace laser beam crosses the electron beam path defines a point on the scattering plane.

The gun is fixed in position on the lower plate of the spectrometer and cannot be adjusted. The analyser, atomic beam source and gas jet were properly adjusted so that they lay in the scattering plane, and pointed at the interaction region. Details of the alignment procedure are presented in the rest of this section.

The alignment was performed by inserting visible laser diodes into each of the spectrometer components, and by turning on the trace laser diode. For each laser diode, the beam passes through a pair of apertures defining the beam direction. Components were then aligned by making the laser beams coincident on the interaction region, and by ensuring that the beams lay in the scattering plane.
3.5.2 Trace Laser

The trace laser is located underneath the spectrometer baseplate, and points vertically upwards. Along with the gun axis, it defines the location of the interaction region and the orthogonal direction to the scattering plane. It traces back along the path that the main laser beam should take into the chamber. When the chamber is closed and under vacuum, this laser is also used to align the main laser beam.

The laser used is a Roithner Lasertechnik ADL-65052TL. These are a small diode lasers which lase at 650 nm. The diodes have a physical width of 6.5 mm, and press-fit into a lens assembly mounted below the baseplate. A plug makes a connection to the terminals on the bottom of the diode, and the circuit is brought outside the tank via the second electrical feedthrough, where it is attached to a laser diode drive unit.

Inside the lens assembly a stack of around 9 to 11 washers, each 0.1 mm thick, space the collimating lens from the laser diode. The exact number required varied depending on exactly how far the laser diode has been mounted inside its housing. The lens sits on the top of the stack and another set of washers holds the lens against a screw fit top.

A bolt secures the lens assembly into an adjustable mount. The mount is stood off from the bottom of the baseplate by a rubber O-ring and held in place by three nuts. The pointing direction of the laser diode is adjusted by tightening or slackening these nuts.

The lower mount for the MAC has two defining apertures for the trace laser beam. When the laser is aligned the beam passes through both apertures. This defines the location of the interaction region in the scattering plane. The trace laser was aligned to pass through these apertures before the rest of the alignment procedure was carried out.
3.5.3 Additional Alignment Lasers

The analyser, oven and gas jet needle must be aligned to aim at the interaction region. This spot should be in line with the centre of the turntable. Everything must be aligned in the same plane, defined so that the trace laser is a normal to the scattering plane.

To perform the alignment, various alignment lasers were used. These are small diode lasers mounted in cases made to fit into the back of the gun, oven, analyser and gas jet needle. The trace laser is also used for alignment.

The gun has a hole drilled into the back of the filament, so as to pass the laser beam through the defining apertures in the gun. With the connector for the filament power supply removed, the alignment laser can slide into the rear of the gun. At the front end of the gun, the front panel was removed. This exposes the triple element aperture lens GL2. A cylinder machined out of brass fits into the lens stack assembly. A small 1 mm hole machined along the axis of this cylinder forms the second defining aperture for the laser beam. The position of the gun cannot be adjusted as it defines the position of the interaction region.

The alignment laser for the oven is a cylinder with the same outer diameter as the crucible. To place this laser into the oven, the back panel and the oven crucible were removed. The laser was then placed into the heater jacket. The first defining aperture is formed at the front of the diode laser assembly and the second is at the output of the skimmer. The six screws on the baseplate can be used to adjust the height and tilt of the oven.

To insert the alignment laser into the analyser, the four screws which hold the back plate onto the analyser were removed. Inside, there are two screws which hold the outer hemisphere in place. These were removed and the hemisphere placed on top of the analyser. The alignment laser slides in from the back and rests inside the analyser. At the front of the analyser, a ‘T’ shaped tool slots into the cone to support the alignment laser at this end, and also defines a second aperture. The first aperture is inside the analyser at the entrance to the energy
selector. The analyser position can be adjusted by means of the two screws at the bottom which move it perpendicular to its defining axis.

The gas jet alignment laser is threaded at the front end to allow it to screw onto the back of the gas jet needle. To access the back of the gas jet needle, the gas hose was unscrewed and a steel block which acts as an adaptor was also unscrewed. The alignment laser for the gas jet needle was then screwed into the back of the gas jet.

The gas jet can be adjusted by adjusting the mount screwed into the top plate of the chamber. This adjustment is rather coarse, but the gas jet beam is poorly defined and so the alignment is not critical.

3.5.4 Performing the Alignment

A single power supply unit drives all the laser diodes except for the trace laser, which runs from a dedicated supply, a Thorlabs LDC500 Laser Diode Controller. Each laser is plugged into one of the ports on the power supply and the current is increased until the unit begins to lase. The lasers can be controlled individually by flicking a switch to turn them on or off.

With the appropriate lasers active, adjustments were made to the oven, analyser and gas jet to bring them into alignment. A small viewing card was used to view the position of the laser beams. Figure 3.20 shows the alignment lasers and the viewing card.

Once the process was completed the components inside the spectrometer were properly aligned, but only as far as the accuracy of this method allows. Smaller misalignments can be corrected to some extent by making use of the deflectors in the gun and analyser.

If there are any major changes to the components inside the chamber, such as the oven being rebuilt, the alignment process should be repeated.
Figure 3.20: The four photographs show (clockwise from top left) the alignment laser for the oven, the alignment laser for the electron gun, the alignment laser for the analyser and viewing the laser spots on the viewing card. The fourth spot is provided by the vertical alignment laser. When the system is aligned, all four spots are coincident with one another, and define the centre of the interaction region. The gas jet laser is not active in these pictures.
3.6 Laser Systems

Two different laser systems were used over the course of the experiment; a Coherent MBR-110 and a Spectra-Physics Matisse TX. Both systems consisted of a tuneable Ti:Sapphire laser pumped by a diode-pumped solid state (DPSS) laser operating at 532 nm. The Ti:sapphire lasers produce infra-red light at 846 nm for the experiments, which is frequency doubled in a resonant cavity to produce the 423 nm light required to excite the $4^1P_1$ optical transition in calcium.

The two lasers systems are similar. Sections 3.6.1–3.6.4 describe the operation of the Coherent laser system, and Section 3.6.5 describes the Spectra-Physics system. The two are then compared and differences highlighted.

3.6.1 Overview of the Coherent Laser System

A representation of the Coherent laser system is shown in Fig. 3.21. There are three main components. The Coherent Verdi V-10 is a DPSS laser which operates at a wavelength of 532 nm with a power of up to 10.5 W. This laser pumps the MBR-110, a tunable Ti:Sapphire laser which is set to lase at $\sim$ 846 nm; this is twice the wavelength of the transition to the $4^1P_1$ state of calcium. The beam from the MBR-110 is passed through steering and collimating optics to a frequency doubler, the MBD-200. This produces the $\sim$ 423 nm radiation used for calcium studies.

3.6.2 Coherent Verdi V-10 Diode-Pumped Laser

The Coherent Verdi V-10 is a DPSS Neodymium Vanadate (ND:YVO$_4$) laser which supplies optical power to the MBR-110 Ti:sapphire tunable laser. It consists of two units; the power supply and the laser head unit. The two are connected by an umbilical cord, and the laser head is actively cooled by a water cooling unit (Coherent T255P).
The power supply is situated remotely from the laser head. Two laser diode bar assemblies housed inside it supply radiation at $\sim 808$ nm which is fed to the laser cavity using multimode optical fibre housed inside the umbilical cord. A fan cooling system draws excess heat away from the laser diodes.

Inside the laser head the pump light is passed through a gain medium, an ND:YVO$_4$ crystal. The crystal is situated inside a laser cavity and lases at 1064 nm. The cavity is a bow-tie configuration and the mirrors are highly reflective at the lasing wavelength. An optical diode inside the cavity ensures operation in only one direction.

To produce the output radiation, an intra-cavity lithium triborate (LBO) crystal generates the second harmonic at 532 nm. The refractive index of the LBO crystal is temperature tuned to optimise second harmonic generation, and the LBO crystal is typically held at temperature of 150°C [96]. The second harmonic is coupled out of the cavity through a mirror which is transparent at the output wavelength.

### 3.6.3 Coherent MBR-110 Ti:sapphire Laser

The MBR-110 is a Ti:sapphire laser capable of delivering laser radiation over the wavelength range 690-1050 nm [97]. The linewidth of the laser is $\sim 100$ kHz.
This is narrow enough to pick out and excite a single hyperfine atomic transition.

The laser optical elements are shown in Fig. 3.22. The cavity is a *bow-tie* or *double-Z* configuration, machined out of a single block of aluminium. The optical elements of the laser are mounted to the block to form a monolithic block resonator (MBR). This gives the cavity a high degree of passive stability, since changes in cavity length would contribute to increased linewidth. The cavity is actively stabilised by means of a piezo mounted mirror (M3), an intracavity etalon (4) and a pair of Brewster plates (5).

The laser radiation from the Verdi V-10 is directed into the MBR-110 via two external input mirrors, and this radiation pumps the Ti:sapphire crystal. The alignment into the input coupler is very critical, and sometimes small adjustments to these two mirrors are necessary to maximise light output from the MBR-110.

The pump beam from the Verdi passes through focussing optics (1) and is coupled in through dichroic mirror M1, which is transparent at the pump wavelength. After passing through the mirror, the pump light is incident on the Ti:sapphire
crystal (2). When excited, the Ti:sapphire crystal emits over a broad band of frequencies. Single frequency operation of the laser is achieved by minimising the losses inside the cavity at the required frequency. Coarse wavelength control is via a birefringent filter [98] (6) which is angle tuned by manually turning a knob on the top of the laser enclosure. This rotates the birefringent filter which in turn rotates the polarisation of wavelengths which are away from the centre frequency. These wavelengths will undergo losses at the Brewster angled surfaces in the cavity, causing it to lase preferentially at the selected frequency. An intracavity thin etalon (4) reduces the linewidth to below 100 kHz, and allows fine tuning of the laser frequency.

A pair of galvanometer mounted Brewster plates (5) are user to scan the laser frequency over a range of ∼40 GHz. Rotating the plates effectively alters the path length of the cavity, which shifts the frequency of the resonant modes.

An optical diode (3) causes high losses in the reverse direction. This is to prevent spatial hole burning, where counter-propagating waves in the laser cavity interfere to prevent lasing at certain frequencies.

To maintain a stable laser frequency, the laser can be locked to the reference cavity (7). The reference cavity is scanned by controlling a piezo which translates the back mirror along the direction of the laser beam. The cavity reflectance and laser beam intensity are monitored with photodiodes (8). The laser is locked though an electronic feedback loop which controls the angle of the Brewster plates and the piezo-mounted mirror M3. This reduces the linewidth to under 100 kHz but the laser still exhibits some long term drift. To correct for this, an external input allows the laser frequency to be scanned. The external scan changes the length of the reference cavity, and so if the laser is locked to it, the laser frequency is also scanned.

To compensate for the long term drift of the laser, an external locking system is used to keep the laser on resonance with the $4^1P_1$ transition. This is explained in more detail in Section 3.7.5.
To monitor the laser wavelength a glass slide is positioned after the output aperture of the laser. This directs a portion of the light, via two steering mirrors, into an optical fibre connected to a Burleigh WA-1500 wavemeter. This measures the laser wavelength to an accuracy of $\pm 1 \times 10^{-4}$ nm.

### 3.6.4 Coherent MBD-200 Resonant Frequency Doubler

The MBD-200 is a frequency doubling unit which is used to produce a laser beam at $\sim 423$ nm. The infrared beam from the MBR-110 is guided into the MBD-200 using a telescope and a pair of beam steering mirrors positioned between the two units. These ensure the correct alignment and focussing conditions are met for the doubler, and that the input beam is mode matched to the cavity.

Inside the MBD-200 is a frequency doubling crystal made from LBO. This nonlinear crystal is used for second harmonic generation (SHG). The infrared beam from the MBR-110 is used to pump the crystal. To increase the efficiency of SHG, the crystal is mounted inside a resonant enhancement cavity. The intracavity intensity is roughly 60 times the intensity of the input beam [99].

The ring enhancement cavity in the MBD-200 is machined from a single block of aluminium. As in the MBR-110, this ensures a good level of passive stability. The mirrors inside the cavity bring the laser light to a tight focus inside the doubling crystal. This maximises the electric field inside the parts of the crystal volume enclosed by the laser beam. The intensity of doubled light produced increases as approximately the square of the electric field intensity, although this falls off at high conversion efficiencies. Typical output powers of $\sim 100$ mW can be achieved.

A H"ansch-Couillaud locking scheme [100] is employed to lock the doubling cavity on to resonance. The cavity must be actively controlled to keep the beam resonant within it. A half wave plate located before the cavity rotates the polarisation of the input beam slightly. The Brewster surface at the crystal causes a frequency dependent elliptical polarisation. This is detected by a polarisation
analyser and produces an error signal which is used to control the optical path length in the cavity by translating a mirror mounted on a piezo. This keeps the cavity on the resonance condition.

When the cavity is not locked, the drive electronics will dither the piezo, thus scanning the cavity and resulting in a maximum in intensity when the cavity goes through the resonance condition. The result is a low average power beam, which is useful for alignment.

3.6.5 Spectra-Physics Laser System

The layout of the Spectra-Physics laser system is shown in Fig. 3.23. Like the Coherent system it utilises a diode-pumped solid state green laser, a tuneable Ti:sapphire laser and a frequency doubler to produce blue laser light at $\sim 423$ nm.

The *Millenia Pro 15sJS* diode-pumped laser provides light at 532 nm. The unit operates in a similar manner to the Verdi-V10. A pair of diode bars in the laser head unit supply pump power to a vanadate crystal inside the laser cavity. An LBO intracavity doubling crystal converts the 1064 nm infrared radiation from the vanadate to 532 nm, which is coupled out of the laser through a dichroic cavity mirror [101]. It has a higher maximum output power of 15 W, compared
The Matisse TX [102], represented in Fig. 3.24, operates on a similar principle to the MBR-110. It is also a Ti:sapphire laser stabilised with a reference cavity. The cavity design is similar, with the addition of two mirrors M2 and M3 along the optical path before the Faraday rotator (5). These act together to cause losses in the reverse direction, since one of the mirrors, M2, is mounted out-of-plane. The combination of Faraday rotator and out-of-plane mirrors form an optical diode, promoting laser action in only one direction in the cavity. An additional intracavity electro-optic modulator (EOM) (2) is used for high frequency adjustments of the optical path length for frequency stability. All the laser optics are mounted on an INVAR baseplate to ensure passive stability and very low thermal expansion.

The reference cavity for the Matisse is external to the laser. This unit contains the reference cavity itself, as well as necessary optics for Pound-Drever-Hall (PDH) frequency stabilisation [103, 104]. This technique is used to keep the laser locked to the reference cavity and works by measuring the reflected light from the reference cell. This can be used to infer whether the cavity is on resonance, since no reflected light should be measured when the laser is resonant with a cavity mode. However when the laser frequency is not coincident with one of the cavity modes, a measure of the reflected light alone is insufficient to adjust the laser fre-
Experimental Apparatus

Figure 3.25: An optical schematic of the Wavetrain frequency doubler. Mode matching and beam steering optics have been omitted for clarity. (1) EOM for PDH stabilisation. (2) Brewster window. (3) Prism and piezo mount. (4) SHG crystal (LBO). (5) Fibre-optic coupler for reflected signal. (6) Brewster window.

frequency back onto resonance, since this measurement provides no information as to the direction of adjustment required. To provide this, an EOM located before the reference cavity is modulated at 20 MHz which effectively dithers the laser frequency by producing a phase modulation. This provides information about the derivative of the signal intensity with respect to frequency and is used in a feedback loop to drive the fast piezo and the EOM such that the laser stays locked to the reference cavity resonance.

The Matisse is controlled and scanned by software on an attached laptop computer, called Matisse Commander. For external control of the laser frequency, a software input allows digital control of the laser frequency by supplying a difference input which is proportional to the difference between the laser frequency and the desired frequency. The laser frequency is monitored by a Toptica WS series wavemeter, which is accurate to $\pm 1 \times 10^{-6}$ nm.

The wavemeter connects to the laptop and this is set up to transmit the laser wavelength measurements to the computer controlling the spectrometer. These measurements are recorded for every data point taken from the spectrometer. This provides a method to check whether the laser was locked to the correct frequency for each data point that was gathered.
Table 3.3: Comparison of various aspects of the two laser systems. All values are approximate.

<table>
<thead>
<tr>
<th>Property</th>
<th>Coherent System</th>
<th>Spectra-Physics System</th>
</tr>
</thead>
<tbody>
<tr>
<td>Year of purchase</td>
<td>1999</td>
<td>2007</td>
</tr>
<tr>
<td>Maximum diode-pumped green laser output</td>
<td>10.5 W</td>
<td>15 W</td>
</tr>
<tr>
<td>Maximum Ti:sapphire laser output</td>
<td>1.2 W</td>
<td>3 W</td>
</tr>
<tr>
<td>Quoted minimum linewidth for Ti:sapphire laser</td>
<td>100 kHz</td>
<td>30 kHz</td>
</tr>
<tr>
<td>Maximum doubler output</td>
<td>100 mW</td>
<td>&gt; 300 mW</td>
</tr>
</tbody>
</table>

The Wavetrain frequency doubler [105] works using an SHG crystal placed inside a resonant enhancement cavity. The optical set up of the cavity is illustrated in Fig. 3.25. The cavity is a delta shape, formed by mirrors M1 and M2 and completed with a prism (3) which bends the optical path and so closes the cavity. The prism is mounted onto a piezo so that the optical path length can be controlled. The cavity is sealed for stability and the beam enters and leaves via Brewster windows (2) and (6). The PDH stabilisation technique is also used here to keep the doubler on the resonance condition. The EOM (1) modulates the incident beam, and the reflection from M1 is coupled into a fibre at (5). This signal is analysed and the piezo at (3) is adjusted accordingly.

3.6.6 Comparison and Discussion of the Two Systems

The Coherent laser system is the older of the two, and advances made in laser technology mean that the newer Spectra-Physics system, built several years later, is the more capable. Briefly; it is more stable; easier to set up, use, and control; and more powerful. Table 3.3 compares some properties of the two systems.

A number of features make the Spectra-Physics system more stable over long operating periods. This has allowed almost continuous running with very little operator intervention. The electronics controlling the Wavetrain doubler are able to relock the cavity quickly once it goes off resonance. The MBD-200 falls out of
lock more readily, and is found to jump out of lock every few hours even when properly set up. This can happen if the piezo in the cavity reaches its maximum travel distance, and also through sudden shifts in the laser frequency or power output.

It should also be noted that on both systems the maximum power attainable from the doubler fell over the course of time. This can be attributed to degradation and gradual misalignment of the optics, and damage to the optics. Occasional cavity mirror readjustments were carried out on both systems which partially mitigated this.

The Matisse Ti:sapphire laser exhibits smaller frequency drift compared to the MBR-110. The MBR-110, when set to the transition frequency and without any external locking system engaged, will stay on resonance only for a few minutes. The Matisse will stay on resonance for several tens of minutes. This is useful for locking the external locking system to the transition frequency, and allows data to be taken for some small periods of time while the external locking system is not operating (for example, when the interaction region is obscured from the quadrant photodiode by the electron analyser).

To summarise, the Spectra-Physics laser system was preferable for taking data from the spectrometer. When this was not available, the Coherent laser system was used to take data. This required more operator intervention and adjustment, and due to the lower laser power the data acquisition rate was lower. Overall using the Coherent system reduced the rate of collecting data.

3.7 Optics

3.7.1 Beam Delivery System

The laser system delivers a beam of laser radiation to the top flange of the spectrometer. The laser frequency is matched to the $4^1P_1$ transition in calcium,
but the polarisation of the beam is not defined. The optics at the spectrometer define this polarisation, and also align and focus the beam into the chamber.

Figure 3.26 shows the optical set up. The first optical element that the beam encounters is a lens. The focal length was chosen to produce a beam with a spot size of around 2 mm in the interaction region. This ensures a high flux of photons which cause more excitations and so improve data gathering efficiency.

After the lens, a mirror directed the laser beam down through the vacuum window and into the scattering chamber. The beam was aligned to be perpendicular to the scattering plane, and to pass through the interaction region. In order to properly align the beam, both this mirror and another beam steering mirror were adjusted. To align the main laser beam, the trace laser diode was switched on and the main beam was aligned so that its path coincided with that of the trace laser. This procedure was only performed when the oven was at room temperature, as operating the diode at a high temperature was found to significantly degrade its lifetime.

The Glan-Laser polariser is positioned in the beam path after the mirror. It
acts to ensure the polarisation of the laser radiation is well defined. The light that leaves the laser system is strongly polarised. The Glan-Laser polariser was aligned to the same axis as this to ensure any other component of polarisation was extinguished from the beam. It was rotated so that the transmitted light from the main beam was at a maximum.

The next optical element was a half wave plate mounted on a rotator. The rotator was driven by a computer controlled stepper motor, described in Section 3.7.2, and this allowed the polarisation vector of the radiation to be rotated.

When circularly polarised radiation was required, a quarter wave-plate was inserted in the optical path after the half wave-plate. With appropriate selection of half wave-plate angle, left- or right-hand circularly polarised radiation was produced.

### 3.7.2 Half Wave-Plate Stepper Motor

The polarisation of the beam into the chamber was controlled by rotating a half wave-plate which was positioned in the path of the laser beam on the top
flange of the vacuum chamber. It was mounted in a Newport RSP-1T rotation mount. This allowed the wave-plate to be rotated continuously through 360°. The rotator was clamped to optical posts on the top flange to hold it in place.

A knob at the corner of the rotator turns a worm gear drive which rotates the wave-plate. To enable the mount to be rotated by a stepper motor, a 60-tooth spur gear was mounted onto this knob. This is illustrated in Fig. 3.27.

The stepper motor was an Astrosyn Y129 12 V motor with a step size of 1.8°. It was mounted to the rotator with a metal plate which screws into both the rotator and the motor. Another spur gear was mounted to the drive shaft of the motor. This gear has 20 teeth, giving a 1:3 gearing ratio between the motor and the worm gear on the rotator.

The motor was connected to a stepper motor drive unit which provides the correct waveforms to run the motor. The drive unit connects to the controlling computer, and allows the motor to be driven using two transistor-transistor logic (TTL) lines; one which selects the direction of the motor, and another which advances the motor by one step when the line is pulsed.

