High Fidelity Readout and Protection of a $^{43}\text{Ca}^+$ Trapped Ion Qubit

A thesis submitted for the degree of Doctor of Philosophy

David Szwer

Trinity Term 2009

St. Catherine’s College, Oxford
Abstract

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This thesis describes theoretical and experimental work whose main aim is the development of techniques for using trapped $^{43}\text{Ca}^+$ ions for quantum information processing.

I present a rate equations model of $^{43}\text{Ca}^+$, and compare it with experimental data. The model is then used to investigate and optimise an electron-shelving readout method from a ground-level hyperfine qubit. The process is robust against common experimental imperfections. A shelving fidelity of up to 99.97% is theoretically possible, taking 100 $\mu$s. The laser pulse sequence can be greatly simplified for only a small reduction in the fidelity. The simplified method is tested experimentally with fidelities up to 99.8%. The shelving procedure could be applied to other commonly-used species of ion qubit.

An entangling two-qubit quantum controlled-phase gate was attempted between a $^{40}\text{Ca}^+$ and a $^{43}\text{Ca}^+$ ion. The experiment did not succeed due to frequent decrystallisation of the ion pair, and strong motional decoherence. The source of the problems was never identified despite significant experimental effort, and the decision was made to suspend the experiments and continue them in an improved ion trap which is under construction.

A sequence of $\pi$-pulses, inspired by the Hahn spin-echo, was derived that is capable of greatly reducing dephasing of any qubit. If the qubit precession frequency varies with time as an $n$th-order polynomial, an $(n + 1)$ pulse sequence is theoretically capable of perfectly cancelling the resulting phase error. The sequence is used on a $^{43}\text{Ca}^+$ magnetic-field-sensitive hyperfine qubit, with 20 pulses increasing the coherence time by a factor of 75 compared to an experiment without any spin-echo. In our ambient noise environment the well-known Carr-Purcell-Meiboom-Gill dynamic-decoupling method was found to be comparably effective.
Acknowledgements

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Chapter 1

Introduction

1.1 Background

1.1.1 Ion Trapping

In 1979, not many decades since the very existence of atoms was a matter for debate \[1\] \[2\], a team at Heidelberg University isolated and observed a single Ba\(^{+}\) ion \[3\]. Suspended by radio-frequency electric fields in a vacuum, illuminated by lasers and laser-cooled to a few tens of millikelvin, such an atom is almost entirely free of the influence of other matter and thus provides an ideal laboratory for testing fundamental physical theories. The history of ion trapping goes back further, to Fischer’s trap of 1959 \[4\] and the quadrupole mass filter (essentially a linear Paul trap, like our own, but with no endcaps) that was first used for mass-spectroscopy in 1955 by Paul and Raether \[5\] \[6\]. But it is the ability to isolate individual atoms that makes the field so exciting today.

As well as the all-electric Paul traps (in various geometries) many experiments are performed with Penning traps, which use constant magnetic and electric fields to trap orbiting ions. Dehmelt and Paul won (half of) the 1989 Nobel Prize for Physics for inventing the Penning and Paul traps \[7\].

1.1.1.1 Laser-Based Studies

One major motivation for developing ion-trap technology is its potential for use in the next generation of atomic clocks. Current caesium fountain clocks boast frequency uncertainties of less than 10\(^{-15}\) \[8\], but only after about one day of averaging. This
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is because they are based on a microwave transition at 9.2 GHz; a clock based on an optical transition at $\sim 10^{14} - 10^{15}$ Hz could reach a similar level in just a few seconds. A trapped ion is almost ideal as such an optical frequency standard: with extremely good isolation, cooling to the ground state of motion and long interrogation time, Wineland et al. say, “...it does not seem unreasonable to think that accuracies and measurement precisions at or beyond 1 part in $10^{18}$ will be achieved” [9]. An example of progress is that the ratio of two ultraviolet transitions, in $^{199}$Hg$^+$ and $^{27}$Al$^+$, has been measured to a fractional uncertainty of $5.2 \times 10^{-17}$ by Rosenband et al. [10]; many other projects are underway using different ions [11, Section 3 and references therein].

Although not yet mature enough to provide a new definition of the second, optical clock research is already producing results in fundamental physics. Frequency ratios, such as that by Rosenband et al. above, depend on the fine structure constant $\alpha$. By repeatedly measuring the ratio over a period of time, changes in $\alpha$ could be detected that are predicted by various theories beyond the standard model [13]. The first ion-based measurement is by Rosenband et al. who deduce a (provisional) limit of $\dot{\alpha}/\alpha = -1.6(2.3) \times 10^{-17}$ [10], consistent with zero and competitive with other bounds from, for instance, the Oklo natural nuclear reactor [13].

Detailed quantum-mechanical calculation methods, such as multiconfiguration Hartree-Fock [14], can be tested by calculating and measuring properties of trapped ions. Excited state lifetimes [14, 15], isotope shifts and hyperfine structure [16] and gyromagnetic ratios [17] have all been used; ratios of light shifts of different levels of an ion have been measured [18, 19] but not yet calculated. Such measurements, as well as measuring transition frequencies, are also useful for calibrating astronomical observations [20, 21].

Experiments have been proposed to measure parity non-conservation in trapped ions, often Ba$^+$ or Ra$^+$. Studying violation of parity symmetry could both test the standard model, even measuring the mass of the Higgs boson, and reveal new physics such as supersymmetry [22, 23].

1.1.1.2 Laser-Free Studies

By forcing an ion to perform orbits, principally at the cyclotron frequency that is inversely proportional to its mass, a Penning trap can be used as an accurate and precise mass spectrometer. One team in this area is the SMILETRAP group at Stockholm
1.1. BACKGROUND

University, which has weighed numerous ions to relative uncertainties below \(10^{-9}\). Measuring the masses of \(^3\)He and \(^3\)H gives the tritium \(\beta\)-decay energy which is needed for measurements of the electron antineutrino mass; masses of silicon isotopes could contribute to a redefinition of the kilogramme based on atomic quantities; masses of \(^{76}\)Ge and \(^{76}\)Se help in the search for neutrinoless double \(\beta\)-decay which would violate the standard model; and the mass of \(^{133}\)Cs allows a calculation of \(\alpha\) (because the photon recoil of caesium atoms has been measured [24] [25].

A similar technique has been used with antimatter. The TRAP collaboration (and later, ATRAP) at CERN has operated a succession of Penning traps over ten years, measuring the relative masses of protons and antiprotons, and improving the experimental precision by a millionfold over that time to show they are approximately equal to 90 parts-per-trillion [26]. The gyromagnetic ratio \(g \approx 2\) has been measured in electrons and positrons, providing further tests of fundamental physics [27, 28].

1.1.2 Quantum Computing

Richard Feynman gave a keynote address at the 1981 MIT Physics of Computation conference, and created a new area of physics [29]. He proposed a universal quantum simulator – a quantum system that could simulate or calculate the behaviour of any other system – and argued that such a thing was needed because the state space of an interesting quantum system is in some senses too large for normal, classical computers. For instance, suppose one wants to simulate a set of \(n\) interacting particles, each of which can be in two states \(|1\rangle\) or \(|0\rangle\). For classical particles, we would simply choose one of the \(2^n\) possible starting states and perform the simulation, and the problem reduces to some kind of numerical integration or similar. But quantum particles can be in superpositions such as \((|1\rangle + |2\rangle)/\sqrt{2}\), and the phenomenon of entanglement means that the superposition must be considered over the system as a whole, rather than for each particle individually. Thus the calculation must work with all of the \(2^n\) states of the system: adding one extra particle doubles the calculation time.