### 3.7.3 Aligning the Wave-Plates

The half wave-plate was mounted in a rotator which was marked with a scale in degrees. This provided a measure of the wave-plate rotation, but could not be used directly to give an absolute measurement of how the polarisation of the beam was aligned relative to the incident electron beam.

The polarisation vector angle was measured relative to the gun axis in the spectrometer. By defining a half wave plate angle of zero to be where the beam is polarised parallel to the gun axis, an absolute measurement of the polarisation vector angle can be obtained. This measurement was carried out by recording the relative rotation of the wave-plate from this zero point, noting that a rotation of 1° on the half wave-plate leads to a 2° rotation in the polarisation vector.
The alignment measurement was carried out by temporarily inserting a polariser below the half wave-plate, as illustrated in Fig. 3.28(a). The polariser was mounted so that it can rotate about an axis defined by the main laser beam. The optic axis is marked on the polariser, and the polariser was accurately aligned with its axis parallel to the gun axis by using two marks on the top flange.

A viewing card placed under the polariser was used to observe the intensity of the transmitted laser radiation. When the half wave plate was rotated so that the observed intensity was at a minimum, the wave plate must be at 90° to the required axis. The zero angle was noted and was recorded in the super-elastic scattering measurements.

When circularly polarised radiation was required, a quarter wave-plate was inserted in the optical path after the half wave plate. The quarter wave-plate will produce circularly polarised light when the incident linearly polarised beam is aligned at 45° to its optic axis. At other orientations elliptically polarised
radiation is produced.

The optical set up pictured in Fig. 3.28(b) was used to find the correct half wave plate rotation to produce circularly polarised light. A mirror was temporarily inserted underneath the quarter wave-plate to reflect the beam back along the optical path. The intensity of the reflected beam after it has passed through the Glan-Laser polariser will be at a minimum when the half wave plate is rotated to be at 45° to the optic axis of the quarter wave plate. This can be shown by considering the polarisation angle of the beam as it passes through the optical system. Such minima were observed at every further 45° rotation of the half wave plate, and these corresponded alternately to left- and right-hand circularly polarised light. The handedness of the polarisation was determined from the super-elastic experiments.

3.7.4 Laser Shutter

The laser shutter was used to block or unblock the beam under the control of a TTL signal. It was placed in the beam path on a laser table away from the spectrometer. This ensured that the magnetic field used to control the shutter did not influence any measurements made in the spectrometer, and prevented mechanical vibrations from being transmitted into the vacuum chamber.

The shutter is a commercial gravity fed laser safety shutter, a Lasermet LS-10-12. When the power was switched off, a beamstop rested in the path of the laser beam, blocking light from travelling through the unit. When adequate current was provided to the shutter, an electromagnet raised the beamstop, allowing the laser beam to pass through.

A simple control unit was devised to open the shutter in response to a TTL signal. The circuit diagram is reproduced in Fig. 3.29. The positive terminal of the shutter’s electromagnet was connected to a 12 V supply. The negative terminal was connected to the drain terminal of a power MOSFET (Q1).
The MOSFET in this circuit acts as a switch. When the gate to source voltage is below threshold, the transistor presents a high resistance in series with the shutter and no current flows. When the gate to source voltage is above threshold, the drain-source resistance drops to a few Ohms and current can flow through the shutter, unblocking the beam.

The TTL input signal is amplified by an LM324 operational amplifier which is configured as a non-inverting amplifier with a gain $G = 2$. This increases the voltage of the input signal to a level that is adequate to drive the transistor gate.

As the LM324 op-amp does not require a negative voltage rail to operate, the control unit runs from a single 12 V supply. A single TTL connection to the controlling computer is sufficient to operate the shutter remotely.

### 3.7.5 Laser Locking System

While the spectrometer was gathering super-elastic scattering data, the frequency of the laser must be resonant with the transition to the $4^1P_1$ state in calcium. When the lasers were turned on, they were set to output laser radiation at the transition frequency. Over time, small changes in the environment, such as changes in temperature and air pressure, cause the laser frequency to drift. This is enough to put the beam out of resonance with the atomic transition, and so small corrections to the laser frequency were continuously required while the
Figure 3.30: Atoms from the oven aperture become spread out in the transverse plane with increasing $t$. The displacement of the excited atoms from the centre of the beam indicates the detuning of the laser. Imaging this with a quadrant photodiode allows control electronics to adjust the laser frequency.

Each of the lasers have an input which allows the laser frequency to be manually scanned. On the Coherent MBR-110, an external scan input specifies an absolute offset from a central reference. On the Matisse TX, a difference signal is used to adjust the laser frequency.

The locking system measures the laser induced fluorescence in the calcium beam to produce a difference signal. This signal relates to the magnitude and direction of any correction needed to the laser frequency. The signal was fed directly to a proportional-integral-differential (PID) control system on the Matisse TX laser, and with appropriate selection of PID factors is able to drive the laser onto resonance.

To lock the Coherent MBR-110, a switch on the back of the locking control box fed the difference signal into an integrator circuit. This integrated signal was used instead of the difference signal to drive the laser.
Figure 3.30 shows a diagram of the locking system. There is a spread of atomic velocities in a direction parallel to the laser beam direction. Assuming that all atoms are emitted from a point at the oven aperture, the perpendicular displacement $x$ of an atom from the atomic beam axis also yields a measurement of its velocity, $v_x$, as long as the time $t$ for the atom to reach the interaction region is known. In this case,

$$x = v_x t$$

where $x$ is the displacement of the atom along the laser beam axis.

Any atom with a perpendicular velocity component directed into the laser beam will have the laser radiation shifted towards the blue end of the spectrum in its frame of reference. If a group of these atoms with similar velocities are fluorescing, the laser has become red detuned. The position of the fluorescence will be shifted away from the centre of the atomic beam axis, in the direction towards the laser (see Fig. 3.30). Conversely, if the velocity component is in the reverse direction, the fluorescence will appear displaced from the atomic beam axis in the opposite direction, indicating that the laser has become blue detuned. The Doppler shift is given by

$$\omega_D = k \times \frac{x}{t}$$

where $k$ is the wavenumber of the radiation, which is travelling in the negative direction. As long as the travel time $t$ can be considered to be constant, the Doppler shift is directly proportional to the displacement of the fluorescence.

In reality, $t$ cannot be calculated exactly for each atom. For an entire ensemble of atoms, the distribution of $t$ values is given by the Maxwell-Boltzmann distribution, defined by the temperature of the atoms leaving the oven. Atoms with different speeds may have the same $x$ displacement, and this leads to a slight ‘smearing’ of the fluorescence.

A lens inside the scattering chamber images the fluorescence through a window onto a QD50-5T quadrant photodiode. It is configured to act as a split photodiode by summing together the signals from the two left detectors (Q1 and Q2 on the
The photodiode is set up initially so that the signals from the left and right sides are equal. As the laser frequency drifts, the position of the fluorescence along the beam axis changes. This alters the position of the image on the photodiode, causing a difference between the signals from left and right. This difference is amplified and produces the difference signal which is used to supply an integrator that corrects the laser frequency. The locking system is able to stabilise the frequency to better than 3 MHz \[106\].

### 3.8 Summary

In this chapter, the design and operation of the super-elastic spectrometer has been detailed. The vacuum system was described, which holds pressure of the scattering chamber low enough to perform scattering experiments. The components of the spectrometer inside the scattering chamber were described, including the oven, electron gun and electron analyser. These provide the target calcium atoms, an electron source, and an electron detector to perform experiments.

The laser system was described, which provided a source of photons to excite the calcium atoms to the \(4^1P_1\) state. The optics used to condition the beam before it entered the chamber were also detailed.

Pieces of equipment used to maintain the correct conditions to run the spectrometer were described; the locking system kept the laser at the correct frequency, and the liquid nitrogen refiller kept the cold trap at \(\sim -200^\circ\text{C}\). Two important maintenance operations were also detailed; refilling the calcium oven, and realigning the spectrometer.

In the next chapter, the power supplies for the electron-optical elements in the spectrometer are discussed. This leads on to a discussion of the computer control system developed to run the spectrometer.
Chapter 4

Electronics and Computer Control

4.1 Introduction

In this chapter the new voltage supplies which provided potentials to the elements in the electron gun and analyser are discussed. In all, the voltage supplies were required to provide 28 different potentials to the lens elements and deflectors in the spectrometer. Two different systems were used for the voltage supplies during the course of these super-elastic scattering studies. The existing supplies were constructed from analogue sections of voltage supply systems developed previously in the atomic physics group. A new system of voltage supplies were also developed as part of the work discussed in this thesis. These supplies are described in this chapter.

A diagram of the older supplies is presented in Fig. 4.1. There are three sections for the supplies. The top crate controls the gun lens element voltages, the gun energy and analyser residual energy. This voltage supply crate is described in [107]. Only analogue amplifier cards were used. These cards have a potentiometer on the front panel which can be adjusted to change the output voltage. There is also a switch which allows the output voltage to be set from a programming voltage accessed via a connector on the front of the card, instead of manually from the potentiometer.
Figure 4.1: The analogue voltage supplies, made up of a top and bottom crate holding analogue voltage cards, and a separate low voltage supply. The labels for each voltage supply show the voltage that the card supplies, as defined in Section 3.3. The low voltage supply allows fine control of the gun and analyser voltages, and also supplies the voltage for the grid.
Below the top crate is another crate of voltage supplies. The cards inside this crate are of a later revision and have a digital to analogue converter (DAC) onboard which allows the output voltage to be digitally controlled. These supplies are described in [108]. Again they were only operated in their analogue mode using a potentiometer on the front to set the output voltage.

Below the two crates is a low voltage supply for the gun energy and the analyser residual energy. The higher voltage gun and analyser supplies in the top crate sit on top of these low voltage supplies, which can be digitally controlled to allow a scan over a small energy range. The low voltage supply for the grid was also located in this enclosure.

These analogue supplies are very stable, with noise and ripple measured at less than a millivolt, and drifts on the order of 100 ppm over a 24 hour period [107]. All cards were designed to be digitally controlled, however they were only used as analogue supplies for the experiments described in this document, since a new set of computer controlled supplies were designed and built to be operated using LabVIEW [109].

The process of adjusting the spectrometer voltages to obtain the optimum signal is referred to here as tuning. With sufficiently high count rates, it is straightforward to do this manually, the operator simply adjusts the supplies to optimise the count rates.

For super-elastic scattering data taken at low energies (typically < 10 eV), count rates from the analyser were very low. This made manual tuning of the spectrometer voltages difficult. The situation is illustrated in Fig. 4.2. This example shows how changing the x-deflector voltage might affect the number of counts from scattering events. The x-deflector controls the angle of the electron beam out of the gun.

There is an optimal value which causes the electron beam to pass through the centre of the interaction region. This will produce a scattering maximum since more electrons pass through the interaction region to scatter from the target.
With count rates from this scattering higher than a few tens of Hertz, it is simple to tune the deflector voltage manually. As an example consider a ratemeter with an audible output, as is used in the experiments. This will produce a loud, high frequency tone when set at the correct scale if the deflector voltage is set to produce a maximum in scattered intensity. This situation is illustrated in Fig. 4.3(a).

The super-elastic scattering cross-section reduces significantly at low energies, leading to low count rates. This makes it very difficult to manually tune the gun when these count rates reduced to less than \( \sim 10 \) Hz. Returning to the example of the audible ratemeter, it will now only generate a series of clicks which correspond to individual electron counting events. It is no longer easy to tell where the scattering maximum is. This is illustrated in Fig. 4.3(b).

To address these difficulties at low energies, a new set of voltage supplies were developed to provide digital computer control of the spectrometer voltages. These supplies are described in the remainder of this chapter.

A fully computer controlled voltage system allows the experimenter to acquire counts at specified voltage levels over extended periods of time. With a computer system in place, it is then possible to accurately optimise the spectrometer voltages using the methods described in Section 4.5.6.
Figure 4.3: An illustration of the tuning process with (a) high count rates and (b) low count rates, with an audible ratemeter. In the first case the audible tone allows the operator to judge the optimal voltage. In the second case the low count rate produces only clicks from the ratemeter corresponding to individual counting events. This makes the optimal voltage much harder to judge.
4.2 The New Voltage Supply Crate

4.2.1 Overview and Block Diagram

The new digital voltage supply is contained within a 19 inch rack mounted enclosure which houses all component parts. A block diagram showing the basic operation of the supply is presented in Fig. 4.4. Voltages from the supply are generated from cards which slot into a backplane. The cards are powered from separate rectifier boards which are remotely located away from the voltage cards, thereby reducing AC pickup.

On the front of the unit are a set of buttons and control knobs, and a display. The output voltages can be set by rotating the control knobs, and the buttons can be used to access other functions of the power supply. The display shows...
estimates of the channel output voltages. The front panel interface is described in Section 4.4.5. In addition to the front panel controls, the voltage supply may be controlled via a universal serial bus (USB) connection to a computer. This allows the computer to set the output voltage levels under software control, as described in Section 4.5.

The system of voltage supplies is digitally controlled by a microcontroller which communicates with each voltage card via the backplane. The microcontroller sets the output voltages using either the controls on the front panel, or from communication with a computer via a USB connection. Each voltage card floats independently, and produces either four or eight different output voltages. By combining several voltage outputs onto a single voltage card, advantage can be taken of the fact that many of the electron optical elements are referenced to the same voltage point.

The backplane is the central component in the voltage supply design. It is a printed circuit board (PCB) with six 43-pin double-sided edge-connector sockets placed at equally spaced intervals. The edge connectors are soldered into mounting holes in the PCB. Voltage cards inserted into the front of the chassis slide along guiding rails to mate with the edge connector, which is positioned inside the voltage supply. The two sides of the edge connector were electrically connected to one another to make signals available to either side of any card inserted into a socket. The pins assignments of the backplane edge connector are defined in Fig. 4.5.

There are 43 pins shown on the diagram, numbered from 0–42. They are divided into three groups.

The interface pins provide inputs to control the board voltages. The board is referenced to 0 V and logic power is supplied from VTTL. There are four physical address lines A0–A3, although only three of these are implemented in practice. SYNC, CLK and D control the interface logic that provides the output voltages when the card is being addressed. These lines are shared between all six card slots.
The output pins OP1–OP8 are used to connect the individual voltage outputs from a card. Wires from the backplane supply these voltage levels to ‘D’ connectors on the back panel, and these in turn connect to the spectrometer. V0REF is the reference analogue potential for the card.

The power pins supply power to the card. Each slot has its own independent floating power supply located remotely from the card. The high voltage +800 V, +250 V and -250 V lines supply unregulated DC power to the card. The VCC, VDD and 5 V lines supply power to the lower voltage components on the card. The VCC and VDD lines are set to supply power to the operational amplifiers (op-amps), voltage regulators and references.
Connections from the voltage outputs of the backplane were brought out to the rear connection panel. The rear connection panel was made from an array of six 25-pin ‘D’ connectors, of which five were used and one is a spare. This transferred the voltage output from the card to the connections on the outside of the supply. The arrangement of the voltage outputs on the rear panel are shown in Fig. 4.6.

4.2.2 Rectifier Boards

Mains power at 240 V AC is brought into the supply through an IEC socket at the rear of the chassis. The mains voltage was split between a bank of six transformers. Each transformer supplies a rectifier module. This is a PCB which provides a number of DC lines to a single backplane socket. Each rectifier module floats independently of every other, allowing the zero volt reference for each voltage card to be defined independently.

The transformers were tapped to provide two sets of output voltages. The first set supplied ±18 V RMS, and was centre tapped between these two voltages to provide a zero volt level. The second set of voltages were between zero and 150 V RMS. The zero volt level from the two sets of outputs were tied together to provide a common reference. These levels were chosen to supply the correct rectified voltages to the edge connector. This in turn provided the correct supply level for the voltage cards.

The backplane was specified to provide six different DC voltage levels for each card slot. Since each of the voltage supply cards have different voltage requirements which depend on their output capabilities, all voltage levels were not required for each card. This led to several different designs of rectifier module, as it was not necessary to build a full set of voltage outputs onto each rectifier module.

Figure 4.7 shows the four different regulator designs that were used in the voltage supply, and their output capabilities. The voltage supply was built with
Figure 4.6: Connections on the rear panel of the voltage supply, viewed from the outside of the supply chassis. The connection layout is the same as the old analogue supplies, allowing the cables to the spectrometer to be swapped from one to the other easily. The analyser lens element connection uses a different cable and so the ordering of the connections was not preserved.
one very high voltage module, labelled VHV, one positive high voltage module, ANAHR, one bipolar high voltage module, SPLIT, and three low voltage modules, LV. The output capabilities of each rectifier module are shown in the diagram.

The internal design of each of the rectifier modules is shown in Fig. 4.8. Each module takes AC input from one of the transformers and distributes this to regulator blocks located on the module. Each block produces certain output voltages and these are routed to a jumper on the end of the module which plugs into the relevant socket on the backplane.

Each of the voltage cards requires a positive and negative rail (VCC and
Figure 4.8: Variations of rectifier boards used in the voltage supply. The board type used varies depending on the voltage requirements of the card in its specified slot. For example, there is no need for the 800 V rail for a deflector card. Each rectifier board is supplied with AC from a transformer tapped at the RMS voltages shown. The DC voltage levels supplied by the board are distributed to a backplane slot via the jumper shown on the right of the diagram. One, two or three rectifier blocks are used to supply the correct output voltages for each board. The circuit diagrams for the rectifier blocks are given in Fig. 4.9.
VDD) and an additional 5 V rail, and this is provided by a low voltage rectifier and regulator block, which is contained on every rectifier module. The low voltage module LV contains no rectifier blocks other than this.

The VHV rectifier module contains two additional rectifier blocks. A voltage quadrupler is used to provide a $\sim 800$ V output, and a $+250$ V output is provided by a half-wave rectifier block. A half wave rectifier must be used here instead of a full-wave rectifier, as the voltage quadrupler must be referenced to 0 V. This references the high voltage transformer winding to 0 V, making it unsuitable for use with a full-wave rectifier since this would require the high voltage winding to be floating.

The ANAHR rectifier module also contains the half-wave rectifier block, which provides a $+250$ V output. A full-wave rectifier may have been used here instead, although the half wave rectifier was found to produce sufficient output current.

The SPLIT module provides $\pm 250$ V outputs using two half-wave rectifiers. These use either the positive or negative half of the AC signal to supply positive and negative DC.

In Fig. 4.9 the circuit diagrams for the various regulator blocks are presented. This shows how the various DC output voltages are supplied from the AC inputs.

4.2.3 Microcontroller Board, Keypad and Display

The operation of the voltage supply is controlled by the microcontroller, which is located on a separate board to the power supply units. The microcontroller sets the voltage levels that are supplied from the voltage cards. These voltages are set either in response to controls on the front panel, or through communication with a computer via a USB port.

The microcontroller is situated on a board which provides connections for the USB and for a programming header. The header is used to configure the microcontroller, as described in Section 4.4. The connections that the microcontroller
Figure 4.9: Circuit diagrams for regulator blocks shown in Fig. 4.8. The **Low Voltage Rectifier/Regulator** block uses a full wave rectifier, smoothing capacitors and regulators to provide regulated ±15 V and 5 V DC. The **Half-Wave** and **Dual Half-Wave** rectifier blocks use the positive or negative going parts of the AC signal to provide unregulated DC output. The voltage quadrupler uses an arrangement of diodes and capacitors to multiply the input voltage. The chain of RQ resistors discharge the quadrupler when power is removed.
board makes the the rest of the supply were shown in Fig. 4.4.

The microcontroller board connects to the voltage cards in the crate via the backplane. This connection is a 9-pin ‘D’ sub-miniature which connects from the board to the address and data lines on the backplane.

A $16 \times 8$ character dot matrix liquid crystal display (LCD) is mounted to the front panel and connects to the microcontroller board via a 15-pin interface. The display is used to show status messages from the microcontroller, for example the voltage level of a channel.

The microcontroller board also connects to a front panel board, called the keypad. Mounted on this board are a bank of twelve rotary encoders, four switches and three LEDs. This is the front panel control interface to the voltage supply. Voltages may be adjusted manually by turning the control knobs and depressing the switches. The front panel controls are described in Section 4.4.5.

Each switch on the front panel uses one digital channel. Each of the rotary encoders uses three digital channels, two to encode rotation information and one to indicate whether the encoder has been depressed. This is a total of 40 digital lines. The state of any of these digital lines determines which key events have occurred on the keypad. The number of digital lines required to transmit this information is reduced from 40 by segmenting the digital lines into groups of 5 bits, with each group selected by a 3-bit address. A total of eight pins on the microcontroller are therefore used to read the keypad state.

4.3 Card Designs

4.3.1 Overview

In this section the design of the voltage supply cards will be discussed. There were four designs of voltage cards, summarised in Section 4.3.5. Each of the voltage cards plugged into the backplane, and supplied either four or eight voltage
channels. Each channel was provided by an amplifier block. There were three different types of amplifier block, described in section 4.3.3, each with specific output capabilities, and it was the selection of amplifier blocks that distinguished one card from another.

Each of the different types of card were built to a similar design, and this is described in the following section. The different types of amplifier blocks will then be described, and the different types of card summarised.

4.3.2 Common Components

The voltage supply cards were based on the same design, shown in Fig. 4.10. Each card was split into two distinct regions, each electrically isolated from the other. The interface section contained the interface logic to the card, and was referenced to the same 0V level as the microcontroller board. The analogue section of the card could be referenced to any required voltage on another card, this is the analogue section.

An edge connector on the left edge of the card plugs into the backplane and electrically connects the card to the rest of the voltage supply. This powers the card, connects the card to the microcontroller and connects the voltage outputs to the lens elements in the spectrometer via the backplane.

The interface section receives address and data signals from the backplane. The address of the card is set using three dual inline package (DIP) switches. A bank of optocouplers labelled ‘Opto’ allows digital signals to be transmitted from the interface section to the analogue section while maintaining their electrical isolation.

Address selection logic compares the state of the DIP switches with the address signal. If these match, then the data signals are transferred to the optocouplers. These signals travel across the isolation barrier to an Analog Devices AD5666 or AD5668 multi-channel DAC. An activity LED on the front of the card is
The layout of a voltage supply card. The edge connector on the left plugs into the back panel. The top and bottom sections of the card are referenced to different supply voltages; the interface section is referenced to the microcontroller board and the analogue section is powered by an independent supply. The parts labelled A1 to A8 are amplifier blocks. Some voltage cards only implement A1 to A4.

connected to the address select logic, and flashes whenever the card is selected and data is sent.

The analogue section contained either four or eight amplifier blocks, depending on the specific card. These are labelled A1 to A8 in the diagram. The multi-channel DAC provided a programming voltage between 0 and 5 V to each amplifier block on the voltage card. The DAC has either four or eight channels, depending on the number of amplifier blocks on the card. The four channel variant of the DAC was the AD5666, and the eight channel was the AD5668.

The DAC was situated in the analogue section of the voltage card so that the output voltages were referenced to the same level as the amplifier blocks. The DAC output voltages are programmed via three digital lines. These are the signals transmitted from the interface section via the bank of optocouplers. The output level for the DACs are set digitally using a DAC programming code which is a number between 0 and \(2^{16} - 1\). This selects an output voltage from the DAC between 0 and 5 V. The relationship between the programming code and
the output voltage is guaranteed to be linear \cite{110}. The amplifiers were then designed so that their output voltage was linearly related to the programming voltage, which would be supplied from the DAC.

4.3.3 Amplifier Blocks

4.3.3.1 High Voltage Supply

The high voltage supply was required for the spectrometer lens elements, the reference voltages GUNE and A1RSE, and the Faraday cup voltage FCUP. A single high voltage amplifier block is a unipolar supply which could be configured to have an output voltage up to $\sim 700$ V. The amplifier was not designed to source or sink high currents. The amplifier could also be configured to give either a positive or negative output voltage by appropriate selection of components.

The high voltage amplifier block can be described simply by the circuit presented in Fig. 4.11. This design was used in all of the voltage cards capable of creating a potential difference of over 20 V. In this diagram current flows from an unregulated high voltage supply, labelled HV, to the 0 V terminal through the transistor and the resistors R2 and R3.

The design of the high voltage amplifier block was based around a metal oxide semiconductor field effect transistor (MOSFET) Q1, which is represented as a variable resistor in Fig. 4.11. The MOSFET can act as a variable resistor because a voltage at its gate terminal (not shown on the diagram) controls the current that can flow through it from the drain (D) to the source (S).

To analyse the behaviour of the circuit, it is useful to consider the output voltage in the cases when the transistor is: fully on and conducting; or not conducting. In the first case, no current flows through R2 and R3, as the transistor provides a low impedance path to the 0 V rail. The voltage at the drain terminal, and hence the output voltage $V_{\text{out}}$, is then almost zero volts. Under these conditions, the amplifier dissipates maximum power, since $P \approx V^2/R_1$, where $R_1$ is
the resistor between the drain terminal of the transistor and the high voltage line held at voltage $V$.

In the second case the transistor is not conducting and presents a very high impedance. Current must therefore flow through R2 and R3. The voltage at $V_{\text{out}}$ can now be calculated by considering the voltage divider formed by R1, R2 and R3. If $R_3 << R_2$, the maximum voltage at the output is $V_{\text{out}}^{\text{max}} \approx V_{HV} R_2 / (R_1 + R_2)$. The amplifier dissipates the least current at its maximum output voltage, since in this case $P = V_{HV}^2 / (R_1 + R_2 + R_3)$.

Between these two extremes, current is split between the two branches of the circuit, with the proportion in each branch controlled by the effective resistance presented by the transistor. The voltage $V_{\text{out}}$ therefore can be varied continuously between the maximum voltage $V_{\text{max}}$ and $V_{\text{min}} \approx 0$.

The amplifier monitors the output voltage by sampling a proportion of it at the voltage divider formed by R2 and R3. This provides the voltage $V_{\text{samp}}$. Resistor R3 was chosen such that the potential between 0 V and $V_{\text{samp}}$ did not exceed 5 V.
An OPA4277 op-amp was used to compare the sample voltage to a programming voltage $V_{\text{prog}}$ supplied to the amplifier block. The output from the op-amp drives the gate of the MOSFET, and therefore determines the current that flows through Q1. The op-amp adjusts its output to keep the difference between its two input voltages $V_{\text{prog}}$ and $V_{\text{samp}}$ at zero. This forms a negative feedback loop and ensures that the output from the high voltage section of the amplifier is linear in relation to the programming voltage. The gain of the circuit is therefore:

$$G = \frac{V_{\text{out}}}{V_{\text{prog}}} = \frac{R2 + R3}{R3}$$

The full circuit design for the high voltage amplifier is shown in Fig. 4.12. The diagram shows an amplifier which is capable of producing output voltages from 0 V up to $V_{\text{out}}^{\text{max}} \approx 180$ V. The gain, determined by the selection of R2 and R3, is $G = 45$. With $V_{\text{prog}}$ at its maximum voltage, 5 V, the output from the amplifier stage would be 225 V, however the actual output voltage achieved was limited to the maximum voltage of the amplifier stage, $V_{\text{out}}^{\text{max}}$. 
The voltage output was provided from the drain terminal of a Fairchild Semiconductor FQP3N80C N-channel enhancement mode power MOSFET [111] specified for high drain to source voltages. This transistor was driven by a precision Burr Brown OPA477 series op-amp [112], which provided a voltage at the gate terminal that controls the output voltage of the amplifier block. A voltage of about 10 V at the gate was required for the transistor to be fully conducting.

Due to the magnitude of the voltages over the amplifier, the resistor R1 was split into two resistors, R1A and R1B, this allowed cheaper standard resistors to be used, as a single resistor here dissipated more than the maximum rated power. Similarly, the resistor R2 was split into R2A and R2B, to ensure that the voltage over a single resistor did not approach the maximum rated value.

To prevent the output voltage from oscillating, capacitor C4 and resistor R6 were used to adjust the phase of the amplifier output so as to suppress high frequency oscillations. Capacitors C1 and C2 filter high frequencies on the high voltage input and regulated output respectively.

By changing the voltage on the HV line and adjusting R1, R2 and R3 accordingly, the gain and maximum voltage of the amplifier block can be altered. To provide the voltages of up to 600 V for the gun elements GL1B and GL2B, an amplifier block was required with a higher maximum output voltage. The modified amplifier block used an unregulated 800 V on the HV line, and values of 660 kΩ, 6.6 MΩ and 47 kΩ for R1, R2 and R3. This gives a gain \( G \approx 140 \), and a maximum output voltage of 700 V, which is not limited by the maximum output voltage, as in this case \( V_{\text{out}}^{\text{max}} > 700 \text{ V} \).

To provide the required voltages for A1RSE and GUNE, negative voltages were supplied. The N-channel MOSFET shown in Fig. 4.12 was hence replaced with a P-channel MOSFET, the IRF9610 [113], while the resistor values were retained as in Fig. 4.12. This circuit was then driven with a negative programming voltage to produce the desired outputs, which in practice meant that the signal from the DAC which drives the high voltage amplifier was fed through an OPA4277 op-amp configured as an inverting amplifier.
In Fig. 4.13, the measurements taken to confirm the linearity of the amplifier are presented for the 200 V amplifier block and the 700 V amplifier block. Both exhibit a linear response to the DAC programming code. The 200 V supply is only linear up to around 180 V, where it clips as the output reaches the maximum. The 700 V amplifier shows some deviation from linearity, although the scale of these deviations are small compared to the output voltage.

4.3.3.2 Deflector Supply

The voltages which connect to the deflector plates were required to be bipolar. The output $V_{\text{out}}$ to these supplies should be adjustable approximately within the range $-20 \text{ V} < V_{\text{out}} < +20 \text{ V}$. This is within the range of many commercially available op-amps and so the Burr Brown OP552 [114] was used with supply rails at $\pm20 \text{ V}$. This allowed a comparable voltage swing at the output.

The circuit diagram for this amplifier block is shown in Fig. 4.14. It requires two voltages, the programming voltage, $V_{\text{prog}}$, and a trim voltage $V_{\text{trim}}$.

The circuit shown in Fig. 4.14 maps the $0 \rightarrow 5 \text{ V}$ range of the programming voltage onto the output range $-20 \rightarrow +20 \text{ V}$. The output voltage was calculated to be:

$$V_{\text{out}} = \frac{R_1 + R_2}{R_1} V_{\text{in}} - \frac{R_2 V_{\text{trim}}}{R_1}$$

To map the programming voltage onto the desired output range, a gain of 8 and an offset of $-20 \text{ V}$ were required. The resistors were chosen to provide the correct gain, $R_1 = 1.2 \text{ k}\Omega$ and $R_2 = 8.2 \text{ k}\Omega$. The required trim voltage was found using

$$V_{\text{trim}} = -\frac{R_1 V_{\text{ofs}}}{R_2}$$

and should therefore be set to $V_{\text{trim}} = 2.93 \text{ V}$. This sets the zero point of the deflector amplifier to the midpoint of the DAC scale.

The trim voltage is supplied by a trim potentiometer elsewhere on the deflector
Figure 4.13: High voltage amplifier linearity measurements for the 200 V and 700 V amplifier blocks. For each amplifier, the points on the top graph show the variation of output voltage with DAC programming code. The dotted line is a fit to the linear region of the graph. The bottom graph shows the deviation of each data point from the fit line. These are on the order of a few hundred parts per million. The error bars show the measured AC component of the signal, these are on the order of a few tens per million.
board which was buffered using another OPA4277 op-amp. This arrangement supplies the trim voltage to all deflector amplifier blocks on the card, and so it was not possible to precisely define the zero point for all the amplifiers. Instead it was only necessary to set the zero point approximately, since the process of calibrating the DACs, described in Section 4.4.3, assured that the program voltage required to set the output to zero was known.

In practice the trim voltage was adjusted by first setting the programming voltage for all DAC channels to mid-scale and then adjusting the trim voltage until the output from the OP552 op-amps were around zero.

The resistor $R_3$ was chosen to be equal to the parallel combination of $R_1$ and $R_2$. This cancels the input voltage offset caused by the op-amp input current.

4.3.3.3 Grid Supply

The amplifier block for the grid supply was only used on the gun voltage card. The voltage for the grid element on the gun is required to be negative, with a
typical output voltage of $\sim 3\,\text{V}$, as discussed in Section 3.3.1. As with the other amplifier blocks, a programming voltage $V_{\text{prog}}$ is required to select the output voltage $V_{\text{out}}$ of the stage.

The circuit diagram for the grid supply is given in Fig. 4.15; it is simply an inverting op-amp with a gain $G \approx -3$, this value of the gain being due to the values of the resistors $R_1$ and $R_2$. The op-amp used for this supply was an OPA4277, powered from the $\pm 12\,\text{V}$ regulators on the voltage card. This limits the maximum output voltage to within around a volt of the negative supply; roughly $-11\,\text{V}$.

The current limiting resistor $R_3$ on the output protects the op-amp from excessive loads on the output pin. For the OPA4277 this is unnecessary since the amplifier has current limited outputs.

### 4.3.4 On-Board Regulators

The on-board regulators supply regulated DC power to the op-amps on the analogue section of the voltage card. A positive and a negative DC voltage were supplied to the on-board regulators via two pins on the edge connector, VCC and VDD.

To operate the deflectors with a range approaching $\pm 20\,\text{V}$, the voltages supplied to the op-amps in the deflector amplifier blocks must be $\pm 20\,\text{V}$. This required the specialised OP552 op-amps, since most will not operate with their supply voltages at these high levels.
The HV and grid amplifier blocks are operated with the supplies to the op-amps held at ±12 V. This is acceptable since the op-amp contained within the high voltage amplifier block is required only to output a maximum of around 10 V to operate the MOSFET, and the typical grid supply voltage is around -3 V. Therefore if a voltage card contained deflector supplies, then the op amp supply rails would need to be held at ±20 V. Otherwise they were held at a lower voltage.

For cards where ±12 V rails were used, 7812 and 7912 series regulators on the VCC and VDD lines generate the local ±12 V levels to use on the card. The circuit is illustrated in Fig. 4.16(a). As specified in the datasheets the regulators are decoupled with 0.1 µF capacitors and protected from reverse currents by 1N4007 diodes DP1–DP4.

The deflector cards, which require ±20 V rails, use a pair of adjustable regulators set to ±20 V instead. The circuit diagram is shown in Fig. 4.16(b). The adjustable regulators used were the LM317 [115] and LM337 [116] types for the positive and negative rails, respectively. These were chosen as they were readily available. The value of the sensing resistors RRN1 and RRP1 were chosen as per the datasheet for the respective regulators. The level of the output was set using a chain of fixed resistance to 0 V from the ADJ pin for each regulator, with a small adjustment possible using trim potentiometers. This allowed for some fine tuning of the output level.

4.3.5 Card Types

In Table 4.1, the various different types of voltage card are listed. The type of card is defined by the selection of amplifier blocks and their configuration. There are four different types of card, and the choice of amplifier blocks in each is selected to supply the correct voltage ranges for specific parts of the spectrometer.

The bias voltage card was referenced to ground. This card supplied the voltages GUNE, A1RSE and FCUP, which were all specified relative to zero volts. The gun elements were referenced to GUNE and the analyser elements to A1RSE.
Figure 4.16: Circuit diagram showing: (a) the ±12V regulators, and (b) the adjustable regulators. The 1N4007 diodes are for protection against reverse bias across the regulators, as specified in the datasheet. The output voltage for the adjustable regulators was set by the value of the sensing resistor RRN1 or RRP1, and the resistance between the ADJ pin and the 0V reference.
<table>
<thead>
<tr>
<th>Card Type</th>
<th>n×</th>
<th>Amp Blocks</th>
<th>Voltage Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>E266 Bias Voltage</td>
<td>2×</td>
<td>High voltage</td>
<td>-200 → 0</td>
</tr>
<tr>
<td>E257 Gun Voltage</td>
<td>4×</td>
<td>High voltage</td>
<td>0 → +200</td>
</tr>
<tr>
<td></td>
<td>2×</td>
<td>Grid supply</td>
<td>-12 → 0</td>
</tr>
<tr>
<td>E288 Analyser Voltage</td>
<td>4×</td>
<td>High voltage</td>
<td>0 → +200</td>
</tr>
<tr>
<td>E292 4-Channel Deflector</td>
<td>4×</td>
<td>Deflector</td>
<td>-20 → +20</td>
</tr>
<tr>
<td>E352 8-Channel Deflector</td>
<td>+4×</td>
<td>Deflector</td>
<td>-20 → +20</td>
</tr>
</tbody>
</table>

**Table 4.1:** The four different voltage card types. The deflector card may be built with either four or eight deflector amplifiers on the card. The workshop number, displayed in the table as $E_{nnn}$, is written on the PCB and may be used to identify the card. The bias voltage card supplies the potentials for GUNE and A1RSE which are required to be negative.

The FCUP voltage supplied a bias voltage to the Faraday cup. This card has one unused amplifier block.

The gun voltage card supplies the voltages for all the gun elements, apart from the deflectors. The card is referenced so that its 0 V level is at GUNE voltage. The card has six high voltage amplifier blocks and two grid amplifier blocks. All the amplifier blocks supply positive voltages; four supply up to 200 V and the other two supply up to 700 V. One of the 200 V supplies is unused and one of the grid amplifier blocks is unused.

The analyser voltage card supplies the voltages for all the analyser elements, apart from the deflectors. This card is referenced to the A1RSE voltage from the base voltage card.

The deflector card supplies voltages for the deflector plates. There were two versions of this card built, one with four deflector amplifiers, and one with eight. These are used for the gun and analyser deflectors.

The voltage reference point for each card is not defined in the voltage supply...
but instead by connections made in a voltage junction box. A list of cards and their reference voltages is given in Table 4.2.

### 4.4 Microcontroller

The voltage supply is controlled by a *microcontroller*, a computer contained on a single chip. The microcontroller chosen was a Microchip PIC18F4550 [117]. The chip provides a number of connections which are used to interface to the separate parts of the voltage supply, including the backplane, the front panel, the display and a controlling computer via a USB port. Internally, the chip contains a non-volatile program memory, a volatile working memory called the data memory, and a small amount of high-endurance non-volatile data memory. The sizes of these memories are summarised in table 4.3. The microcontroller contains a number of *peripherals*, this is hardware located on the chip but external to the processing unit. Those used for the voltage supply were the digital ports, the timers, the interrupt controller and the USB controller.

The microcontroller sequentially executes coded instructions located in the program memory. These instructions may operate on the internal state of the controller, allowing it to change arbitrary values in memory and perform calculations. Instructions may also operate to change the state of peripherals, for example allowing the controller to exchange data with connected components.
Memory | Size (bytes) | Volatile?
--- | --- | ---
Program memory | 32768 | No
Data EEPROM memory | 256 | No
Data memory | 2048 | Yes

**Table 4.3:** PIC18F4550 microcontroller memory sizes. A volatile memory only retains its contents while power is applied to the device.

Additionally, program control instructions allow the controller to branch the execution point to a non-sequential location in the program memory. These branch instructions may depend on the outcome of a condition (a *conditional branch*).

Figure 4.17 illustrates the controller’s view of the voltage supply. The display is a 16 × 2 LCD, and the display controller is a clone of an Hitachi HD44780U. The *ICD header* connects to the computer for programming and debugging purposes only.
A 4 MHz crystal oscillator was used to provide a clock source for the microcontroller. The microcontroller was set to derive a 48 MHz clock signal from this external oscillator. This frequency was determined by the USB peripheral, which must run at this speed. The microcontroller uses four oscillator periods per instruction cycle, so each instruction cycle takes around 80 ns. Most instructions take one instruction cycle to complete, apart from conditional branch instructions, which take two.

4.4.1 Controller Firmware

The behaviour of the controller is determined by the firmware. This is a list of coded instructions that the microcontroller will follow when the power is applied. The firmware was generated on a computer using Microchip MPLAB 8 [118], and was written onto the microcontroller’s non-volatile program memory using a programmer, the Microchip ICD 2 [119]. The programmer connected to the programming pins on the microcontroller via a programming port.

The firmware was written using the C programming language [120], and compiled using the Microchip C18 Compiler [121]. The output from the compiler was then used to produce a firmware file which was written to the microcontroller.

The initialisation routine, the interrupt service routine and the main program loop are located in main.c. The rest of the program code is split into several different files which group related subroutines together.

The interrupt service routine handles events from two of the timers built onto the microcontroller. These timers are called TMR0 and TMR1, and are configured and enabled during the initialisation routine. Each timer counts down at a specified rate until it reaches zero, at which point the timer overflows and program execution is interrupted to pass control to the interrupt service routine.

The uses for the two timers are listed in Table 4.4. The first timer, TMR0, is used to poll the keypad at a regular interval of ~ 40 ms. This polling interval
Interrupt driven timer events

<table>
<thead>
<tr>
<th>Timer</th>
<th>Purpose</th>
<th>Source File</th>
</tr>
</thead>
<tbody>
<tr>
<td>TMR0</td>
<td>Keypad polling.</td>
<td>keypad.c</td>
</tr>
<tr>
<td>TMR1</td>
<td>Additional software timers.</td>
<td>timers.c</td>
</tr>
</tbody>
</table>

Table 4.4: Interrupt driven timer events. The microcontroller has a number of hardware timers, one is used to regularly poll the keypad, and one is multiplexed to eight low resolution software timers.

was chosen to be long enough to act to debounce the mechanical switches and encoders on the front panel, but also short enough to be sensitive to the waveform between each detent on the rotary encoders.

The keypad state is stored in a ring buffer and processed later in the main program loop. This ensures that the microcontroller spends a minimal amount of time processing interrupts, as this halts execution of the main program code.

The second timer, \( \text{TMR1} \), is multiplexed to eight low resolution software timers with a resolution of around 150\( \mu \text{s} \). Function calls defined in the file \text{timer.c} allow simplified access to these timers. The function \text{tmr_u_delayset()} activates a timer by setting it to a positive non-zero value. Every time that \( \text{TMR1} \) overflows, the timer is decremented by one. When it reaches zero the timer is deactivated. A second function, \text{tmr_u_waitorrelease()} will return true if the timer has elapsed, and will release the timer.

The remainder of the firmware is organised as a number of finite state machines. This is a method of specifying the behaviour of each sub-system by describing each possible state of that sub-system, and defining when to transition to another state. Each sub-system is tasked with controlling a given piece of hardware which makes up the voltage supply. A list of the state machines and their function is given in Table 4.5.

The main program loop repeatedly calls each state machine in turn. If the state machine is waiting for a transition then it is idle, and so will immediately return control to the main program loop. If the state machine has transitioned to
Table 4.5: State machines implemented on the microcontroller. The final two on the list are from the Microchip USB Library.

<table>
<thead>
<tr>
<th>Name</th>
<th>Function</th>
<th>Source File</th>
</tr>
</thead>
<tbody>
<tr>
<td>cmd_sm</td>
<td>USB command interface.</td>
<td>cmd.c</td>
</tr>
<tr>
<td>dac_sm</td>
<td>Interface to voltage supply cards.</td>
<td>dac.c</td>
</tr>
<tr>
<td>dsm</td>
<td>LCD display driver.</td>
<td>display.c</td>
</tr>
<tr>
<td>kph_sm</td>
<td>Key responder.</td>
<td>keyhandle.c</td>
</tr>
</tbody>
</table>

State machines (USB Library)

<table>
<thead>
<tr>
<th>Name</th>
<th>Function</th>
</tr>
</thead>
<tbody>
<tr>
<td>CDC_TX</td>
<td>USB serial emulation driver.</td>
</tr>
<tr>
<td>USBDeviceTasks</td>
<td>Low level USB tasks.</td>
</tr>
</tbody>
</table>

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Writing the program code using state machines has the advantage that different hardware control routines can run concurrently. As an example, consider the process of updating a voltage output from the supply. These are controlled via a number of DACs, accessed via seven digital pins on the microcontroller which connect to the backplane. The DACs are clocked at a much lower speed than the microcontroller, at around 3 kHz. Updating a single DAC voltage takes around 20 ms. If no other tasks are running, the microcontroller is idle for most of this period, while it is waiting to send data on the next clock transition.

Now consider a second task which may be requested at the same time; writing a character to the display. To program a character onto the display also requires a digital waveform of a finite length, in this case around 1 ms. Using a conventional sequential programming model, the amount of time taken for both updates would be equal to the sum of the two times, as one is processed after the other. This is illustrated in Fig. 4.18(a).