Feynman believed the only solution was a computer that also played by quantum rules: that harnessed the massive parallelism provided by superposition and entanglement, and efficiently simulated quantum problems by scaling as fast as the problems did. He didn’t know whether a universal quantum simulator was possible, and it wasn’t shown to be true until Seth Lloyd proved it in 1996 [30, 31]. But in the meantime David
Deutsch had a subtly different idea: the universal quantum computer.

By analogy with the Church-Turing hypothesis (every “function which would naturally be regarded as computable” can be computed by a universal Turing machine), Deutsch presented a quantum version of a universal Turing machine \[32\]. He also described a toy problem that a quantum algorithm could solve faster than any classical one – this became known as the Deutsch-Jozsa algorithm \[33\], and was improved by Cleve et al. \[34\].

Arguably the most important quantum algorithms so far discovered are those that have implications for codebreaking: Shor’s factorisation algorithm for instance. The RSA public-key cryptography system depends on the fact that classical computers cannot factorise an \(n\)-digit number in time that is any polynomial function of \(n\): this is generally taken to mean that it is unfeasibly slow. The \(n\)-digit number is published and used to encrypt messages; its factors are kept secret and used to decrypt messages. Shor’s algorithm \[35\] can factorise it in time that is polynomial in \(n\), allowing the cryptosystem to be broken.

Another important algorithm is Grover’s search, which allows an unstructured list of \(n\) items to be searched in time proportional to \(\sqrt{n}\) (classical computers obviously take time proportional to \(n\) \[36\]). This speeds up solving NP-complete problems like the travelling salesman, as well as minimising functions and numerical integration \[37\] (although the efficiency gain is less than the exponential improvement of Shor’s algorithm). Stephen Jordan \[38\] has compiled a long list of quantum algorithms.

1.1.2.1 The DiVincenzo Criteria

David DiVincenzo \[39\] identified 5 key features that a useful quantum computer should have. These are:

1. **A scalable physical system with well characterized qubits.** A quantum bit (qubit) is a two-level quantum system such as a spin-1/2 particle. It is also possible to use qutrits (three-level quantum systems) and higher, making certain operations more efficient \[40\] \[41\], although the great majority of work uses qubits.

2. **The ability to initialize the state of the qubits to a simple fiducial state, such as \(|000\ldots\rangle\).**
3. **Long relevant decoherence times, much longer than the gate operation time.**

4. **A “universal” set of quantum gates.** The general rule is that one must be able to apply arbitrary single-qubit gates (rotations by any angle about any axis, which can of course be synthesized from as few as two rotations), and at least one two-qubit gate such as controlled-NOT or controlled-Z (in which a NOT gate or a phase rotation, respectively, is applied to one qubit if-and-only-if the second, control qubit is in state $|1\rangle$). A quantum computer might be more efficient if a wider variety of gates (such as controlled-NOT with more than one control qubit) is possible.

5. **A qubit-specific measurement capability.**

### 1.1.2.2 Decoherence and Error Correction

A classical computer has a negligible error rate for its fundamental operations, but quantum computers will probably be much less robust. Peter Shor and Andrew Steane independently developed quantum error correction: a set of subtle techniques for separating the error from the computer’s state, so that the error can be measured and corrected without disturbing the delicate superpositions and entanglements of the state itself. Nielsen and Chuang [42] has a detailed account of the subject.

The basic idea is to encode a single logical qubit $(a|0\rangle + b|1\rangle)$ in several logical qubits. The simplest scheme, for example, “copies” one logical qubit onto three physical qubits $a|0\rangle + b|1\rangle \rightarrow a|000\rangle + b|111\rangle$. After being stored for a time, or transmitted along a noisy channel, the encoding process is repeated and two of the qubits are measured. The measurements obtained tell us whether or not one of the qubits was flipped, and which one it was. This allows us to correct the remaining qubit if necessary, and restore the original state. This scheme can only correct single bit-flip errors, but it is possible to make more complex codes that can correct any general error, even complete loss of a physical qubit.

Fault-tolerant quantum computing extends error-correction to the quantum gates.

---

1. Of course, it is impossible to truly copy a qubit. $(a|0\rangle + b|1\rangle) |0\rangle \rightarrow (a|0\rangle + b|1\rangle) (a|0\rangle + b|1\rangle)$ is banned by the no-cloning theorem ([13][14] and [12] Box 12.1)); but $(a|0\rangle + b|1\rangle) |0\rangle \rightarrow (a|00\rangle + b|11\rangle)$ can be done, and is the basis of quantum error correction.
CHAPTER 1. INTRODUCTION

The logical qubits remain encoded throughout the computation, and each logical gate is made up of many physical gates. The error rate of the logical gates can be made as low as desired, provided that the physical-gate error probability is below some threshold. The threshold is typically estimated to be around $10^{-4}$, well below the error rate of current experimental gates.

1.1.2.3 Implementations

Numerous physical systems have been proposed for implementing quantum computing (QC). Trapped ions are, of course, the main subject of this thesis and will be considered separately. Other important systems include nuclear magnetic resonance (NMR), using the spins of nuclei in (usually liquid) molecules as qubits. An NMR machine has used a 7-qubit molecule to perform Shor’s algorithm and factorise 15 [45], the largest number of qubits so far used in any quantum algorithm. However there are doubts about its ability to scale to larger processors [46].

Photons having, say, two orthogonal polarisation states, have been used as qubits, with two groups having demonstrated 2-qubit Grover searches [47, 48]. Most QC proposals use the “circuit model”, where quantum gates, measurements etc. are consecutively applied to the qubits. This turns out to be highly inefficient with photons because they can only be entangled with a small probability [49]. Instead, the Grover implementations used “one-way” quantum computing: photons were created in a specific entangled “cluster” state, and then the algorithm was performed just by measuring the photons (carefully choosing which photons to measure, and in what basis). A recent review of one-way QC is by Briegel et al. [50].

Solid-state systems, such as quantum dots in semiconductors or superconducting circuits, are very attractive in terms of being potentially highly scalable. However, they currently have very high decoherence rates. Recently a two-qubit superconducting processor was used to perform the Deutsch-Jozsa and Grover’s algorithms [51].

There are also ideas such as topological QC, in which quasiparticle “anyons” are moved around each other to perform gates that could be highly resistant to errors [52]; or adiabatic quantum computing, in which a Hamiltonian is slowly altered so that the final ground state encodes the solution to the problem [53].
1.1.3 Quantum Computing with Trapped Ions

Ion trapping is one of the most advanced and promising implementations of quantum computing. It is advanced because most of the DiVincenzo criteria have been demonstrated, along with some simple algorithms; and it is promising because there is much progress being made towards scaling up to a full scale computer, and reducing error rates below the error-correction threshold. Häffner, Roos and Blatt have recently published a comprehensive review of the subject [54].

1.1.3.1 DiVincenzo Criteria applied to Trapped Ions

A scalable physical system with well characterized qubits. A qubit is stored in two Zeeman states of an ion’s ground energy level (using the electron’s spin); or in two hyperfine-split levels (using the combined nuclear and electron spins); or in two energy levels separated by an optical-frequency transition. Optical qubits have the disadvantage that the upper level usually has a significant decay rate (e.g. 1/1.17 s for a qubit in the $S_{1/2}$ and $D_{5/2}$ levels of Ca$^+$. [55]), setting a hard limit to the coherence time.

If an ion has hyperfine structure, it is possible to choose two qubit states whose separation becomes independent of the magnetic field (to first order) at some choice of magnetic field. These are often called “clock states” because of their obvious application in atomic clocks. Such a qubit is highly resistant to magnetic field noise. The states can be in the ground level, or separated by an optical transition.

The ability to initialize the state of the qubits to a simple fiducial state, such as $|000\ldots\rangle$. Ion qubits are easy to initialise by optical pumping – illuminating the ion with light of a single polarisation or frequency so that the ion enters a dark state. A naïve method, such as simply using polarised light, may not be able to reach the fault-tolerance threshold (in that case, because even small amounts of polarisation impurity can significantly reduce the fidelity). 99.9% accurate state preparation was achieved by the Innsbruck ion-trap group by exploiting the frequency selectivity of a narrow quadrupole transition [56].