However, as the display is accessed via different physical pins to the DACs, it is possible to program them during the time that a DAC is being updated. The total time to perform the two updates is equal only to the time that the longest
Figure 4.18: Concurrent signalling using a state machine. Each block on the diagram represents a length of time taken to update either a DAC voltage, or a character on the display. The height of a box corresponds to the length of time that an update takes. In each diagram the time, $t$, increases in a downwards direction.

(a) A sequential update. A DAC voltage is updated first, followed by a display update. This takes the longest time.

(b) The DAC update and the display update are carried out in parallel in this diagram. The total time taken is equal to the length of time that the longest task takes, in this case the DAC update.

(c) Multiple display updates cannot be carried out in parallel. This diagram shows multiple display updates being carried out sequentially while a DAC is being updated.
update takes, in this case this is the DAC update. Figure 4.18(b) illustrates this case. Additional display updates are then possible while the DAC update is completing, as shown in in Fig. 4.18(c).

While communicating with hardware in this way, the microcontroller still spends most of its time idle and waiting to send the next clock transition, but importantly this idle time is made available to the other sub-systems. This is essential for the USB sub-system which must maintain constant and timely communication with the host computer if it is connected. It also helps to make the system responsive, so for example while a knob is being rotated on the front panel, the display can be updated continuously while the rotation events continue to be detected and interpreted.

A disadvantage to the state machine approach is that it leads to program code that can be difficult to interpret. In the next section, a schematic diagram and description is provided for the main sub-system responsible for setting the voltage output levels.

4.4.2 Performing a Voltage Update

The microcontroller communicates with the voltage cards via the backplane. Each card contains some address select logic to ensure that the DAC on a specific card can only respond when its address is selected. There are three address lines, labelled $A_0$, $A_1$ and $A_2$. These address lines are used to select a physical slot in the voltage supply chassis in which a specific card sits. Figure 4.19 shows how the physical slots are assigned.

The DAC on each voltage card controls the levels of either four or eight voltage outputs from the supply. Depending on the number of channels the DAC used is either an Analog Devices AD5666 (four channels) or an AD5668 (eight channels) [110]. These voltage outputs are controlled from separate output channels on each of the DACs. As discussed in Section 4.3.3, the voltage from each DAC channel passes through an amplifier. This maps the output range of
the DAC on the card to the necessary voltage range required for a specific element of the spectrometer.

Each DAC is programmed using three control lines, \texttt{SYNC}, \texttt{CLK} and \texttt{D}. These lines are used to transmit a 32-bit \textit{control word} to the DAC. A specific channel on the DAC is selected via three bits in the control word; these bits are referred to as \texttt{D0}, \texttt{D1} and \texttt{D2}. For the four channel DAC, the value of \texttt{D2} is ignored.

The physical slot address and the channel number are combined to generate a unique six bit address for each voltage channel on the supply. The binary channel address is defined as follows:

\[
\text{Channel address} = \text{Card Address} \oplus \text{DAC number} = \overline{A2} A1 \overline{A0} \overline{D2} \overline{D1} D0
\]

Table 4.6 lists the voltage supply channels and their corresponding address. These are used by the firmware to select a specific channel, and are used to identify a specific channel when a computer is attached via the USB connection.

To update the voltage output from a DAC channel, a specific pattern of bits must be transmitted along the three control lines, as illustrated in Fig. 4.20. The DAC is ready to receive data when the \texttt{SYNC} line is taken low. A \textit{control word} made up of 32 data bits \texttt{DB31} to \texttt{DB0} is clocked into the DAC on the falling edge of the \texttt{CLK} line. This changes the output voltage according to a 16-bit binary
<table>
<thead>
<tr>
<th>Channels (Gun)</th>
<th>Name</th>
<th>EID (Hex)</th>
<th>Slot</th>
<th>Wire colour</th>
<th>Voltage Range (V)</th>
</tr>
</thead>
<tbody>
<tr>
<td>GUNE</td>
<td>000 010 (0x02)</td>
<td>1</td>
<td>Blue</td>
<td>-200 → 0</td>
<td></td>
</tr>
<tr>
<td>ANQD</td>
<td>001 000 (0x08)</td>
<td>2</td>
<td>White</td>
<td>0 → +200</td>
<td></td>
</tr>
<tr>
<td>GRID</td>
<td>001 110 (0x0E)</td>
<td>2</td>
<td>Red</td>
<td>-15 → 0</td>
<td></td>
</tr>
<tr>
<td>GL1B</td>
<td>001 100 (0x0C)</td>
<td>2</td>
<td>Yellow</td>
<td>0 → +700</td>
<td></td>
</tr>
<tr>
<td>GL2B</td>
<td>001 101 (0x0D)</td>
<td>2</td>
<td>Orange</td>
<td>0 → +700</td>
<td></td>
</tr>
<tr>
<td>GL1C</td>
<td>001 001 (0x09)</td>
<td>2</td>
<td>Purple</td>
<td>0 → +200</td>
<td></td>
</tr>
<tr>
<td>D1X+</td>
<td>010 000 (0x10)</td>
<td>3</td>
<td>White</td>
<td>-20 → +20</td>
<td></td>
</tr>
<tr>
<td>D1X−</td>
<td>010 001 (0x11)</td>
<td>3</td>
<td>Purple</td>
<td>-20 → +20</td>
<td></td>
</tr>
<tr>
<td>D1Y+</td>
<td>010 010 (0x12)</td>
<td>3</td>
<td>Blue</td>
<td>-20 → +20</td>
<td></td>
</tr>
<tr>
<td>D1Y−</td>
<td>010 011 (0x13)</td>
<td>3</td>
<td>Green</td>
<td>-20 → +20</td>
<td></td>
</tr>
<tr>
<td>D2X+</td>
<td>011 000 (0x18)</td>
<td>4</td>
<td>White</td>
<td>-20 → +20</td>
<td></td>
</tr>
<tr>
<td>D2X−</td>
<td>011 001 (0x19)</td>
<td>4</td>
<td>Purple</td>
<td>-20 → +20</td>
<td></td>
</tr>
<tr>
<td>D2Y+</td>
<td>011 010 (0x1A)</td>
<td>4</td>
<td>Blue</td>
<td>-20 → +20</td>
<td></td>
</tr>
<tr>
<td>D2Y−</td>
<td>011 011 (0x1C)</td>
<td>4</td>
<td>Green</td>
<td>-20 → +20</td>
<td></td>
</tr>
<tr>
<td>D3X+</td>
<td>011 100 (0x1B)</td>
<td>4</td>
<td>Yellow</td>
<td>-20 → +20</td>
<td></td>
</tr>
<tr>
<td>D3X−</td>
<td>011 101 (0x1D)</td>
<td>4</td>
<td>Orange</td>
<td>-20 → +20</td>
<td></td>
</tr>
<tr>
<td>D3Y+</td>
<td>011 110 (0x1E)</td>
<td>4</td>
<td>Red</td>
<td>-20 → +20</td>
<td></td>
</tr>
<tr>
<td>D3Y−</td>
<td>011 111 (0x1F)</td>
<td>4</td>
<td>Brown</td>
<td>-20 → +20</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Channels (Analyser)</th>
<th>Name</th>
<th>EID (Hex)</th>
<th>Slot</th>
<th>Wire colour</th>
<th>Voltage Range (V)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A1RS</td>
<td>000 011 (0x03)</td>
<td>1</td>
<td>Green</td>
<td>-200 → 0</td>
<td></td>
</tr>
<tr>
<td>A1L1</td>
<td>100 000 (0x20)</td>
<td>5</td>
<td>White</td>
<td>0 → +200</td>
<td></td>
</tr>
<tr>
<td>A1IH</td>
<td>100 001 (0x21)</td>
<td>5</td>
<td>Purple</td>
<td>0 → +200</td>
<td></td>
</tr>
<tr>
<td>A1AM</td>
<td>100 010 (0x22)</td>
<td>5</td>
<td>Blue</td>
<td>0 → +200</td>
<td></td>
</tr>
<tr>
<td>A1OH</td>
<td>100 011 (0x23)</td>
<td>5</td>
<td>Green</td>
<td>0 → +200</td>
<td></td>
</tr>
<tr>
<td>ADX+</td>
<td>101 000 (0x28)</td>
<td>6</td>
<td>White</td>
<td>-20 → +20</td>
<td></td>
</tr>
<tr>
<td>ADX−</td>
<td>101 001 (0x29)</td>
<td>6</td>
<td>Purple</td>
<td>-20 → +20</td>
<td></td>
</tr>
<tr>
<td>ADY+</td>
<td>101 010 (0x2A)</td>
<td>6</td>
<td>Blue</td>
<td>-20 → +20</td>
<td></td>
</tr>
<tr>
<td>ADY−</td>
<td>101 011 (0x2C)</td>
<td>6</td>
<td>Green</td>
<td>-20 → +20</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Channel (Faraday Cup)</th>
<th>Name</th>
<th>EID (Hex)</th>
<th>Slot</th>
<th>Wire colour</th>
<th>Voltage Range (V)</th>
</tr>
</thead>
<tbody>
<tr>
<td>FCUP</td>
<td>000 000 (0x00)</td>
<td>1</td>
<td>White</td>
<td>0 → +200</td>
<td></td>
</tr>
</tbody>
</table>

Table 4.6: Voltage lines and channels
number encoded in the control word.

The microcontroller is able to change the digital signals on the control and address lines under the control of the firmware. This allows the DAC voltages to be programmed. The functions associated with controlling the DACs on the voltage cards are located in the file `dac.c`, and together make up the DAC sub-system. This file also contains the code for the state machine. While the state machine is running it allows DAC updates to occur without blocking execution of the main loop, so that other sub-systems can run in parallel.

The DAC sub-system keeps a record of the output voltages using a DAC value table stored in the microcontroller’s volatile memory. This table contains a list of the 16-bit codes that were used to program each DAC. To alter an output voltage, the relevant DAC must be programmed with a new code using the function `dac_setval()`. The sub-system writes the new code to the table and marks that entry to show it has not yet been programmed to the DAC.

A simplified state diagram for the sub-system is shown in Fig. 4.21. In the diagram, each state is represented by a box, drawn with rounded corners. Inside each box is the title of the state, at the top, followed by a list of actions. These actions are only carried out once, when a transition to that state occurs. Transitions on the diagram are represented by arrows, with the condition for the transition to occur written beside them. The system will remain in a given state

---

**Figure 4.20:** The digital waveforms required to write to the AD5668/AD5666 16-bit DACs used in the voltage cards. This diagram is adapted from [110].
**Figure 4.21:** A representation of the state machine for updating voltages. This diagram represents the state machine implemented in the `dac_sm()` function located in the file `dac.c`. Each of the rounded boxes represents a state. The top line is the title of the state and the contents of the box are a list of actions which occur directly after a transition. This is a simplified representation of the state machine, and does not show procedures necessary for updating the non-volatile memory to reflect changes to the values, or the procedures for queuing an update to the display.
until one of these conditions is met, at which point it will transition to the state indicated. The diamond boxes, labelled ‘A’ and ‘B’ are pseudostates, from which the state machine will transition immediately.

The sub-system begins in the ‘idle’ state. An algorithm periodically scans the DAC value table while in this state. If an updated entry (marked as unprogrammed) is found in the table, the algorithm stores the relevant DAC address and channel, and the state machine transitions to the ‘initialise’ state.

The ‘initialise’ state sets the address lines to point to the correct DAC. An array called \texttt{data[ ]} is used to hold the control word, and contains the values for data bits \texttt{DB31} to \texttt{DB0}. The array is zero indexed, so the first element is \texttt{data[0]}. This array encodes the new value to be programmed to the DAC, and the channel on the DAC which is to be updated.

The variable \texttt{sm} is used by the state machine to identify which part of the waveform is currently being transmitted. While clocking in 32 bits of data, the \texttt{CLK} line will make 64 transitions, so \texttt{sm} must count up to 64. The \texttt{CLK} line inverts every time \texttt{sm} is incremented, and the next data bit is written to \texttt{D} every two increments.

In the initialise state, the \texttt{SYNC} and \texttt{CLK} lines are taken low in preparation for clocking data out into the DAC. The first element of data, \texttt{data[0]} is prepared on the \texttt{D} line, and the variable \texttt{sm} is set to 1 to indicate that the \texttt{D} line has already been set to the first element in \texttt{data[ ]}.

The initialise state sets a software timer to count down from 300 $\mu$s. When the timer elapses, a transition occurs to a pseudostate ‘A’ which checks whether the variable \texttt{sm} is an odd or even number, and makes a transition to the appropriate state.

In the ‘sm=odd’ state, the \texttt{CLK} line is set to the logic low state. The DAC detects this falling edge on the clock line, and reads data in from the \texttt{D} line. The state machine increments the position counter \texttt{sm}, and a software timer is allocated to count down from 300 $\mu$s. When the timer elapses, the sub-system
transitions to pseudostate ‘B’.

The ‘sm=even’ state sets the clock line high and prepares the next bit of data on the D line. This state also adds one to the position counter sm and sets a software timer to count down from 300 \( \mu \text{s} \). The sub-system will transition to the ‘B’ pseudostate when this timer elapses.

At the ‘B’ pseudostate, the position counter sm is checked to see whether it is below 64. In this case the system transitions to state ‘A’ which then checks the parity of the counter and continues to clock data onto the DAC.

At the end of the waveform sm is 64 and this causes a transition to the ‘clean up’ state. This sets the CLK and SYNC lines high and then immediately transitions to the ‘idle’ state.

By this point, the DAC will have been updated with the new value. This will cause the corresponding output voltage to change in a way that is linearly related to the output voltage from the DAC.

### 4.4.3 Calibration and Deflector Potential Mirroring

To establish the relationship between the 16-bit binary number written to the DAC, and the voltage that appears on the output of a channel, a set of routines were developed to convert between DAC programming codes \( n \) and output voltages, \( v \). There is a linear relationship between \( n \) and \( v \), as discussed in Section 4.3.3, since the AD5666/8 DAC used in the deflector cards is guaranteed to give a linear relationship between its output voltage and the programming code [110]. The output voltage from the DAC then drives an inverting amplifier, which has a linear output with respect to its input.

The code responsible for conversions and calibrations is contained in the file cal.c. This file also contains the calibration table for the voltage supply. The calibration table is stored in a simple format. For each channel, four numbers are stored, \( n_a, n_b, v_a \) and \( v_b \). The calibration process was carried out by using a high
precision digital voltmeter to measure the voltage at each channel. The DAC output was set using the code $n_a$, and the voltage recorded as $v_a$. The process was repeated for $n_b$ and $v_b$. As the output from both the DAC and the amplifier stage are linear with respect to their inputs, this information is sufficient to map a 16-bit code $n$ to an output voltage $v$. The calibration table was computer generated using a separate program, this process is described in Section 4.5.4.

To make a conversion between $n$ and $v$, the controller calculates a multiplicative factor $m$ (the \textit{slope}), and an additional constant $c$ (the \textit{intercept}). For a particular channel these are given by:

$$m = \frac{v_a - v_b}{n_a - n_b}, \quad \text{and} \quad c = \frac{n_a v_b - n_b v_a}{n_a - n_b}. \quad (4.1)$$

With $m$ and $c$ defined in this way,

$$v = mn + c.$$

The voltage supply uses this conversion to display an estimate of the output voltage $v$ on the front panel, using the supplied DAC code for the channel, $c$.

These routines are also used to set the deflector voltages. For each $x$– and $y$– deflector, there are a pair of deflector plates. The voltages on the two plates are held at equal magnitude and opposite polarity.

When the voltage on one of the plates is changed, the voltage on the opposing plate must also be changed to the correct value. The firmware handles this automatically. The channel that is explicitly changed is the \textit{master}, and the corresponding channel to be updated is the \textit{mirror}.

The firmware performs the following calculation to find the correct code to set the mirror $n_-$ from the master, $n_+$:

$$n_- = n_+ + \frac{2c}{m}$$

The mirror is then updated using the code $n_-$, which ensures that the pair of
The microcontroller firmware contains a further three state machines apart from the DAC sub-system and the Microchip USB drivers. These handle display updates, keypad events, and USB commands, and were listed in Table 4.5.

The display sub-system firmware code is contained within the file `display.c`. A state machine defined in this file is called from the main program loop and reads pending display updates from a ring buffer. In a similar manner to the DAC state machine, the data is clocked to the LCD driver via four data lines and three control lines. Various functions defined in this sub-system allow for the drawing of characters to the display, or for other control functions to be executed, for example the screen may be cleared or the cursor relocated.

The keypad sub-system handles key events on the keypad, located on the front panel. The state machine, defined in the file `keyhandle.c`, therefore defines the user interface to the voltage supply when it is operated via the front panel. This includes updating the correct output voltage in response to a rotation of a rotary encoder, and saving and restoring a DAC value when the appropriate buttons are pressed.

For the USB command sub-system, a state machine is defined which handles the state of the USB serial command processor. This state machine, defined in the file `cmd.c`, contains additional nested state machines for each command in the command set.

The front panel of the voltage supply is laid out as in Fig. 4.22. The supply can be controlled from a bank of 12 rotary encoders `EN01` to `EN12` and four switches
Figure 4.22: The front panel of the voltage supply. The rotary encoders are shown numbered EN01 to EN12. The LEDs are marked DS1 to DS3.

SW1 to SW4. Three LEDs DS1, DS2 and DS3, and a 16 × 2 character dot matrix LCD provide visual indicators of the state of the voltage supply. The LED DS1 remains illuminated as long as power is applied.

The 12 rotary encoders are used to change the power supply voltages. These were used to manually tune the spectrometer voltages. As there are fewer encoders than voltage channels, each encoder may change one of three different voltages when it is rotated. The voltage that it changes is determined by the mode to which the voltage supply is currently set. The mode can be advanced through states A, B and C by pressing switch SW4. The current mode is represented by the state of two LEDs; DS2 and DS3.

The voltages that each rotary encoder may change are shown in Fig. 4.22. For example, encoder EN01 changes GUNE in mode A, D1X+ in mode B and A1RS in mode C. As a voltage is being changed, the name of the voltage, the code sent to the DAC and the estimated output voltage are shown on the display.

Depressing a rotary encoder knob into the panel (instead of rotating it) changes its resolution. A coarse resolution allows the full voltage range to be scanned more quickly but with less accuracy. A fine resolution then allows for
the voltage to be set more precisely.

Buttons SW2 and SW3 allow for the current DAC code to be stored or recalled respectively. The microcontroller is able to store a separate value for each voltage channel. This may be recalled later to return to a known tuning condition.

4.4.6 USB Interface

When the voltage supply is connected via the USB interface, the output voltages can be controlled by sending commands over the USB cable.

The firmware contains some code from the Microchip USB Library [122]. This library is configured so that the voltage supply appears as a serial port when it is attached to a computer. A terminal program capable of communicating over a serial line, such as PuTTY [123], may then be used to interface with the voltage supply using a simple command set.

The command set may also be used to communicate with a higher level program to produce more complicated behaviours. Such a program is demonstrated in Section 4.5 in this example. This program combines control of the voltage supply with spectrometer measurements to automate various functions of the spectrometer.

To use the terminal program to communicate with the voltage supply, the supply was first powered on, and then connected to the controlling computer via the USB port. The voltage supply was then recognised by the operating system, which assigned a name to the device.

The terminal program was then configured to communicate with the voltage supply by using this device name for identification, allowing the computer to send and receive data via the USB connection. The voltage supply is controlled via the simple command set described in Table 4.7. This allowed the DAC codes to be set or read for each channel, and also provided a notification when the voltages were changed on the front panel. There are also other commands to control the
state of the supply and to interrogate the internal state of the microcontroller, these are discussed in the table.

An illustration of a typical serial session is given in Fig. 4.23. A higher level program, as described in the next section, can interface to the voltage supply by sending commands in this fashion and interpreting the text that is returned.

4.5 Computer Control Software

4.5.1 Introduction

A suite of computer control software was developed to control the spectrometer and take experimental data. The software was programmed using LabVIEW [109]. An individual program in LabVIEW is referred to as a virtual instrument (VI). The interface to a VI is the front panel. A front panel may contain controls and indicators. These are used to specify the inputs to and outputs from the VI.

The logic that controls the front panel is contained in the block diagram. The block diagram specifies the behaviour of the VI graphically using a programming language referred to as ‘G’. G is a dataflow programming language. The block
USB Command table

<table>
<thead>
<tr>
<th>Command</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>HLP</td>
<td>Displays the full command list and version number</td>
</tr>
<tr>
<td>SET dac value</td>
<td>Set the specified dac to value. Table 4.6 lists the dac channel codes that correspond to each voltage. The value is a number between 0 and ((2^{16}) - 1) which is scaled according to the calibration to produce an output voltage.</td>
</tr>
<tr>
<td>GET dac</td>
<td>Returns the value of the specified dac. The DAC code and the returned value are as specified in the SET command.</td>
</tr>
<tr>
<td>REP {1</td>
<td>0}</td>
</tr>
<tr>
<td>LOC {1</td>
<td>0}</td>
</tr>
<tr>
<td>DLY time</td>
<td>Delay for a time specified in multiples of 150 µs, and then return to the command prompt. Used for testing the software timer.</td>
</tr>
<tr>
<td>MEM addr [newval]</td>
<td>Examines or optionally modifies one byte in the controller’s volatile memory. The addr parameter specifies the memory location to examine. The optional newval argument, if specified, will write this new value to the memory, overwriting the old value.</td>
</tr>
<tr>
<td>EEC addr [newval]</td>
<td>Examines or optionally modifies one byte in the controller’s high endurance non-volatile memory. The addr parameter specifies the location in this memory to examine, and if the optional newval argument is supplied, the new value will be written to the memory. This non-volatile memory is used to record the voltage levels for each channel.</td>
</tr>
</tbody>
</table>

Table 4.7: USB command table. Each command is three letters long and is followed by zero or more numeric arguments. All arguments to commands are specified in hexadecimal.
diagram is made up of icons representing functions (like addition and multiplication), controls, indicators, and other VIs. These are connected together by wires which represent the flow of data in the program.

When a VI runs, an individual function in the block diagram will only execute when all the data required at its input terminals is available. The order in which the functions are executed is not explicitly specified, as it would be in a procedural language, such as C.