Long relevant decoherence times, much longer than the gate operation time. Qubits stored in ground-level clock states can have very long coherence times. In $^{171}$Yb$^+$, a $T_2$ (phase-coherence) time of 2.5(3)s was measured [57], while our group used $^{43}$Ca$^+$.
and could detect no decoherence over 1 s \cite{58}. Both experiments used spin-echo pulses to compensate for static errors in the qubit frequency (Langer et al. \cite{59} achieved $T_2 = 14.7(1.6)$ s in $^9$Be$^+$ even without a spin-echo). In the extremely stable field of a Penning trap, coherence times of several minutes have been observed \cite{60} (the other experiments were in Paul traps). These times are far longer than current experimental gate times of $10^{-5}$-$10^{-4}$ s (see below). As technology improves it seems very likely that gates will get faster (as motional frequencies of traps increase) and coherence times longer (as magnetic field stabilisation improves, or high-field clock states are used).

**A “universal” set of quantum gates.** Single-qubit gates seem straightforward: a coherent pulse of laser light, microwaves or radio waves are applied to drive Rabi oscillations between the qubit states. The difficulty comes with individually addressing ions that may be separated by just a few $\mu$m. If using lasers, the beams can be tightly focused on the ions; the ion spacing can be increased during certain portions of the algorithm to make this easier \cite{61,62}. Longer-wavelength radiation cannot be focused so the ions must be distinguished in frequency space, either by a magnetic field gradient \cite{63,64} or by using a laser beam to selectively light-shift a certain ion \cite{65}. In a microtrap, it may be possible to use DC voltages on the segmented electrodes to push selected ions radially so that they experience micromotion; the resulting sidebands allow a laser to selectively address them despite illuminating all ions in the string \cite{66}.

Multi-qubit gates (almost always two-qubit) require the ions to be coupled by a “bus”: a single quantum mode that the ions can couple to in a controlled manner. In most cases, two ions interact via their Coulomb repulsion and share a motional mode. Lasers are used to state-selectively couple the ions to the mode, and the bus mediates a phase shift or bit-flip.

There are three common two-qubit gates. The Cirac-Zoller gate was the first to be invented \cite{67} (effectively initiating the field of trapped ion QC), and the core steps were experimentally demonstrated the same year \cite{68}. One of the qubits is directly mapped to the motional mode using a sideband $\pi$-pulse. The second qubit is then driven around a complete $2\pi$ Rabi oscillation with some auxiliary energy state, this pulse being tuned so that it only occurs if the ions’ motion is excited, and the ions pick up a differential phase shift of $\pi$. Then another sideband pulse on the first ion undoes the motional excitation. The upshot is a two-qubit phase gate, enough for universal QC. Cirac-Zoller
gates (with a modification to the $2\pi$ step) have been performed with 92.6(6)\% fidelity at Innsbruck [69] using optical qubits in $^{40}\text{Ca}^+$, each gate taking 500 $\mu$s. The Cirac-Zoller gate requires single-ion addressing and good ground-state cooling of the motional mode.

A Mølmer-Sørenson gate [70] is much less sensitive to the motional mode’s temperature and does not need single-ion addressing. Two laser beams illuminate the ions equally such that the light’s sum frequency is twice the qubit splitting, but with each individual beam tuned close to (but not resonant with) a motional sideband (one to a red sideband, the other to a blue). The effect is to produce Rabi oscillations of the collective two-qubit state, and this leads to a universal two-qubit gate. Innsbruck have used this gate to entangle two $^{40}\text{Ca}^+$ optical qubits, with a fidelity of 99.3(1)\% and a gate time of 50 $\mu$s [71]; and also two $^{43}\text{Ca}^+$ optical clock states, with a fidelity of 96.9(3)\% and a gate time of 100 $\mu$s [72]. The ion-trap group at the University of Michigan have created all four Bell states with average fidelity 79\% and a gate time of 80 $\mu$s [65]; they used clock-state hyperfine qubits in $^{111}\text{Cd}^+$.