Figure 4.24 shows the front panel of the VI used to calculate the calibration parameters. This program was named getslope.vi. In this example, the calibration parameters can be entered using the controls on the left of the front panel. When the program is executed, the indicators on the right display the calculated value of the slope and intercept.

The function of the block diagram for getslope.vi was programmed to carry out the calculation from (4.1) with the supplied values of the calibration parameters, and display the result. This block diagram is shown in Fig. 4.25.

The diagram represents the individual mathematical operations that make up
the calculation of the slope and intercept. By tracing the path of the wires, it should be clear that the diagram will compute values at the ‘slope’ and ‘intercept’ terminals which match the expressions for \( m \) and \( c \) from (4.1).

Instead of having an operator manually interact with a VI, the VI may be wired into another block diagram as a sub-VI. This is analogous to a subroutine in a procedural language. In practice, getslope.vi is not used to calculate the slope and intercept values manually, but is instead called upon by other parts of the software to perform the calculation when required.

The remainder of this section will discuss the software used to control the spectrometer. This will begin with details of how the signals are interfaced between the computer and spectrometer, using a data acquisition (DAQ) card.

### 4.5.2 Data Acquisition

The DAQ card is the interface between the computer and most of the equipment attached to the spectrometer. The DAQ card is inserted into a peripheral component interconnect (PCI) slot inside the controlling computer. An external
I/O connector block makes the physical connections to the various instruments that make up the spectrometer. The connector block connects to the DAQ card via a cable, and is housed inside an aluminium chassis which has various connectors mounted on the outside.

The DAQ card used was the National Instruments PCI-6221 [124]. This card is able to measure analogue signals with 16-bit precision. There are 24 digital I/O ports, at 5 V level, used for signalling with some digital devices. The card provides two on-board counters which are used for electron counting and measuring the Faraday cup current. The break-out board was a National Instruments CB-68LP and contained screw terminal blocks at which the electrical connections to the spectrometer were made.

A diagram of the break-out board chassis is given in Fig. 4.26. This shows the location of the connections to the spectrometer. These signals are described further in Section 4.5.5.

Some equipment does not interface with the computer via the DAQ card. The
voltage supply discussed earlier was connected via the USB port. The Spectra-Physics wavelength meter is controlled via a separate laptop computer used to control the Spectra-Physics laser system (see Section 3.6.5). This computer transmits the current laser wavelength along with a timestamp to the spectrometer computer once every second, using a network connection.

4.5.3 Main Interface

The main interface to the computer control functions is shown in Fig. 4.27. This VI is named commcore.vi. When the program is started, it prompts for the USB port that the voltage supply is attached to. Once this is correctly selected, the front panel shown in the figure is displayed. This is the main entry point to all the computerised spectrometer functions. These functions can all be accessed by clicking on their respective buttons. The program was terminated, when needed, by clicking the red ‘STOP’ button in the upper-right corner of the window.

The voltage supply could be controlled directly by pressing the button labelled ‘vpanel’ (short for virtual panel). This causes the window shown in Fig. 4.28 to appear. Twelve of the spectrometer voltages can be represented at one time using this interface. They are tiled in a $6 \times 2$ grid of channel displays. The voltages may be entered manually, or varied by using the mouse to drag a ‘slider’ control in the vertical direction.

A menu at the bottom of the window allows a specific control set of twelve voltages to be chosen to show in the window. For example the channel displays
could be set to show all the gun deflector voltages. It is also possible to define an arbitrary control set by clicking on the voltage name in the displays, and changing it to display a different voltage channel.

The interface also allowed the output level of all the channels to be written to a channel data file stored on the computer. This provided a quick method to record the state of the voltage supply outputs. The voltage supply could be restored to any of the saved states by selecting an appropriate file to load. A separate program `dacrepgen.vi` was used to generate a formatted list of the output channels from the channel data file, which could be sent to a printer when a hardcopy of the channel settings was required.

By using the virtual panel VI, it was possible to obtain low level control of the
voltages using only the computer interface. This may be used to tune the spectrometer voltages as well as the controls on the front panel. Section 4.5.6 shows how a simplex algorithm has been implemented which in some cases was preferable to manually tuning the spectrometer (for example when the spectrometer is running unattended).

### 4.5.4 Calibration Procedure

The voltage supply outputs were calibrated by pressing the ‘calibrate’ button in the main window. This opens the interface for calibrating the voltage supplies.

The procedure for calibrating an individual voltage channel was to vary the output from the DAC controlling the channel, and measure the voltage output from the amplifier.

The calibration VI provided a method to update the calibration data interactively for each voltage channel in the supply. The front panel is pictured in Fig. 4.29. Calibration data is adjusted for the channel specified by the ‘dac index’ numerical entry field at the top of the window.

To adjust the calibration data for the channel, a DAC code at the low end of the scale was entered into ‘nb’. Clicking the ‘set from B’ button programmed the channel using this code. The output voltage from the channel was measured using a Hewlett Packard 34401A high precision multimeter and recorded into the
The same process was repeated for ‘na’ and ‘va’ to obtain the calibration data for the channel. The calibration was then verified by entering another code into the ‘send code’ field. This would cause the channel to be updated with the new code, and a voltage estimate was generated based on the new calibration data. This estimate would match the voltage displayed on the voltmeter if the calibration process was successful.

Once the calibration has been calculated, it was then saved to the DAC firmware. This allows the voltage estimate to be displayed on the front panel of the power supply.

To format the calibration data for inclusion in the firmware, a separate VI was produced named `exportcal.vi`, pictured in Fig. 4.30. This generated the C program code for a table of calibration data. This was then inserted into the firmware code file `cal.c`. 

Figure 4.30: The DAC calibration export. The calibration data is formatted as a C struct definition so that it can be inserted into the relevant part of the firmware code, see text.
4.5.5 Spectrometer Control and Monitoring Signals

Table 4.8 summarises the computer controlled parts of the spectrometer and which VIs are used to interact with them. Those labelled *core signals* are used to run the experiment and take data.

The *health monitoring signals* are used to record the condition of the spectrometer as data is being taken. Although these did not contribute to the experimental results, if a discrepancy was found in the data, it was possible to ascertain the condition of the spectrometer while a specific data point was being measured, and then check whether the spectrometer had been operating correctly.

4.5.6 Grid Search and Simplex Tuning

The voltage supply control software has two methods to assist in finding the optimum tuning parameters for the spectrometer. These are the grid search, and the simplex tuning algorithm.

A grid search is a process which scans the spectrometer voltages and records the signal strengths as it is doing so. The grid search implemented in the control software may be configured to take place over one or two dimensions, although more are generally possible. Optimum voltages may then be found by examining the result of the scan.

The simplex tuning algorithm actively searches for the optimum tuning conditions by attempting to scan selected spectrometer voltages until the signal reaches a maximum. This section will describe both grid search and simplex tuning as they are implemented in the control software.

The grid search and simplex tuning programs were started from the main panel by pressing either the ‘gridsearch’ button or the ‘simplex’ button. Both of these programs combine control of the power supply with feedback from the spectrometer to aid in the tuning of the electron-optical elements in the gun and
### Core Signals

<table>
<thead>
<tr>
<th>Dir.</th>
<th>Signal</th>
<th>VI Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>←</td>
<td>Analyser Counts</td>
<td>analysercounts.vi</td>
<td>Counts the number of electron detection events in a specified time period.</td>
</tr>
<tr>
<td>←</td>
<td>Faraday Cup</td>
<td>readfcupcurrent.vi</td>
<td>Reads the current measurement from the electrometer connected to the Faraday cup.</td>
</tr>
<tr>
<td>→</td>
<td>Half Wave-Plate</td>
<td>stepperctl.vi</td>
<td>Rotates the half wave plate by a specified amount by sending TTL signals to the stepper motor driver.</td>
</tr>
<tr>
<td>→</td>
<td>Laser Shutter</td>
<td>shutterctl.vi</td>
<td>Opens or closes the laser shutter by sending the appropriate TTL signal level.</td>
</tr>
<tr>
<td>→</td>
<td>Analyser drive</td>
<td>movetoangle.vi</td>
<td>Rotates the analyser around the turntable by sending TTL signals to the stepper motor driver.</td>
</tr>
</tbody>
</table>

### Health Monitoring Signals

<table>
<thead>
<tr>
<th>Dir.</th>
<th>Signal</th>
<th>VI Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>←</td>
<td>Pressure</td>
<td>mptf.vi</td>
<td>Measures the pressure of the chamber using the Ion-Combi gauge.</td>
</tr>
<tr>
<td>←</td>
<td>Oven Temperature</td>
<td>mptf.vi</td>
<td>Analogue output from thermocouple amplifier supplies the measurement of oven temperature.</td>
</tr>
<tr>
<td>←</td>
<td>Fluorescence</td>
<td>mptf.vi</td>
<td>Laser locking control electronics; one of the analogue outputs corresponds to total fluorescence.</td>
</tr>
<tr>
<td>←</td>
<td>Laser Wavelength</td>
<td>multiscan.vi</td>
<td>The current laser wavelength as measured by the computer attached to the laser. File sent over network and read during the data file write.</td>
</tr>
</tbody>
</table>

**Table 4.8:** Spectrometer control and monitoring signals, and the VIs which are used to interface with them. The *Dir.* column specifies whether the signal is an input to the computer (left pointing arrow) or an output (right pointing arrow).
<table>
<thead>
<tr>
<th>Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>fcup</td>
<td>Faraday cup current, units are calibrated to scale on electrometer.</td>
</tr>
<tr>
<td>a1</td>
<td>Count rate from the channeltron in the electron analyser.</td>
</tr>
<tr>
<td>a2</td>
<td>Count rate from a second analyser; not used in the super-elastic spectrometer as this has only one analyser.</td>
</tr>
<tr>
<td>a1a2</td>
<td>The product of count rates a1 and a2; again, not used in the super-elastic spectrometer.</td>
</tr>
<tr>
<td>super</td>
<td>The super-elastic signal from the analyser, calculated by subtracting the count rate with the laser blocked from the rate with the laser unblocked.</td>
</tr>
<tr>
<td>zero</td>
<td>This counting source is always zero.</td>
</tr>
<tr>
<td>random</td>
<td>This counting source returns random numbers scaled to the time interval requested.</td>
</tr>
</tbody>
</table>

The super-elastic spectrometer is able to provide a current measurement from the Faraday cup, named fcup. The signal from the analyser is named a1. A VI named getratebyname.vi was used to sample a counting source for a specified period of time. From this measurement an estimate of the counting rate could be obtained.

The super-elastic signal super is a measure of the analyser count rate when the laser beam is blocked, subtracted from the count rate while the laser is exciting the calcium atoms. The laser beam is blocked or unblocked by controlling the laser shutter.

The grid search that was implemented in the control software is able to sample every point in a one- or two-dimensional space defined by either one or two spectrometer voltages, specified over a certain range. For each point, the value of a specific counting source was recorded. In Fig. 4.31, the front panel for the

**Table 4.9**: Counting sources defined by the software. The a2 and a1a2 sources are not implemented on the super-elastic spectrometer, since it does not have a second analyser. The zero and random sources do not depend on measurements and were used for testing the software.
one-dimensional grid search is presented. Changing the channel selected as the ‘x channel’ determined which voltage to scan; in the figure GRID has been selected. The ‘x range’ control determines the extent of the scan, Fig. 4.31 shows this set to range from $-7 \rightarrow -2\,\text{V}$.

The resolution of the scan was varied by changing the value of ‘grains’; this determined the number of measurements to take within the specified voltage range. The ‘time’ was the number of milliseconds to spend sampling each point. A higher number produced a more accurate estimate of the counting rate. The ‘settle time’ determined the amount of time to wait after changing the voltages before sampling the next point.

The counting source was set by entering text into the ‘monitor’ control. In the figure, the text $\text{fcup}$ was entered, and so the counting rate estimate was proportional to the Faraday cup current.

The scan was commenced by clicking the ‘start scan’ button. The results
Figure 4.32: Two dimensional grid search showing the voltage channels GRID and ANOD being scanned against the Faraday cup current.

were displayed as a graph with the voltage along the horizontal axis and the count rate on the vertical axis. The graph in the figure shows that the optimal tuning voltage for the grid lies at around -4.7 V, although this is dependent on the voltages at the other gun elements, particularly ANOD.

The one-dimensional grid search was also used to take energy loss spectra by varying either GUNE or A1RS. Additionally the two voltages could be varied simultaneously by using the ‘link channel’ option which was located in the virtual panel VI.

A two-dimensional grid search could be carried out in a similar manner to a one-dimensional search. The ‘dual channel’ tab was selected and a voltage channel selected for the ‘y channel’. Figure 4.32 shows the VI for the two-dimensional case. In this example GRID and ANOD were scanned.

There is no option for grid searches in more than two dimensions. The grid search is an inefficient method of finding the optimum tuning conditions as it be-
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Figure 4.33: Tuning the spectrometer using the simplex algorithm. Each line on the graph corresponds to one coordinate value of one vertex on the simplex, at each iteration of the algorithm. The scale is arbitrary and each line is offset from every other for clarity. The upper line on the graph is the value to optimise, in this case the Faraday cup current. The GRID and ANOD voltages quickly settle to a level where the Faraday cup current is maximised.

comes another order of magnitude slower for every extra dimension to be searched. This algorithm also wastes time as it samples the signal in areas where the maximum is unlikely to be found.

A better algorithm to use is the downhill simplex optimisation algorithm [125], which has been used to run the (e,2e) spectrometer at Manchester [126]. A VI called simplexmonitor.vi was programmed to implement this algorithm on the spectrometer. A screen capture of the front panel is shown in Fig. 4.33.

A simplex is a geometrical object with a number of vertices equal to one more than the number of dimensions of the space in which it is defined. To start the algorithm, an initial simplex, and the voltages to be optimised, are defined in a configuration file. The file was specified using the ‘select programme’ control shown in the figure. The number of channels to be optimised determines the...
dimensionality of the optimisation problem, the number of dimensions being one more than the number of channels. The configuration file also specifies a counting source to use as the figure of merit for the optimisation, as well as a number of other parameters for the optimisation.

While the algorithm was running, it reflects, expands or contracts the simplex in such a way that it ‘falls’ into the region where the signal is at its peak. This procedure hones in on the voltage where the signal is at a maximum, rather than scanning every point as the grid search does. The coefficients for transforming the simplex are defined in the configuration file.

Using the simplex algorithm on the various electron optical elements while monitoring the Faraday cup current or super-elastic count rate allows the spectrometer to be tuned with no operator intervention.

4.5.7 Data Collection System

The spectrometer counts electron detection events for a specified number of seconds through a range of half wave-plate angles and at a defined angle of the analyser. This is one scan. The specifics of the scan process are described in Section 5.3. For each scattering angle, a scan may be repeated many times to improve the statistics of the data. Each of these sets of scans was assigned a name, called the namebase, which allowed a set of scans taken together to be easily identified. Additionally all the data recorded would belong to a named data group. The group name was changed every time the spectrometer was opened to air, for example when the calcium oven needed to be refilled.

During a scan, counts were recorded for a specified interval with the laser beam blocked and also with the beam unblocked. This is a single data point. The half wave-plate was then advanced so that the next point could be taken. For every point, a value of the fluorescence from the chamber was recorded, again with the beam blocked and unblocked. This was to verify that the shutter was working correctly and to help assess the time at which the calcium oven would
run out. This created four different data files for each scan detailing the count rates and measured fluorescences when the laser was blocked or unblocked. Each of these files is simply a list of numbers corresponding to the measurement at each point.

Additionally, the software would create another file which described the conditions of the scan, and the filenames of the data files. This file was named using the namebase text, and the index number of the scan within the namebase. For example if the namebase was CAP121094, then the 38th scan for this namebase would be described by the file CAP121094x38.mtf. A list of each of the data fields recorded in this file is given in Table 4.10.

Data was collected by pressing the ‘scan’ button on the main panel. This displayed the front panel of multiscan.vi which allowed super-elastic scattering data to be collected from the spectrometer. A screen capture of this panel is shown in Fig. 4.34.

Most of the data description file parameters from Table 4.10 were entered using the controls on the left of the scan panel (Fig. 4.34). This also allowed the
### Field Description

<table>
<thead>
<tr>
<th>Field</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>type</td>
<td>Type of measurement being taken, either P12 for a measurement of $P_{ln}$ and $\gamma$, or P3 for an $L_{\perp}$ measurement.</td>
</tr>
<tr>
<td>angle</td>
<td>Angle of the analyser.</td>
</tr>
<tr>
<td>x0</td>
<td>Angle in degrees of half wave plate for first measurement.</td>
</tr>
<tr>
<td>dx</td>
<td>Angle of half wave-plate between each data point measurement.</td>
</tr>
<tr>
<td>group</td>
<td>Data group that this scan belongs to.</td>
</tr>
<tr>
<td>delay</td>
<td>Amount of time that counts were taken with the laser unblocked.</td>
</tr>
<tr>
<td>rbkdelay</td>
<td>Amount of time that counts were taken with the laser blocked.</td>
</tr>
<tr>
<td>steps</td>
<td>Number of stepper motor steps to advance after each data point.</td>
</tr>
<tr>
<td>direction</td>
<td>Direction of rotation of the half wave-plate stepper motor.</td>
</tr>
<tr>
<td>timestamp</td>
<td>Time that the scan started.</td>
</tr>
<tr>
<td>timeend</td>
<td>Time that the scan finished.</td>
</tr>
<tr>
<td>oventemp</td>
<td>Temperature of the oven, measured at the end of the scan.</td>
</tr>
<tr>
<td>pressure</td>
<td>Pressure of the chamber, measured at the end of the scan.</td>
</tr>
<tr>
<td>superfile</td>
<td>Name of the file that stores a list of the counts with the laser unblocked.</td>
</tr>
<tr>
<td>rbkfile</td>
<td>Name of the file that stores a list of the counts with the laser blocked.</td>
</tr>
<tr>
<td>fluorescefile</td>
<td>Name of the file that stores the fluorescence measurements while the laser beam is unblocked.</td>
</tr>
<tr>
<td>xfluorescefile</td>
<td>Name of the file that stores the fluorescence measurements while the laser beam is blocked.</td>
</tr>
<tr>
<td>namebase</td>
<td>Namebase that this scan belongs to.</td>
</tr>
<tr>
<td>lambda</td>
<td>Laser wavelength as measured by the Toptica wavemeter on the Spectra Physics laser system, along with the time that the measurement was taken.</td>
</tr>
</tbody>
</table>

**Table 4.10:** Fields in the data description file. Each entry is recorded for every scan.
number of repeat scans to be selected by entering the desired number into the ‘scans’ numeric entry box. This specified the number of scans that will be present in the namebase.

Before a scan is carried out the half wave-plate angle was set by pressing the ‘adjust HWP’ button. This presents the window shown in Fig. 4.35. The rotation angle of the wave plate was set so the polarisation vector of the radiation from the wave plate would be in line with the gun axis, as described in Section 3.7.3.

To set the wave plate correctly, ‘enter current angle’ was selected from the drop down box and a value of zero was entered into the entry box labelled ‘value’ below. Pressing the ‘run’ button stored the new configuration, and then pressing ‘exit’ would dismiss the window.

To start a scan or series of scans the ‘start’ button was pressed in the scan window (Fig. 4.34). This controls the shutter and half wave-plate orientation to collect data and store it into the data files specified, as explained earlier.

The scan program may also be run independently from the commcore.vi by running multiscan.vi separately. This allows data to be collected when the analogue voltage supplies are conected.

To fully automate collection of data from the spectrometer, a batch control program was developed. Batch mode allows the operator to define a sequence of operations for the spectrometer to perform. For example, the spectrometer can be set to collect data over a range of angles and over several energies, while retuning gun and analyser voltages where necessary.

Using the batch control VI, show in Fig. 4.36, a list of spectrometer tasks
Figure 4.36: The batch control main window. Tasks can be added or removed using the controls on the left. Individual tasks can be configured using the pane on the right.

<table>
<thead>
<tr>
<th>Task</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>sleep</td>
<td>Waits for the specified amount of time, in milliseconds.</td>
</tr>
<tr>
<td>angle</td>
<td>Change the angle of the analyser.</td>
</tr>
<tr>
<td>simplex</td>
<td>Perform the simplex optimisation routine as specified by a configuration file.</td>
</tr>
<tr>
<td>scan</td>
<td>Perform a scan or number of scans with the parameters that are specified.</td>
</tr>
</tbody>
</table>

Table 4.11: Batch commands implemented by the batch control VI. Placing a number of these commands in sequence allows the spectrometer to gather large volumes of data unattended.

were specified, these are then executed sequentially until the end of the list was reached. A full list of the possible batch operations is given in Table 4.11.

The batch command list could be modified using the batch program main window and saved by pressing the ‘save’ button. Each batch task could be configured using the pane on the right of the window. Once the command list has been entered, pressing the ‘exec’ button caused the tasks to be executed.
4.6 Summary

In this chapter, the voltage supplies used to provide the correct potentials for the gun, analyser and Faraday cup were described. The various elements of the voltage supply are described and the assembly and construction of the unit detailed.

The voltage supply is controlled by a microcontroller. The firmware that was programmed onto the microcontroller was discussed, and the details of how the firmware acted to change the output voltages were described.

The final part of the chapter described the computer software that interacted with the power supply and the rest of the spectrometer. This allowed the electron gun and analyser to be tuned, and super-elastic scattering data to be recorded onto the controlling computer.

In the next chapter, the experimental results and analysis will be presented. Data collected using the automated data collection programs, and data characterising the voltage supplies presented and analysed.
Chapter 5

Method, Results and Analysis

5.1 Introduction

This chapter describes the acquisition of experimental results, including the ACPs, for calcium. First, the steps taken to calibrate the gun and analyser are described. Energy loss spectra of helium and calcium were taken to verify the calibration.

The ACPs are derived from the pseudo-Stokes parameters, which are found from the super-elastic electron scattering rates at different incident laser polarisations. New results at 65 eV, 10 eV and 8 eV are then presented. This chapter will explain the procedure followed for manually fitting the data for each experimental run, and then explain how the method was extended and automated to work with large data sets comprising many runs.

For working with the large data sets that the experiment would eventually produce, a computer-based system for automatically analysing the data was developed. For runs at a high energy where the super-elastic count rates were high, there were fewer data files and so it was possible to fit to the experimental data manually. At lower energies, the count rates were markedly reduced and it became necessary to repeat measurements multiple times to compensate for this.
This repetition generated a large amount of data and as a result it became impractical to manually process the data sets from each run, some of which could contain hundreds of files.

5.2 Initial Measurements

5.2.1 The Contact Potential

The electron beam is produced inside the electron gun, at the filament. The energy of the electrons is controlled by the gun bias voltage, $V_{\text{GUNE}}$. This voltage sets the potential at the filament so that potential energy of a test charge placed here would be $U_F$ with respect to ground. By the time the electrons leave the gun they will have acquired kinetic energy due to the potential difference between the filament and the exit aperture of the gun. From here electrons proceed to the target region. At this point the kinetic energy is defined to be $U_T$.

There are various processes at work which cause a difference between the two energies $U_F$ and $U_T$. In these experiments, this is referred to as the contact potential,

$$\phi = U_F - U_T. \quad (5.1)$$

Processes which may cause the contact potential are illustrated in Fig. 5.1. This shows the production of an electron at the filament, its journey to the interaction region, and the subsequent detection at the electron analyser.

Towards the left of the figure, the gun filament is shown, heated by a constant current supply, which provides $\sim 2$ A through the tungsten wire. The current supply circuit is biased from one of the voltage supplies (GUNE) in such a way as to hold the tip of the filament at the negative bias voltage, $V_{\text{GUNE}}$. For an electron to be released, it must overcome the work function of the filament. The electron will therefore lose an amount of energy as it leaves, which contributes to the contact potential.
Figure 5.1: Causes of the contact potential. This diagram shows effects which may contribute towards a shift in the energy of an electron. In the region between the gun and analyser a dashed line is drawn to represent the change in energy the electron may undergo as a result of any stray electric fields. For details, see text.
After the electron leaves the gun, any stray electric fields around the interaction region will cause changes in the kinetic energy of the projectile. These stray fields are often caused by insulating surfaces in the scattering chamber becoming charged by stray electrons. In the super-elastic spectrometer described in this thesis, calcium which was deposited on spectrometer surfaces would oxidise, forming an insulating layer of calcium oxide. Electrons incident on such layers negatively charge these surfaces, causing small perturbations of the electric field inside the scattering chamber.

If the electric field potential in the interaction region is negative compared to the 0 V level in the spectrometer, the electrons which interact with the target will do so at an energy $\Delta E_I$ lower than would otherwise be expected.

The entrance and exit apertures on the electron gun and analyser (respectively) are both at the same potential. As the electric field is conservative, a detected electron scattered from the interaction region will have gained energy $\Delta E_I$ once it reaches the analyser.

The energy changes $\Delta E_I$ cancel one another and this effectively masks the effect of the stray fields in energy-loss scattering measurements performed in the chamber, including the super-elastic experiment. This is because the relative difference between the energy of the created and detected electrons will remain the same, whatever the field at the interaction region. However, since the energy of the electrons at the interaction region does depend upon the contact potential and stray fields, the collision process between the electron and atom may be different, particularly at low energies.

The flow of electrons between the gun and analyser effectively forms a junction between the two metals at the external surfaces. The two metals are dissimilar; the material at the exit aperture of the gun is grade 310 stainless steel and the cone forming the entrance aperture of the analyser is made from molybdenum. As the work functions of these two metals differ, this forms a potential difference which also contributes to the contact potential.
5.2.2 Calibrating the Gun and Analyser

The gun and analyser were calibrated so that electrons could be produced and detected at a known energy. The energy resolution of the gun was $\sim 0.6$ eV. The energy resolution of the analyser was set to be at a similar scale to the gun resolution as discussed in Section 3.3.2.

The analyser residual energy, set from the power supply A1RSE, selects the detection energy for electrons. For convenience, the analyser was calibrated so that the potential difference in volts, $-V_{\text{A1RSE}}$, was numerically equal to the energy in electron volts of the electron to be detected. This calibration was performed by adjusting the voltages from the power supplies A1IH and A1OH, which change the potential on the inner and outer hemispheres, and A1AM, which controls the analyser pass energy.

The correct voltages for the analyser elements had been determined previously from simulation in an electron-optics computer model, and then refined by carrying out scattering measurements on the autoionising states of argon. This process always ejects electrons at the same characteristic energies, and so detection of these electrons allows the analyser energy to be calibrated, since it was not sensitive to the calibration of the gun. The voltages used to correctly calibrate the analyser were shown in Section 3.3.2, and were $V_{\text{A1IH}} = 31.94$ V, $V_{\text{A1OH}} = 8.11$ V for $V_{\text{A1AM}} = 15.00$ V.

Calibration of the gun energy was performed by performing elastic scattering measurements on helium, which has a $2^2S$ negative ion resonance as observed by Brunt, King and Read [127]. This resonance occurs at $19.366 \pm 0.005$ eV, and is useful to measure because it occurs only at this absolute value of incident electron energy. This means that the effects of stray fields in the interaction region do not cancel, and so a measurement of the contact potential and the effect of stray fields can be made.

An incident electron at the energy of the resonance will temporarily become bound to the nucleus to form $\text{He}^-$. This ion is short lived and decays by ejecting
the captured electron. The waveform defining the direct elastic scattering process and that for the creation of the negative ion then interfere to cause a Fano resonance in the scattering profile [127].

To take the data, a plot of elastic scattering yield against incident energy is produced at a given scattering angle. When the gun is emitting electrons at the correct energy, a resonance in the elastic scattering cross section is observed. The shape of the feature is dependent on the scattering angle, and at $\theta_e = 90^\circ$ it manifests as a dip. Measurements were taken at this angle since it is easiest to fit to this shape, and the resonance is quite strong compared to the background signal.

To calibrate the gun, the position of the dip was measured with respect to $V_{\text{GUNE}}$, the bias potential of the gun. This allows the contact potential of the electron gun to be found. The electron energy is then related to the bias potential of the gun by

$$U_T = -V_{\text{GUNE}} - \phi$$

(5.2)

in electron volts, where $\phi$ is the contact potential. It was found that the contact potential would change over time, and this was thought to be due to calcium depositing inside the chamber as the experiment progressed.

When taking scattering measurements to find the contact potential of the gun, helium gas was introduced into the scattering chamber through the gas jet nozzle, which was aimed into the interaction region. The turbomolecular pump then removes the helium from the chamber. At equilibrium, the amount of gas which enters is the same amount that is removed, and a constant pressure is established. The flow of helium was controlled by a needle valve. A pressure of $1 \times 10^{-5}$ mbar was found to give good signal levels.

With the contact potential unknown, the gun was set to emit electrons around the energy of the resonance by setting $V_{\text{GUNE}} = -19.4$ V. This provided a good starting point from which to find the contact potential, which was on the order of one or two volts. Next, the analyser was set to the elastic scattering peak by
manually scanning the analyser voltage $V_{\text{AIRSE}}$ through a range around the gun voltage until the maximum count rate for elastically scattered electrons was found. This procedure set the spectrometer to detect electrons which have elastically scattered from the helium atoms in the gas jet.

The helium elastic spectrum was taken by scanning the analyser and gun voltages ($V_{\text{AIRSE}}$ and $V_{\text{GUNE}}$) together, at the same rate and in the same direction. The analyser continues to detect electrons from the elastic peak during the scan, but the energy of those electrons on the peak changes. This allows the helium resonance to be found, as long as it lies within the scan range.

The results of measuring the $2^2S$ resonance in helium are presented in Fig 5.2. Using simple methods, the voltage $V_{\text{GUNE}}$ at the dip was determined to be $-18.2 \pm 0.1$ V. This means that, using (5.2), the contact potential is $\phi = -1.2$ eV.
<table>
<thead>
<tr>
<th>State</th>
<th>Transition</th>
<th>Energy (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$2^3S$</td>
<td>$(1s)^2 \rightarrow 1s2s$</td>
<td>19.820</td>
</tr>
<tr>
<td>$2^1S$</td>
<td>$(1s)^2 \rightarrow 1s2s$</td>
<td>20.616</td>
</tr>
<tr>
<td>$2^3P$</td>
<td>$(1s)^2 \rightarrow 1s2p$</td>
<td>20.964</td>
</tr>
<tr>
<td>$2^1P$</td>
<td>$(1s)^2 \rightarrow 1s2p$</td>
<td>21.218</td>
</tr>
<tr>
<td>$3^3S$</td>
<td>$(1s)^2 \rightarrow 1s3s$</td>
<td>22.718</td>
</tr>
<tr>
<td>$3^1S$</td>
<td>$(1s)^2 \rightarrow 1s3s$</td>
<td>22.920</td>
</tr>
<tr>
<td>$3^3P$</td>
<td>$(1s)^2 \rightarrow 1s3p$</td>
<td>23.007</td>
</tr>
<tr>
<td>$3^1D$</td>
<td>$(1s)^2 \rightarrow 1s3d$</td>
<td>23.074</td>
</tr>
<tr>
<td>$3^3D$</td>
<td>$(1s)^2 \rightarrow 1s3d$</td>
<td>23.074</td>
</tr>
<tr>
<td>$3^1P$</td>
<td>$(1s)^2 \rightarrow 1s3p$</td>
<td>23.087</td>
</tr>
<tr>
<td>Ionisation potential:</td>
<td></td>
<td>24.587</td>
</tr>
</tbody>
</table>

Table 5.1: Energy levels of neutral helium, showing the electronic configurations and the energies needed to excite each transition. Only levels up to $n = 3$ are shown, and energy level splitting of the triplet states is not shown.

5.2.3 Helium Energy Loss Spectrum

An energy loss spectrum is a plot of the scattering cross section against energy loss for electron collisions. Electrons are directed at the atomic target and the scattering rate is recorded over a range of energies.

Most electrons are elastically scattered and lose no energy in the interaction; these are detected at an energy loss of 0 eV and lead to a large peak in the scattering cross section at this energy.

If an electron is inelastically scattered, the electron gives up some of its energy to the atom to excite a specific state. These electrons leave the collision with a lower energy, and are seen as peaks in the energy loss spectrum. The position of the peaks indicates the energies needed to excite different atomic states.

Energy loss spectra may be taken using two methods. The first is to keep the gun voltage at a fixed value and then scan the analyser energy, and the second method is to do the reverse; scan the gun energy whilst keeping the analyser voltage fixed. In the data recorded in this section, the gun voltage was fixed since the optimal gun tuning parameters were found to be more strongly dependent on the bias voltage, compared to those in the analyser.
An energy loss spectrum for helium is shown in Fig. 5.3. A table of the corresponding energy levels for various states of helium is given in Table 5.1. These energies are well established [128]. In the energy loss spectrum, two distinct peaks can be seen.

The resolution of the spectrometer was too low to resolve close lying individual transitions in helium. The larger of the two peaks is due mainly to the $2^1P$ state, with some contribution from the weaker $2^1S$ state. The second, smaller peak is due to a combination of the $n = 3$ states, which occur at similar energies.

These two peaks are labelled in the figure, and can be seen to be close to the published values. This measurement confirmed that the energy calibration of the electron analyser was correct to within a reasonable accuracy of $\pm 0.2 \text{ eV}$.
5.2.4 Calcium Energy Loss Spectrum

A similar spectrum to the helium energy loss spectrum can be obtained for calcium. The state which will be studied in the super-elastic experiments is the $4^1P_1$ state. The energy needed to excite this state from the ground state is $2.93\text{ eV}$, causing a peak in the energy loss spectrum at this value. The $4^1P_1$ state may also be excited with radiation at $422.67\text{ nm}$ from the laser. With the laser beam properly directed into the interaction region, a portion of the calcium atoms will be laser excited into the P-state. Some electron collisions with these excited atoms result in the incident electron gaining energy as the atom de-excites, and these events are detected as a super-elastic peak, with negative energy loss.

An energy loss spectrum for laser excited calcium atoms is given in Fig. 5.4. Three distinct peaks are seen, which correspond to the super-elastic, elastic and inelastically scattered electrons, as discussed. The super-elastic interaction is the least likely, and has a correspondingly low count rate, almost two orders of magnitude lower than the elastic peak.
magnitude smaller than the elastic peak. Both the super-elastic and inelastic peaks occur at the same relative energy, around ±2.9 eV from the elastic peak, as would be expected.

5.3 Measuring the Atomic Collision Parameters

In order to determine the ACPs at different scattering angles, the super-elastic signal must be monitored as the polarization of the laser light is changed. This process was controlled using either the multiscan program, or the earlier version called SuperStep, which controls the rotation of the half wave plate while recording count rates from the analyser. The multiscan program was described in detail in Section 4.5.7.

The ACPs from the super-elastic scattering experiment can be related to the conventional coincidence experiment through the optical pumping parameters, which were detailed in Section 2.2.5. For calcium these parameters evaluate to unity and so the results for the conventional coincidence experiment and the time-inverse experiment are directly related.

5.3.1 Measuring $P_{\text{lin}}$ and $\gamma$

Exciting the calcium atoms with linearly polarised light allows measurements of $P_{\text{lin}}$ and $\gamma$ to be made as a function of the scattering angle, $\theta_e$. The angle of the polarization vector $\theta_{\text{pol}}$, is set using the half wave plate, where $\theta_{\text{HWP}} = 2\theta_{\text{pol}}$. As this angle changes, the scattering yield was seen to vary.

A plot of the scattering rate against the angle of the polarization vector produces a sinusoidal curve. The dependence of the scattering intensity on the angle of the polarization vector was given in equation (2.17). Here it is recast in terms of three variables $A$, $B$ and $C$,

$$S(\theta_{\text{pol}}, \theta_e) = A(\theta_e) + B(\theta_e) \cos^2(\theta_{\text{pol}} - C(\theta_e))$$  (5.3)
where the scattering rate, $S(\theta_{pol})$ represents the rate of electron counts due to super-elastic scattering, with the linear polarisation of the incoming laser radiation set to $\theta_{pol}$ with respect to the gun axis. Fitting this to the data allows values for $A$, $B$ and $C$ to be obtained. For a single fit, it was sufficient to use a fitting program such as Kaleidagraph [129]. This uses the Levenberg-Marquardt least squares fitting algorithm [130] to fit an equation in the form of (5.3) to the data points.

By way of example, Fig. 5.5 illustrates the result of fitting this equation to experimental data taken over a range of analyser angles, in this case at 12 eV. The resulting fitting coefficients and derived values of $P_{lin}$ and $\gamma$ are shown.

Once values for the coefficients from (5.3) have been computed, the calculation to find $P_{lin}$ is straightforward [53]:

$$P_{lin}(\theta_e) = \frac{B(\theta_e)}{2A(\theta_e) + B(\theta_e)}$$

(5.4)

The value of $\gamma$ is related to the fitting coefficient $C$, as is explained in the next section.

The error on $P_{lin}$ was found by using error propagation techniques on the above equation (5.4), to give

$$\sigma_{P_{lin}}^2 = \left(\frac{\partial P_{lin}}{\partial A}\right)^2 \sigma_A^2 + \left(\frac{\partial P_{lin}}{\partial B}\right)^2 \sigma_B^2$$

$$\therefore \sigma_{P_{lin}}^2 = \left(\frac{2A}{(2A+B)^2}\right)^2 \sigma_A^2 + \left(\frac{-2B}{(2A+B)^2}\right)^2 \sigma_B^2$$

(5.5)

where $\sigma_A$ and $\sigma_B$ are the errors on the $A$ and $B$ coefficients respectively. These errors were supplied by the fitting routines.

### 5.3.2 Obtaining $\gamma$ in the Correct Geometry

In a conventional coincidence experiment, the $x$-axis of the natural frame is aligned with the electron gun axis, as discussed in Section 2.2.2. Angles in the
Figure 5.5: Data points showing the super-elastic scattering rate with the random background subtracted, for data recorded at 12 eV. The solid line shows the fit to the data. The polarization vector angle is the angle from the gun axis. Positive angles go anticlockwise looking along the $z$-axis from above the scattering plane. The fitting parameters for the four graphs are shown below, along with the computed parameters for $P_{\text{lin}}$ and $\gamma$.

$\theta_e = 50^\circ$ (t = 20 s)

\[
\begin{align*}
A &= 88 \pm 5, \\ B &= 424 \pm 5, \\ C &= 127 \\
P_{\text{lin}} &= 0.70 \pm 0.01, \\ \gamma &= -77^\circ \pm 3^\circ
\end{align*}
\]

$\theta_e = 55^\circ$ (t = 20 s)

\[
\begin{align*}
A &= 69 \pm 3, \\ B &= 239 \pm 5, \\ C &= 133 \\
P_{\text{lin}} &= 0.63 \pm 0.01, \\ \gamma &= -78^\circ \pm 3^\circ
\end{align*}
\]

$\theta_e = 60^\circ$ (t = 30 s)

\[
\begin{align*}
A &= 78 \pm 2, \\ B &= 114 \pm 3, \\ C &= 209 \\
P_{\text{lin}} &= 0.42 \pm 0.01, \\ \gamma &= -89^\circ \pm 3^\circ
\end{align*}
\]

$\theta_e = 65^\circ$ (t = 30 s)

\[
\begin{align*}
A &= 69 \pm 1, \\ B &= 52 \pm 2, \\ C &= 146 \\
P_{\text{lin}} &= 0.27 \pm 0.01, \\ \gamma &= -81^\circ \pm 3^\circ
\end{align*}
\]
scattering plane are then conventionally measured from this axis. As the analyser angle is changed, the natural frame remains static relative to the lab frame. This is illustrated in Fig. 5.6.

As explained previously, a super-elastic scattering experiment is the time-inverse of the coincidence experiment. To compare super-elastic results with an equivalent conventional coincidence experiment in the natural frame, the locations of the gun and analyser are reversed. Now as the analyser is rotated around the interaction region, the natural frame must rotate with it, since in the conventional coincidence experiment (which is the time-inverse), this would be equivalent to moving the gun. The orientation of the natural frame in this case in shown in Fig. 5.7. Hence when moving the analyser, the natural frame rotates about its z-axis, with its x-axis aligned to the analyser detection axis.

The angle of the polarization vector which gives the maximum scattering yield is given by the fitting parameter $C$. This was measured with respect to the gun axis in the super-elastic experiment in Manchester, and not the analyser axis, so a rotation is required to express it in the natural frame. This is illustrated

Figure 5.6: The natural coordinate frame in a conventional coincidence experiment. The $x$-axis is parallel to the incoming electron momentum vector, $k_{\text{in}}$. The scattering angle, $\theta_e$ is measured as positive as shown, and $\gamma$ is also positive in this direction by convention.
in Fig. 5.8(a). The diagram shows the angle where scattering is at a maximum makes an angle of $C$ with the gun axis. The analyser makes an angle of $\theta_e$, measured from the same axis. The angle between the analyser and the gun is $(\pi - \theta_e)$. By rotating the angular positions of the gun and analyser clockwise through this angle, the polarization vector now makes an angle of

$$\pm \gamma = C + \theta_e$$

(5.6)

to the analyser axis.

By convention, the scattering angle should always be positive after rotation. When this is not the case, as in Fig. 5.8(b), symmetry considerations allow the diagram to be flipped along the analyser axis. The condition that the gun angle must be positive fixes the sign of $\gamma$.

The error on $\gamma$ is given simply by the error on the fitted $C$ parameter and the error on the scattering angle:

$$\sigma^2_\gamma = \sigma^2_C + \sigma^2_{\theta_e}$$

(5.7)
Figure 5.8: These diagrams are a pictorial representation of how an experimental measurement of $C$ may be translated to a measurement of $\gamma$. Each diagram shows the position of the analyser (A) and gun (G) in the scattering chamber. Two examples are shown; in (a) the angle $\theta_e$ is positive and in (b) it is negative. The solid line indicates the path of a super-elastically scattered electron which travels from the gun, gains energy in the interaction region, and is scattered towards the analyser. The dotted horizontal line in each diagram represents the $x$-axis in the natural frame. The dashed line is the direction of maximum scattering amplitude, $C$, which is measured in a clockwise direction from the $x$-axis.
The error due to the fit, $\sigma_C$, is usually small, and so the greatest contribution to the error on $\gamma$ is the uncertainty in the analyser angle.

5.3.3 Measuring $L_\perp$

The parameter $L_\perp$ is directly related to the $P_3^S$ pseudo-Stokes parameter when the optical pumping parameters are unity by the following relationship [53]:

$$L_\perp = +P_3^S$$

(5.8)

The $P_3^S$ pseudo-Stokes parameter can be found as in equation (2.15) from measurements of the scattering intensities for excitation from left-hand and right-hand circular polarised radiation:

$$P_3^S = \frac{S_{RHC}(\theta_e) - S_{LHC}(\theta_e)}{S_{RHC}(\theta_e) + S_{LHC}(\theta_e)}$$

(5.9)

The experimental arrangement for producing circularly polarised radiation was discussed in Section 3.7.1. Inserting a quarter wave plate after the half wave plate changes linearly polarized light to circularly polarized light when the polarization vector is aligned at multiples of 90 degrees to the quarter wave plate axis. Either left hand circular, or right hand circular light is produced, depending on the birefringent properties of the wave plate.

The sign of the polarisation measurement was deduced by comparing to earlier data [59] where the sign of $L_\perp$ was well known.

The measurement of the scattering intensities from left-hand or right-hand polarised radiation are formed from the averages of several measurements. The error on these measurements was estimated from the standard error of the mean.
5.4 Results at 65 eV Equivalent Energy

5.4.1 Method

The first data set presented here was collected at 65 eV equivalent energy. Therefore the analyser in the super-elastic experiment was set to detect electrons at 65 eV, and the gun was set to emit electrons at \((65 - E_e)\) eV, where \(E_e = 2.93\) eV, the energy of the transition from the ground state to the \(4^1P_1\) state. The equivalent incident energy of 65 eV was chosen because at the time of writing, no other such results had been taken at this energy.

These measurements were taken before the multiscan program had been fully developed, and so an earlier version of the data collection program was used, called SuperStep, to record the scattering data.

To take the \(P_{lin}\) and \(\gamma\) measurements, the wave plate was taken through one full rotation, stopping at ten degree intervals to determine the scattering rate. This rotated the polarisation vector of the radiation incident on the interaction region through \(720^\circ\). The procedure was then repeated with the wave plate rotated in the opposite direction. This ensured that any systematic error in the calibration of the stepper motor was cancelled. The count rates were then averaged for each polarisation angle. A background count rate was then taken, by blocking the laser beam and measuring the number of counts over 100 seconds. This background rate was subtracted from the signal. This methodology implicitly makes the assumption that the background rate can be considered to be constant over the time of the measurements. This assumption was reasonable for the acquisition times used at this energy.