The third common gate, called a “geometric phase gate” or “wobble gate”, is a variant of Mølmer-Sørenson – whereas the Mølmer-Sørenson gate minimises the excitation of the motional mode at all times, the wobble gate causes a large motional excitation but minimises its effect on the (populations of the) qubit states. The lasers are used to apply a state-dependent force to the ions that forces them into a wobbling motion, as the name suggests, and that motion causes a phase shift. I give a longer description in section 5.1. The gate was first described and implemented by the National Institute of Standards and Technology (NIST) in Boulder, Colorado. They produced an entangled Bell state with 97\% fidelity in $^9\text{Be}^+$ hyperfine qubits [73], with a gate time of 39 $\mu$s. Our group has achieved 83\% fidelity with $^{40}\text{Ca}^+$ Zeeman qubits [74, 75], using a gate time of 88 $\mu$s. Wobble gates have the same advantages as Mølmer-Sørenson gates, and could also be performed faster for a given fidelity. However the standard wobble gate will not work with clock states [76], and although a variant [77] overcomes this problem it has yet to be tested.

A bonus of both the wobble and Mølmer-Sørenson gates is that they can be used to entangle multiple ions at the same time. NIST have used a Mølmer-Sørenson gate to entangle up to four ions [78], and a wobble gate to entangle up to six [79]. Note however that the Innsbruck group created entangled states of up to eight ions using individual ion addressing, more like the Cirac-Zoller method [80].
Alternative gate methods have been performed or conjectured. For instance, a strong magnetic-field gradient would allow the qubit and motional states to be coupled using microwave radiation, leading to laserless two-qubit gates [S1]. This eliminates photon-scattering as a source of decoherence, and takes advantage of the fact that it is much easier to generate and control highly-coherent microwaves than light.

A qubit-specific measurement capability. Almost all trapped-ion experiments perform readout by fluorescence. Laser light is shone on the ion(s) such that one qubit state scatters photons, and the other is dark. Viewing the ion with a photomultiplier tube (PMT) or a camera allows the state to be deduced with extremely high accuracy. For a $^{40}$Ca$^{+}$ optical qubit our group achieved an average fidelity of 99.99% in 145 µs [S2]. That is an example where the dark state is a metastable level; that level is often called the “shelf”. Electron-shelving was invented by Dehmelt [S3], who proposed using it to measure the frequency of the 202.2 nm transition in Tl$^{+}$. To measure a Zeeman or hyperfine qubit, it must first be mapped to an optical qubit. This thesis describes readout of a $^{43}$Ca$^{+}$ hyperfine qubit in this manner, with 99.77(3)% fidelity (Chapter 4) experimentally achieved with a 400 µs shelving pulse and simulations predicting that both fidelity and speed can be greatly improved.

Several ions can be simultaneously read-out by imaging the fluorescing ions onto a camera. The ions’ images, not being point-like, will overlap to some extent; but a well-designed (classical) algorithm can deduce the states with the minimum of cross-talk. Our group has used an electron-multiplying Charge-Coupled Device (CCD) camera to read-out from four $^{40}$Ca$^{+}$ optical qubits. Even though $\approx 4\%$ of the signal at one ion comes from its nearest-neighbours, an iterative maximum-likelihood analysis method was developed such that cross-talk contributed only $1(1) \times 10^{-3}\%$ to the detection error [N4].