To measure \(L_{\perp}\), the SuperStep program was used to take counts at half wave plate angles of 0, 45, 90, 135, 180, 225, 270 and 315 degrees to the quarter wave plate axis, which alternated between right and left hand circular polarization (in that order). They were then taken again in the reverse direction to return the half wave plate back to zero degrees. In this way, counts were accumulated for
left and right hand circularly polarized light.

For the measurements using both linearly polarised light and circularly polarised light, the acquisition time was ten to fifty seconds per data point, depending on the signal rate. The computer generated one file per analyser angle which contained a list of the number of electrons counted at each polariser angle in the clockwise and anticlockwise directions.

### 5.4.2 Results and Discussion

The combined results of the $P_{\text{lin}}$, $L_\perp$ and $\gamma$ measurements at 65 eV are shown in Fig. 5.9. These have been published in a conference proceedings [131]. The final graph is $P_{\text{tot}} = \sqrt{P_{\text{lin}}^2 + L_\perp^2}$, which should not exceed unity [63]. Major contributions to the errors include uncertainties in the angles of the analyser and half wave plate, and the errors on the fitting parameters.

The data for $P_{\text{lin}}$ shows a sharp dip at $\theta_e = 22.5^\circ$, which extends down to $P_{\text{lin}} \approx 0.22$. There is a broad, shallow dip at $\theta_e = 90^\circ$, and a small dip at $\theta_e = 55^\circ$.

The data for $\gamma$, the charge cloud alignment angle, has a simple structure. In the measurements, this parameter increases to $\gamma \approx 0^\circ$ at $\theta_e = 45^\circ$. Beyond here the direction of rotation with increasing $\theta_e$ changes, and the angle decreases until $\gamma = -77^\circ$ at a scattering angle of $80^\circ$. There is some evidence of a cusp shaped feature at an angle of $65^\circ$. At larger scattering angles, the value of gamma begins to increase again. In almost all cases, the alignment angle is negative.

In the graph for $L_\perp$, two large peaks and two troughs are evident. The peaks are at scattering angles $25^\circ$ and $75^\circ$, and extend up to $L_\perp \approx 0.93$ and $L_\perp \approx 0.63$ respectively. The troughs at scattering angles of $55^\circ$ and $85^\circ$ have values of $L_\perp \approx -0.31$ and $-0.67$. Small features are evident beyond $\theta_e = 85^\circ$, where $L_\perp$ remains negative. Positive values of $L_\perp$ at smaller angles indicate that the charge cloud angular momentum is clockwise, whereas negative values at larger angles
Figure 5.9: Results showing variation of ACPs with analyser angle at 65 eV equivalent energy. For discussion, see text.
indicate this is anticlockwise.

The graph of the coherence parameter, $P_{\text{tot}}$, shows that there was some loss of coherence in the interaction between scattering angles of 65° and 100°. This has been seen at other energies, and may indicate that spin flip processes are occurring in the interaction.

Theoretical calculations for the ACPs at different scattering angles are not available at 65 eV. However the work may be compared to earlier results at 45 and 55 eV, for which calculations are available. This is shown in Fig. 5.10, and was the subject of a paper [60]. The calculations shown on the plots were made by Chauhan et al. using an RDW model [57]. The ACPs are shown over a full range of scattering angles, since the MAC device was used to take some of the data points [59]. Comparing the data taken at 65 eV with that taken previously shows that the new data follows the general trend.

In the results for $P_{\text{lin}}$ shown in Fig. 5.10, a sharp dip at just under 30° is seen, along with a large, shallower dip at around 90°. This is also apparent in the data at 65 eV, where the angular positions and magnitudes of these two dips were similar. The results for $\gamma$ also show similarities, with minima around the 20° and 80° regions of the plot. One difference in the 65 eV data is that the onset of the maximum, where $\gamma$ approaches zero, occurs at a larger scattering angle than at 55 eV and 45 eV. In the $L_\perp$ results, peaks exist at around 30° and 70° as in the results shown in Fig. 5.10. The trough at an angle of 55° is shallower than in the previous studies, and at 65 eV there is also some evidence of a peak around 140°.

To summarise, the 65 eV data are seen to be broadly similar in structure to the data collected at 45 eV and 55 eV, although the positions and magnitudes of some of the features are seen to have changed.
Figure 5.10: Earlier results taken measuring the ACPs at 45 and 55 eV. The solid line indicates the predictions made by [57]. The other data points shown are from experimental work by the Flinders group [41] and by Kleinpoppen et al. [52].
5.5 Low Energy Measurements at 12 eV and 10 eV Nominal Energies

5.5.1 Considerations for Data Collection at Low Energies

When the spectrometer is operating and the analyser is tuned to detect super- elastically scattered electrons, it may seem reasonable to assume that all of the electrons detected are due to this scattering process. This is because the laser is only exciting the $4^1P_1$ transition with an energy $E_\phi = 2.93\, \text{eV}$, so that

$$E_{\text{out}} = E_{\text{in}} + E_\phi$$

and the analyser is set to detect electrons with energy $E_{\text{out}}$, which is higher than the energy of electrons from the gun $E_{\text{in}}$. The laser interaction should be the only source by which the electrons may gain energy in the scattering chamber.

To verify this, background counts were taken with the laser beam blocked. For high energies this works well, and count rates of less than one per second were detected. These counts may be attributed to elastically scattered electrons that have sufficient energy to reach the CEM. Both the elastic peak and the detection function of the analyser have a Gaussian form, which gives a small probability that elastically scattered electrons at the extreme ends of the Gaussian are detected. By comparison, with the laser incident on the interaction region, a super-elastic count rate of many thousands per second was measured.

At lower energies the signal to noise ratio deteriorates, and with the equivalent energy reduced to 10 eV, background counts can number several hundred per second, with the laser making a difference of only tens of counts at the super-elastic peak. This was due to the degraded performance of the electron gun at these energies producing electrons that could reach the detector.

The electron gun is designed to work best at energies above 20 eV, where the beam of electrons that it produces is well defined. In order to record low energy
super-elastic data at 12 eV and 10 eV, the gun was required to emit electrons at energies 2.9 eV lower than these energies. The gun was therefore set to operate at 9.1 eV and 7.1 eV to allow data collection.

With the electron optics set up correctly, the electron beam should have a small pencil angle and zero beam angle at the interaction region. At low energies the correct focussing conditions cannot be met, as this would require the electron beam diameter to be large inside the second lens element of the gun. The aperture lenses used in the gun suffer from large aberrations when the fill factor of the lens is high, leading to poor focussing due to increased spherical aberrations [132]. Furthermore, a large width of the electron beam would not allow it to pass through the exit aperture of the gun.

As the desired focussing condition cannot be reached with this gun at these energies, the electron beam was not as well formed. This can be seen in Fig. 5.11, which shows a simulation of the electron gun set to emit electrons at 7 eV.

The voltages shown on the diagram are representative for operation of the gun at this energy. The electron beam at the interaction region has a diameter of several millimetres, compared to a ~1 mm diameter beam at a higher energy, as it can no longer be accurately controlled. As the beam was not focussed well at the target, this was compensated for by running the electron beam at a higher current of 5–10 µA, as detected on the Faraday cup.

At these high beam currents and low energies, the computer model indicates that the onset of space charge effects become significant. This serves to further reduce the beam quality, increasing aberrations and causing the beam to diverge further. Space charge also makes the predictions from this model unreliable, and so the values for the voltages at low energy were found by tuning manually to maximise the super-elastic signal.

As the beam has a larger angular divergence, electrons are more likely to stray from the beam axis and scatter from structural parts of the chamber. These electrons may ingress through small gaps in the sides of analyser and be detected
**Figure 5.11:** The electron gun as simulated in SIMION 7 [86], operating at 7 eV, and with space charge effects modelled. The path of the electrons from the filament is shown in black, going across the page from left to right. Field lines of constant potential due to the electrostatic lens elements are drawn in red. Representative voltages for the gun elements at this energy are labelled. These were found to produce the best super-elastic signal. The simulation shows that at low energies the beam is not as effectively focussed at the interaction region, compared to higher energies, and the beam has a larger diameter in the interaction region (cf. Fig. 3.6). The interaction region is at the far right of the diagram, space charge effects cause the beam to begin to diverge by this point.
in the CEM, having bypassed the angular and energy selection mechanisms. This results in spurious electron counts, and explains why taking data with the low energy beam, which is poorly collimated, has a large background count rate compared to a well collimated beam at higher energy. The background count rate is a combination of these electrons which have made their way to the CEM by means other than the analyser assembly, and also those electrons detected from the extreme end of the elastic scattering energy peak.

The problem of high background counts is compounded by a lower super-elastic signal at these energies. This is mainly due to the poor focussing of the gun, and a lower cross-section for super-elastic scattering at low energies. This makes the required signal very small. This is where the difficulty lies in taking low energy measurements, and why it was necessary to accumulate significantly more data at these energies compared to previous studies.

5.5.2 Data Collection Method

The data collection process was described in Section 4.5.7. Briefly, to obtain data at low energies, measurements were recorded using multiscan, which was the data collection software developed for this purpose. For each specified angle of rotation of the half wave-plate, two measurements were taken. These were a count of the number of electrons detected with the laser beam blocked (the background noise counts) and counts with the beam incident on the interaction region (the laser-on counts). The difference between the two gave the super-elastic counts, and dividing this quantity by the acquisition time for the data point gave the super-elastic count rate. The data collection system also collects many other readings relating to the condition of the spectrometer as data is being gathered, as was described earlier in Section 4.5.

As the signal rate at 12 eV and 10 eV was very low, data had to be recorded over a longer period to accurately determine the super-elastic scattering rate. One way to do this would be to simply increase the acquisition time for each data
point. For some angles, acquisition times of around five minutes per point were required to discern any super-elastic signal from the data. Over these timescales it was found that fluctuations in the background signal made the measurements unreliable.

To solve this problem, a number of different scans were performed for each angle, which together formed a set of scans. The acquisition time for each data point in a scan was set to be no more than 30 seconds. Each data point consisted of a measure of laser-on and background counts, and the background level was assumed not to fluctuate over this time.

The super-elastic count rate is deduced by subtracting the background from the laser-on counts, measured over a short time for each data point in the set. As the time period is short, the deduced super-elastic signal is noisy and has a large error associated with it.

By then combining the super-elastic signal from every congruent data point in a set, the signal can be recovered from the data. This is because the background rate for each point is sampled over a small time interval, during which it is less likely to undergo a large fluctuation.

To analyse the linear polarisation measurements which determine $P_{\text{lin}}$ and $\gamma$, the super-elastic counts were added together for each data point in the set, and divided by the total acquisition time. This allowed the super-elastic count rate to be determined as a function of the polariser angle $\theta_{\text{pol}},$

$$S(\theta_{\text{pol}}) = \sum_i \frac{a_i(\theta_{\text{pol}}) - b_i(\theta_{\text{pol}})}{t_i}$$  \hspace{1cm} (5.10)

where the index $i$ defines a specific scan in a set, $a$ are the counts recorded with the laser on, $b$ are the counts of the background noise with the laser blocked, and $t_i$ is the acquisition time. The weighting assigned to each of the data points was defined from the standard error of the mean.

The fit from equation (5.3) was applied to the dataset $S$ to obtain values
for the ACPs \( P_{\text{lin}} \) and \( \gamma \). The error estimates were then derived from the errors on the fit, where again a Levenberg-Marquardt fitting algorithm was used which incorporated the weighting on each point.

For the \( P^S_3 \) measurements which determined \( L_\perp \), the procedure from Section 5.3.3 was followed. Each scan would record consecutive LHC and RHC measurements as the half wave-plate was advanced through steps of 45°, which produced radiation at the correct polarisation from the quarter wave-plate. The range of angles was chosen to take the half wave-plate through a full rotation. This was to correct for any asymmetries in the wave-plate. The \( L_\perp \) parameter was found from (5.9) and (5.8), where the measurements for LHC and RHC were averaged to give \( S_{\text{LHC}} \) and \( S_{\text{RHC}} \), with the errors on each quantity estimated from the standard error.

The value of \( L_\perp \) for the set of scans was then determined by performing a weighted average of each of the values computed for each scan, with the error on the weighted average \( \sigma_L \) defined as in the literature [133].

### 5.5.3 Online Analysis Software

The online analysis software was developed to automate the task of combining the data from individual scans, fitting to the data, and deriving the values of the ACPs for each of the scattering angles \( \theta_e \). This software was a necessity since processing the volume of data generated by the spectrometer manually would have been impractical; the data for the 10 eV results contained almost 30,000 files. Using the computer, this could typically be processed in around ten seconds to produce results for all ACPs.

As with the spectrometer control software, described in Section 4.5, the online analysis software was written using LabVIEW [109]. To view the data from a single scan, a scan file editor, called mtfeditor was developed. This is pictured in Fig 5.12, and allowed the data from a scan to be viewed by selecting the appropriate file. It also allowed the attributes of the scan to be edited, so that a
Figure 5.12: The scan file editor, which displays the attributes of an individual scan and allowed all the data from the scan to be viewed.

To analyse a set of scans together, another program, comboviewer, was written. The interface to this program is shown in Fig. 5.13. The program was able to group the data files representing each of the scans into sets. For linear polarisation data, selecting a data set would perform the necessary summing and fitting calculations, and compute values of $P_{\text{lin}}$ and $\gamma$. For the circular polarised data, values for $L_\perp$ were computed directly.

Finally, to create the full set of plots for the three ACPs, a program was developed called plgplots, shown in Fig. 5.14. This program would take a list of directories on the computer containing the data files, and examine the contents of the files in each of these directories to generate the plots. All data taken at the same angle, and in the same data group, was plotted as a single point on the graph.

The online analysis software, particularly plgplots, was useful in identifying trends or mistakes in the data while it was being taken, as graphs of the ACPs
Figure 5.13: The data view program, which groups together a set of scans in the same set and calculates the ACPs together.

could be readily generated from the ‘live’ data. The calculated values from the software could be exported so that they could be used in a professional graphing program.

5.5.4 Results and Discussion

The data at 12 eV and 10 eV equivalent energy was taken using the older power supplies, as the new supplies described in Chapter 4 had not been completed at this point. Correctly tuning the gun and analyser directly at these energies was not possible, and so the tuning process was carried out by tuning to the super-
Figure 5.14: The ACP plot viewer, displaying graphs of $P_{\text{lin}}$, $\gamma$ and $L_{\perp}$ against the scattering angle (horizontal scale). The plot shows a subset of the 10 eV data. The errors on $\gamma$ are small as the software only shows the errors due to the statistics, without including those due to experimental sources, which were added at a later stage.
elastic peak at a higher energy, 25 eV. With the electron optics optimised at this energy, the gun and analyser energies were slowly decreased simultaneously in 5 eV steps until the desired energy was reached.

The results of the low energy measurements were the subject of a publication [61]. The data is shown in Fig. 5.15 for 12 eV and 10 eV nominal equivalent energies. These energies correspond to the assumed detection energy of the analyser for the super-elastic measurements, and are nominal to account for the possibility of errors on the energy due to contact potentials and stray fields. For the equivalent conventional coincidence experiment, these would be the energy of the detected inelastically scattered electron.

The graphs show the variation in the ACPs over a range of scattering angles from 25 to 140 degrees. The graphs on the left of the figure show the results at 12 eV, and those on the right show 10 eV.

The top two graphs (a) and (b) show plots of $P_{\text{lin}}$ against scattering angle for an electron energy of 12 eV and 10 eV. At 12 eV, three distinct minima are seen, at angles 60°, 100° and 125°. At these points the minima are seen to extend down to $P_{\text{lin}} \approx 0.27$, $P_{\text{lin}} \approx 0.46$ and $P_{\text{lin}} \approx 0.35$ respectively. In the remainder of the angular range, the value of $P_{\text{lin}}$ varies, and approaches unity at some points; the greatest value is seen at $\theta_e = 115^\circ$, where $P_{\text{lin}} \approx 0.93$.

The 10 eV data for $P_{\text{lin}}$ has a similar structure. The first minimum, which occurs at 60° is shallower, with $P_{\text{lin}} \approx 0.55$, and also broader. The dip around 125° extends to a similar depth at both energies, and is broader in the 10 eV data. The variation of $P_{\text{lin}}$ with respect to $\theta_e$ is also much smoother. There is some evidence at around 80° of an additional dip as seen in the 12 eV data, although the statistics at 10 eV may be too poor to reliably resolve a feature here.

The data point at $\theta_e = 100^\circ$ suggests a very sharp minimum in the 10 eV data, where the value of $P_{\text{lin}}$ drops from $\sim 0.95$ down to $\sim 0.30$ within 5°. As the change is so sharp and the error bar is large for this point, some explanation of this data point is warranted. When taking data at this scattering angle, the
Figure 5.15: Measurements of the ACPs at 12 eV and 10 eV (nominal energy), calculated from the scattering data over the angles shown.
rate of super-elastic counts was found to vary between around 0.3–0.7 Hz. The count rates derived from the measurements of the electron counts at different polarisation angles for $\theta_e = 100^\circ$ are plotted in Fig. 5.16. Clearly when compared to Fig 5.5 the statistics are much poorer. This manifests itself in a large error on the $A$ and $B$ coefficients in equation (5.3), which propagates to a large error on $P_{\text{lin}}$. Attempts to take more data to reduce the error were hampered since low scattering yield at this angle made successful measurements very dependent on stable operating conditions; out of over 200 attempted runs only 14 produced useful data. This data point will be discussed further below.

The middle two graphs (c) and (d) in the figure show the variation of the alignment angle $\gamma$ with scattering angle. For the 12 eV data, this shows a gradual and smooth variation at low angles $\theta_e \leq 70$, where $\gamma \approx -80^\circ$, with a small dip at $\theta_e = 60^\circ$ which brings the value of $\gamma$ down to $-90^\circ$. At $70^\circ < \theta_e < 130^\circ$, the rate of the variation with $\theta_e$ increases, and crosses through zero at $\theta_e \approx 115^\circ$. This point corresponds to alignment of the charge cloud with the photon polarisation vector. Where $\theta_e \geq 130^\circ$, the measured values for $\gamma$ stay around $-55^\circ$.

At 10 eV, variations in $\gamma$ as a function of the scattering angle is gradual. Unlike the 12 eV data, the alignment angle remains negative throughout the scattering
angles that were measured. From $\theta_e = 25^\circ$, the alignment angle gradually increases from $\gamma = -70^\circ$ to $\gamma = -55^\circ$ at $\theta_e = 95^\circ$. There is evidence of a small dip around $\theta_e = 65^\circ$, although to confirm this, additional data points would need to be taken. Above $\theta_e = 95^\circ$ there is a sharp increase to $\gamma = 0^\circ$, after which the alignment angle can be seen to gradually reduce back to $\gamma = -55^\circ$ at $\theta_e = 140^\circ$.

The lower pair of graphs (e) and (f) plot $L_\perp$ against scattering angle for the two energies. The $L_\perp$ plots have a relatively simple structure compared to $P_{\text{lin}}$ and $\gamma$, the main feature of both of these plots is the large central dip, the position of which is dependent on the energy. At 12 eV, this dip is seen at $\theta_e \approx 100^\circ$, and peaks occur either side at scattering angles $\theta_e \approx 65^\circ$ and $\theta_e \approx 125^\circ$. The values measured for $L_\perp$ range over almost all permissible values, $-1 < L_\perp < +1$.

For the measurements of $L_\perp$ at 10 eV, the measured range of values lies within the range $-0.53 < L_\perp < +0.80$. A similar structure is apparent compared to the 12 eV data, with the characteristic broad minimum shifted in angle to $\theta_e \approx 85^\circ$. There is clear evidence of a peak at $125^\circ$, but unlike the 12 eV data, the location of another peak at low scattering angles cannot be reliably deduced.

In Fig. 5.17, the results taken at 10 eV nominal energy are presented along with results predicted for this energy by theoretical models. There were four models available for comparison with the experimental data, as discussed in Chapter 1:

**Relativistic distorted wave (RDW)** calculations are from Chauhan, Srivastava and Stauffer [57].

**R-matrix (RM)** calculations were made by Kawazoe, Kai, Chauhan, Srivastava and Nakazaki [54].

**R-matrix using B-splines (BSR)** work was conducted by Zatsarinny, Bartschat, Bandurina and Gedeon [56].

**Convergent close-coupling (CCC)** calculations were taken from the work of Fursa and Bray [58].
Figure 5.17: Data at 10 eV (nominal energy) plotted against theoretical models for 10 eV. There is only very modest agreement with the experimentally measured data.

Figure 5.18: Data at 12 eV (nominal energy) plotted against theoretical models at 10 eV. The CCC and BSR models best fit the measured data. For details, see text.
In all these theoretical calculations, values for the Stokes parameters $P_1$ and $P_2$ were provided to compare with experimental data. These are numerically equivalent to the pseudo-Stokes parameters $P^S_1$ and $P^S_2$ since the optical pumping parameters for calcium are unity. As the experiment in Manchester was designed to directly measure $P_{\text{lin}}$ and $\gamma$, these values were derived from the calculations using the relationship \[ P_1 + iP_2 = P_{\text{lin}}e^{2i\gamma} \] (5.11) which allowed $P_{\text{lin}}$ and $\gamma$ to be found [53]:

\[
P_{\text{lin}} = \sqrt{P_1^2 + P_2^2} \]
\[
\gamma = \frac{1}{2} \arctan \left( \frac{P_2}{P_1} \right)
\] (5.12)

The four plots in Fig. 5.17 show a comparison between the data at a nominal energy of 10 eV, and the theoretical models at that energy. Overall the models do not fit well with the measurements.

Plot (a) shows the measurements for $P_{\text{lin}}$ plotted against scattering angle. Evidence of the dip predicted by all the models at around $125^\circ$ can be seen in the data. There is also some evidence of some of the structure at around $105^\circ$ being reproduced, as predicted by the CCC and RDW models, although the point at $\theta_c = 100^\circ$ sits far away from all theoretical predictions. At angles below $80^\circ$ the agreement with all models is poor. The dip predicted by the R-matrix models and the CCC model is not reproduced in the data, and although the RDW model predicts the dip at around $50^\circ$, there is little agreement at scattering angles below $50^\circ$.

For the alignment parameter $\gamma$, shown in plot (b), agreement between the models and the data is also poor. Below $100^\circ$ the data points do not obviously correlate to any of the models. There is a weak agreement above $120^\circ$, where there is some suggestion of the dip that is predicted by all four of the models. However the additional structure by the models is not apparent in the measurements of $\gamma$. 
In plot (c) $L_\perp$ measurements are shown. The models correctly predict the presence of the broad dip, although all understate the width of this feature. The magnitude of the minimum and maximum values are also underestimated by the models, which all predict values of $L_\perp$ near to +1 and as low as $\sim -0.8$.

The final plot, (d) shows $P_{\text{tot}} = \sqrt{P_{\text{lin}}^2 + L_\perp^2}$. The quantity $P_{\text{tot}}$ should be equal to unity if the interaction was fully coherent. Some loss of coherence is evident in the data, and the RDW model correctly predicts this at $45^\circ$. The other deviations from $P_{\text{tot}} = 1$ are not predicted by any of the theories.

As discussed in Section 5.2.2, the contact potential of the experiment varied. This was thought to be due to layers of calcium depositing on spectrometer surfaces in the chamber. The calcium layers may charge up, causing stray fields which affect the incident and outgoing energies of the electron beam in the target region. This gave rise to an uncertainty of $\sim 2$ eV in the equivalent energy of the interaction. Due to this, it was reasonable to compare the data at 12 eV nominal energy with the models at 10 eV, as the uncertainty in the energy made it possible that the equivalent energy of this data was closer to 10 eV.

In Fig. 5.18, the data at 12 eV nominal energy is hence plotted against the model predictions at 10 eV. For plot (a), showing $P_{\text{lin}}$, the CCC, BSR and RM models predict the dip at $65^\circ$, although the RM model predicts some additional structure which does not appear in the data. The BSR model better predicts the magnitude of the feature here, while the CCC model better predicts the angle. The second dip at $\sim 105^\circ$ is best predicted by the CCC and BSR models, and the third dip at $125^\circ$ is well matched to the RM model, as well as the CCC and BSR models.

The data and models for $\gamma$ are shown in plot (b). There is a very good agreement with the CCC model for scattering angles above $70^\circ$, with the theoretical curve passing through the error bars for almost all points. Below this angle the data points appear offset from theory, although the data follows the shape of the curve. Only the CCC and BSR models show the correct structure, the other models show spurious features which do not present in the data.
For plot (c) showing $L_\perp$, the broad minimum fits best with the CCC calculation, which predict both this feature and a smaller dip at around $45^\circ$. The maximum value of $L_\perp$ is well predicted by the CCC, BSR and RM models. The minimum value is understated by all the models, although CCC and BSR calculations are closest to the measured minimum value. The width of the large minimum is reproduced well by all models except for the RDW calculation.

The final plot (f) shows that for some measurements, particularly as the scattering angle increased, there was a loss of coherence. This was not well predicted by any of the models.

The models at 10 eV therefore show good agreement with the set of data at 12 eV nominal energy. In particular the CCC calculations are able to reproduce many of the features found in the measurements, with a particularly good fit to the alignment angle $\gamma$. The BSR model also reproduced many features well, although with an angular offset in the case of the $L_\perp$ and $P_{\text{lin}}$ data.

Since the models for 10 eV show good agreement with the 12 eV nominal energy data, it is likely that the experimental data is offset by around 2 eV from the stated value. As discussed earlier this was likely due to layers of calcium coating the spectrometer surfaces, an effect which has previously been observed [59, 93].

As the CCC model had been the best fit to the data, a CCC calculation was requested from Prof. Igor Bray at 8 eV [134], to compare with the data at 10 eV nominal energy. This comparison is shown in Fig. 5.19, along with a plot of the data points for 12 eV nominal energy with the 10 eV model. This shows that the data at 10 eV nominal energy generally fits well to the CCC model at 8 eV, strengthening the argument that a 2 eV shift in energy from the nominal values was present.

In the fit to the data at 10 eV nominal energy, the most prominent feature is the large, sharp dip at $100^\circ$ predicted by the model and indicated by the single data point at this scattering angle which was discussed above. The model fits the data well at angles below this point. Above this angle, the CCC model correctly
Figure 5.19: Data at 12 eV and 10 eV nominal energy plotted against CCC model at 10 eV and 8 eV.
predicts the presence of a dip at $\theta_e \approx 130^\circ$. However the CCC model appears to underestimate the magnitude, as the data shows a fall to $P_{\text{lin}} \approx 0.33$, whereas the model only predicts a fall to $P_{\text{lin}} \approx 0.68$.

The model fits the data to $\gamma$ well, with a good proportion of the line within the error bars on the points. At $100^\circ$, the sharp increase to near $\gamma = 0^\circ$ is seen followed by a decrease at higher scattering angles. The dip predicted by the CCC model is not seen at $\theta_e \approx 95^\circ$, which instead remains at $\gamma \approx 55^\circ$ in this region.

The CCC calculation for $L_\perp$ shows the weakest agreement with the experimental data. The general shape of the large feature is reproduced, and the position and magnitude of the peak at $\theta_e \approx 125^\circ$ is well reproduced. However the dip at $\theta_e \approx 85^\circ$ is offset from the model by an angle of around $15^\circ$, and the magnitude $L_\perp \approx -0.54$ is far less than the model, which predicts a drop to $L_\perp = -1$. Finally the magnitude of the peak around $\theta_e = 40^\circ$, where $L_\perp \approx 0.70$ in the data, is overestimated in the CCC model.

The CCC model at 8 eV clearly predicts the data taken at a nominal energy of 10 eV, compared to the model at 10 eV. Along with the good agreement between the 12 eV data and the 10 eV models, this is evidence of an offset of around 2 eV in the energy calibration of the spectrometer.

5.6 Summary

In this chapter, the experimental results obtained from the super-elastic scattering spectrometer were discussed. Initial measurements to calibrate the spectrometer were outlined, and energy loss measurements were taken that showed the spectrometer was performing well.

Data was presented for super-elastic scattering at 65 eV, 12 eV and 10 eV. From these data sets, the atomic collision parameters were deduced by performing various fits to the data. The results were discussed and the errors analysed. Although no direct comparison to theory was available at 65 eV, the results pre-
dicted from RDW calculations were available at lower energies. The data at 65 eV was seen to follow the general structure of the model and of the previous data taken at 55 eV and 45 eV.

At lower energies the scattering cross section reduced substantially, and the levels of background noise increased. This reduction in the signal to noise ratio meant that far more scattering data had to be collected from the spectrometer, compared to previous studies. The volume of data that was generated was impractical to analyse by hand, and a computer program to automatically analyse the data collected from the spectrometer was written and detailed here.

The data collected at nominal energies of 12 eV and 10 eV were presented and discussed. Theoretical calculations were available at 10 eV for RM, RDW, BSR and CCC models. As there was an uncertainty of around 2 eV in the value of the energy, both sets of data were compared to the models, and the quality of the fit in each case was discussed. It was found that the data collected at 12 eV nominal energy was a better match to the models at 10 eV, indicating a discrepancy of 2 eV between the actual and measured values of the incident electron energy. The BSR and CCC models were the better matches to the data at this energy which is not surprising as they are low energy models.

Finally calculations using the CCC model were presented at 8 eV. This was compared to the data at 10 eV nominal energy. The quality of the fit was discussed and this was found to be excellent in general. From this it was concluded that a 2 eV shift in energy was likely from the nominal energy value quoted for the measured data.
Chapter 6

Conclusions and Future Directions

6.1 Summary of Work

In this thesis, the process of super-elastic scattering from laser excited calcium atoms was discussed, experiments were detailed and results presented. During the course of these studies, improvements were made to the spectrometer to allow it to operate in a more autonomous manner, which in turn allowed for more efficient data collection.

Chapter 1 introduced the experiment in the context of earlier studies. Experimental work in the field was discussed, and a review of the relevant theoretical models used to predict the outcome of these experiments was presented.

The atomic collision parameters, which can be used to describe the shape of the P-state excited atom, were introduced in Chapter 2. These would later be used to characterise the outcome of the super-elastic scattering experiments. A QED description of the laser interaction with the calcium atoms was then presented. The optical rate equations were derived and the excited state population calculated for a typical laser power, as used in these experiments.

The equipment used to perform the super-elastic scattering experiments was described in Chapter 3. The scattering experiments were carried out inside a
sealed vacuum chamber. The chamber was held at a pressure of $3 \times 10^{-7}$ mbar during operation by a turbomolecular pump backed by a rotary pump.

Inside the scattering chamber, an electron gun was set to produce a beam of electrons focussed on the interaction region, in the centre of the chamber. An atomic beam oven designed to operate at 800°C supplied a well defined beam of calcium atoms to the interaction region. Scattered electrons were detected with the electron analyser, which could discriminate between electrons at different scattering angles and energies. Atoms in the gaseous phase could also be injected into the target region via a gas jet nozzle for calibration purposes.

For super-elastic studies on the $4^1P_1$ state of calcium, a laser beam was introduced into the target region through a window at the top of the scattering chamber. The laser systems used were capable of delivering over 300 mW of laser power at a wavelength of 423 nm, which matched the energy of the transition in calcium. The minimum laser linewidth that could be achieved was 30 kHz. Long term laser frequency drift was corrected by a laser locking system which used measurements of laser induced fluorescence in the interaction region to determine the offset of the laser frequency from resonance.

The optics used to correctly focus the laser beam and select the polarisation were described. A half wave-plate controlled by a stepper motor produced linearly polarised light that was rotated by a specified amount. Insertion of a quarter wave-plate in the optical beam path produced circularly polarised light, with the handedness of the polarisation then controlled by the half wave-plate.

In Chapter 4, the computer controlled elements of the spectrometer were presented. This included a new digital power supply for controlling the electron optics, and a new computer-controlled acquisition system for recording data. The construction and performance of the new power supplies was discussed, with circuit diagrams provided for all the major elements. Operation of the power supply firmware was also described. A state machine programming model was implemented to allow the controller to efficiently share processing resources between several tasks.
The computer software written to control the spectrometer and take data was described. The software was capable of operating the new power supplies, and so was able to take energy loss spectra, store and recall the state of the voltage supplies, and change the tuning conditions of the electron-optical elements in the spectrometer. The tuning process could be automated using a simplex algorithm to optimise the power supply voltages.

With the new software system in place, most aspects of the scattering experiment could be run automatically. Data pertaining to the state of the spectrometer was also monitored and recorded. The automatic system reduced the amount of operator intervention that was required and ultimately allowed for longer running times, allowing a larger volume of scattering data to be collected. Records of the state of the spectrometer were used to identify any possible problems with the data collection process.

The super-elastic scattering data collected from the spectrometer, along with a discussion of these experimental results, was presented in Chapter 5. This included new super-elastic data recorded at equivalent energies of 65 eV, 10 eV and 8 eV.

The contact potential was described and found to arise from a combination of physical effects; the work function at the gun filament, stray fields in the interaction region, and a potential difference due to the use of dissimilar metals at the entrance apertures of the gun and analyser. The contact potential had to be taken into consideration when assessing the impact energy of the electronic projectile on the target.

The procedure for calibrating the energy of the spectrometer was described. The process of taking a helium $2^3S$ resonance spectrum allowed measurements of the contact potential to be taken. The results of one such measurement were shown which gave the value of the contact potential as $\phi = -1.2$ eV.

Energy loss spectra of helium and calcium were taken to confirm that peaks corresponding to transition energies occurred at the established values. The en-
ergy resolution of the spectrometer allowed the $2^1P$ and $n = 3$ transitions in helium to be deduced at the expected energies. For the calcium energy loss spectrum, 423 nm laser radiation at the energy of the $4^1P_1$ transition was introduced into the interaction region. The resulting spectrum showed both an inelastic and a super-elastic scattering peak for this transition, spaced at energies $\pm 2.93 \text{eV}$ from the elastic scattering peak, also as expected.

A set of ACPs over the angular range $15^\circ$ to $125^\circ$ were calculated from scattering data recorded at an equivalent energy of 65 eV for the $4^1P_1$ transition in calcium. This data was compared to other experimental and theoretical work at lower energies, 45 eV and 55 eV. The new data at 65 eV was found to be in broad agreement with the earlier data.

Measurements were then taken at 10 eV and 8 eV equivalent energy, to test against various theoretical models of the interaction at low electron energy. The four models compared were not consistent with one another and it was hoped that experimental data at these energies would validate one or more of the theoretical approaches.

Taking measurements at these energies involved running the electron gun at energies below those for which it was designed. The consequences of this were discussed and it was shown that the electron beam focusing at the target and the collimation through the chamber were degraded. This led to a smaller super-elastic signal and greater background noise. A large volume of data was collected to compensate for the lower signal rate, which necessitated the development of new analysis software to calculate the ACPs automatically.

It was seen that the CCC model, and to a lesser extent the BSR model, best predicted the super-elastic data. Furthermore it seemed likely that electric fields in the scattering chamber caused by negatively charged calcium coated surfaces had contributed to a 2 eV shift between the nominal energy and the incident electron energy at the interaction region. This was seen from observing the quality of the fit to the models at 10 eV. Comparisons made between the data at 10 eV nominal energy, and new CCC predictions at 8 eV also showed good
agreement, lending further weight to this hypothesis.

6.2 Future Directions

6.2.1 Voltage Supply

The voltage supply cards are connected to the backplane using an edge connector. These were chosen as there was a good supply of them readily available in the lab, however the reliability of these connectors was found to be poor. In particular, the connectors could easily become misaligned if the height of the card was incorrect by only a few millimetres. A change for any future voltage supply would be to replaced these with another connector, for example the DIN41612 Eurocard connectors, which are always correctly aligned by virtue of their design.

Although the voltage supplies were stable enough to undertake the super-elastic scattering studies described in this thesis, the stability and drift characteristics were not equal to the older generation of power supplies [108, 135]. At the resolution of the super-elastic spectrometer, this was found not to be important. However, improvements to these characteristics would be necessary if the power supply were applied to a higher resolution electron spectroscopy application. These improvements could be achieved by careful shielding and further separation of digital and analogue parts of the design, and redesigning and rerouting some of the amplifier circuitry.

One limitation that was encountered while developing the firmware for the microcontroller was that the space available in the various memories was eventually exhausted. This meant that it became difficult to add new functions to the voltage supply firmware, as old code would have had to be removed or made more efficient. Microcontrollers are available with larger memories, for example the PIC18F87J50 [136]. Devices with larger memories generally work at a lower voltage of 3.3 V, instead of 5 V, and so the microcontroller board would have to be redesigned to accommodate the new chip.
With a microcontroller that has more memory, extra commands may be added to the USB interface. These may for example allow output voltages to be set directly, rather than from the DAC code, or for the internal calibration table to be updated without reprogramming the entire unit.

6.2.2 Computer Control and Software

In the experiment of Karaganov et al. [46], the polarisation of the laser radiation is controlled using a pair of quarter wave-plates which may be independently rotated using stepper motors under the control of a computer. Using a pair of stepper motors to rotate appropriate phase retardation plates is advantageous compared to using only a single stepper motor, as it allows for computer selection of either circular or linear polarisation. In the current arrangement, the operator must make this change manually by inserting or removing a quarter wave-plate in the beam path, which must then be realigned.

The large volume of files produced by the spectrometer was not well anticipated. This adversely affected the speed of the data collection and analysis software at some points. The act of accessing each individual file while performing calculations on the data sets presents a large overhead in proportion to the time spent performing calculations on the file. When multiplied by the several thousands of files which were created by the spectrometer, this added up to a significant delay. This suggests that organising the data into separate files is not the most efficient arrangement.

The type of data produced by the spectrometer is well suited to a database, which stores data structured as entities referred to as records. For example, a simple record structure for the experiment would store values for the wave-plate angle, the analyser angle, the time period, and the number of counts recorded in the time period with the laser beam blocked and unblocked. Database software contains functions to allow a subset of this data to be extracted, so for instance the count rates at a single analyser angle could be examined. The time to access
this data would be small as the database may be optimised for this type of query. Database systems are readily available and well developed, one candidate might be the SQLite [137] database library.

Use of a database would increase the overall speed of the analysis software. The increase in speed would allow the analysis software to be integrated with the data collection software. Values could then be automatically generated for the ACPs without delay and then displayed interactively, while the data was being collected. There would no longer be a requirement for a separate suite of programs to analyse the data. Such a scheme would allow for trends or issues with the data to be identified immediately. For example, if such a system were in place for the 10 eV nominal energy data, it would have been immediately clear that more points should have been taken to better characterise the sharp feature that was observed around \( \theta_e = 100^\circ \).

### 6.2.3 Scattering Experiment

Elements with D-shell electronic structure are of interest to theorists, however there is no super-elastic collision data yet available for such targets. The ground to excited state transitions for these atoms are in the ultraviolet portion of the spectrum. This presents a problem for carrying out super-elastic experiments, as these wavelengths are not accessible with the required high-stability single mode lasers at appropriate power levels.

To reach ultraviolet wavelengths using the lasers available to the group, an external frequency doubling cavity would be constructed. This would take the blue light output at \( \sim 400\ \text{nm} \) from the laser system, and use an appropriate frequency doubling crystal to produce ultraviolet radiation at twice the input frequency. The cavity would thus extend the wavelength range of the current laser system.

A list of some of the new targets which could be studied is given in Table 6.1. These targets are considered to be of particular interest, both for theorists, and
Conclusions and Future Directions

Table 6.1: New targets for super-elastic scattering experiments. The vapour temperature is the temperature required to produce a metal vapour suitable for forming an atomic beam, as specified by Ross and Sontag [16]. The transition wavelengths are found from the NIST database [78].

<table>
<thead>
<tr>
<th>Target</th>
<th>Vapour temp. (°C)</th>
<th>Ground state configuration</th>
<th>Transition</th>
<th>Transition wavelength (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cu</td>
<td>1250</td>
<td>(Ar) 3d^{10} 4s^1</td>
<td>4^2S_{1/2} \rightarrow 4^2P_{1/2}</td>
<td>327 nm</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>4^2S_{1/2} \rightarrow 4^2P_{3/2}</td>
<td>325 nm</td>
</tr>
<tr>
<td>Zn</td>
<td>340</td>
<td>(Ar) 3d^{10} 4s^2</td>
<td>4^1S_0 \rightarrow 4^1P_1</td>
<td>214 nm</td>
</tr>
<tr>
<td>Ag</td>
<td>1420</td>
<td>(Kr) 4d^{10} 5s^1</td>
<td>5^2S_{1/2} \rightarrow 5^2P_{3/2}</td>
<td>388 nm</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>5^2S_{1/2} \rightarrow 5^2P_{5/2}</td>
<td>328 nm</td>
</tr>
<tr>
<td>Au</td>
<td>1030</td>
<td>(Xe) 4f^{14} 5d^{10} 6s^1</td>
<td>6^2S_{1/2} \rightarrow 6^2P_{1/2}</td>
<td>268 nm</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>6^2S_{1/2} \rightarrow 6^2P_{3/2}</td>
<td>243 nm</td>
</tr>
</tbody>
</table>

for practical applications; for example there is interest in using zinc for new forms of lighting.

For those targets which exhibit hyperfine structure (gold and silver), the radiation produced from the doubling cavity will need to be resonant with the transition from both of the hyperfine ground states to the excited state. The ground state splitting is 1977 MHz (6099 MHz) for silver (gold), which is large enough to be resolved by the laser. An EOM would be used to produce a sideband from the main beam, which will be doubled inside the cavity along with the fundamental. To ensure the cavity is resonant with both modes, the cavity conditions must be carefully controlled, as the extra mode places an additional constraint on the cavity length.

It is calculated that the maximum ultraviolet output power from the doubling cavity would be \( \sim 40 \text{ mW} \). After losses in the beam delivery system this will be reduced by an estimated 70%, leaving \( \sim 10 \text{ mW} \) at the interaction region. This would not be sufficient to collect an appreciable super-elastic signal at all accessible angles. To amplify the laser power at the target, a resonant enhancement cavity built around the interaction region will be used. This cavity has already been constructed, and is currently being tested in the spectrometer by collecting new super-elastic data from calcium.
As can be seen from Table 6.1, some of the elements to be studied form a vapour at temperatures higher than the current oven can achieve. Due to this, a new high temperature oven will be used to form the atomic beam for use in these new experiments. Work on building this oven is at an advanced stage.

In conclusion, the super-elastic scattering experiments which were performed have provided new data to compare to theoretical work at low energies. Measurements of the atomic orientation and alignment for calcium atoms were taken using the spectrometer, at equivalent energies of 10 eV and 8 eV. In this regime, the CCC model was the most effective at modelling the scattering process. The extension of the super-elastic studies in Manchester to include more atomic targets will provide further data against which to test scattering theories, and assist in progress towards a complete scattering theory, able to fully describe all collisional interactions on this scale.
References


REFERENCES


[69] P. Farrell, W. MacGillivray, and M. Standage, “Quantum-electrodynam- 

[70] B. Hall, Y. Shen, A. Murray, M. Standage, W. MacGillivray, and I. Bray, 
“Superelastic electron scattering from laser excited rubidium at 20eV 
incident energy,” Journal of Physics B (Atomic, Molecular and Optical 

[71] A. J. Murray, A stepwise electron-photon coincidence experiment on the 
$6^1P_1$ state of mercury. PhD thesis, Division of Science and Technology, 
Griffith University, 1989.

[72] M. Harvey, Low Energy Electron Scattering from a Pulsed AC-MOT. PhD 
thesis, School of Physics and Astronomy, University of Manchester, 2009.


[74] J. Ackerhalt and J. Eberly, “Quantum electrodynamics and radiation reac-
tion: Nonrelativistic atomic frequency shifts and lifetimes,” Phys. Rev. D, 


[76] W. MacGillivray and M. Standage, “Stepwise electron and laser excitation 


p. 013409, Jan 2008.


[104] E. Black, “An introduction to Pound-Drever-Hall laser frequency stabiliza-


[111] Fairchild Semiconductor Corporation, *FQP3N80C/FQPF3N80C 800V N-