If readout is poor, a full-scale quantum computer could easily improve it by “copying” one qubit onto several ancillae and measuring them all – relying on the high-fidelity of multi-qubit gates. A variant of this process was demonstrated at NIST. The state of a $^{27}$Al$^{+}$ optical qubit, which cannot practically be read-out by a direct method, is transferred to a $^{9}$Be$^{+}$ ion using a motional bus, and then the beryllium ion’s state is measured by fluorescence detection. Each cool/transfer/measure cycle takes 2 ms and has $\approx 85\%$ fidelity. But the aluminium qubit’s state is not affected by the transfer (other
than collapsing to one the qubit eigenstates, losing any entanglement or superposition it had), so the process can be repeated for a maximum of 99.94% fidelity in \( \approx 13 \text{ ms} \) [85].

The speed of the above methods is fundamentally limited by the ion’s fluorescence rate, but Stock and James [86] have proposed a method that avoids this problem for rapid readout from \( \text{Ca}^+ \). Monochromatic light near 397 nm, 383 nm or 403 nm could drive a four-photon transition that ionises an ion in the \( 4S_{1/2} \) level, but has no effect on the \( 3D_{3/2} \) and \( 3D_{5/2} \) levels. The electron released on ionisation is collected by an electrode (under the influence of the ion-trap’s electric fields, which do not form a trapping potential for an electron) and can be detected by electronics. They estimate readout times of 3 ns and efficiencies > 99%.

### 1.1.3.2 Other Progress with Trapped Ions

Some simple algorithms have been demonstrated. Innsbruck, NIST and Michigan have all demonstrated teleportation of quantum information between ions [87, 88, 89] with respective fidelities 83(1)\%, 78\% and 90(2)\%. The experiments show an interesting contrast: the Innsbruck and NIST teams used two-qubit gates to make the entangled pair that forms the quantum channel for the teleportation protocol. The Michigan team stored two \(^{171}\text{Yb}^+\) hyperfine clock qubits in separate traps 1 m apart, collected photons from the ions into optical fibres and performed Bell-state measurements on the photons: this allowed teleportation from one ion to the other, but could also be generalised into a (non-deterministic) two-qubit gate [90]. The entangling gate only succeeded when a particular photon state was measured, which happened with probability \( \sim 10^{-8} \), although the post-selected fidelity was 89(2)\%.

The basic three-qubit quantum error-correction protocol, described in Section 1.1.2.2, was implemented at NIST [61] on \(^9\text{Be}^+\) hyperfine qubits. Although extremely far from the error-correction threshold (the procedure introduced infidelity of \( \sim 20\% \)), they showed that it could correct bit flip errors. Repetitive error-correction – where a qubit is kept alive for several rounds of correction – has not yet been demonstrated; nor has any more advanced correction protocol. The same group have performed a three-qubit “semiclassical Quantum Fourier Transform” (QFT) [62], a simplified version of the full QFT that is used in Shor’s algorithm. Apart from the initial preparation, a three-qubit entangling gate that also sets the input for the QFT to analyse, the semiclassical QFT uses only measurements, classical communication and single-qubit gates.
Extremely basic quantum simulations have been performed. In Garching, two $^{25}\text{Mg}^+$ hyperfine qubits were used to simulate a magnetic material changing from paramagnetism to ferromagnetism [91]. The wobble gate was used to simulate the spin-spin interaction.

1.1.3.3 Scaling up

A working trapped-ion quantum computer would probably have to use the “quantum CCD” architecture [92]. Instead of storing thousands of ions in a long string, an array of many small ion traps would be micro-fabricated on a chip. The DC electrodes of the traps would be segmented, allowing the ions to be moved around by changing the voltages. Ions would be brought together, a gate would be performed, the ions would be separated, and then moved to storage regions, readout regions or to another gate. Such movements would heat up the motional modes and reduce gate fidelity, so sympathetic cooling [93] would be important. Coolant ions of a different species would be brought into the same potential well as qubit ions, and laser-cooling applied to the coolant ions.
1.2 Structure of this Thesis

The general theme of this thesis is improving the fidelity of basic operations with trapped ions. The problem is addressed directly, by simulating and implementing high-fidelity readout and dynamical decoupling; and indirectly, by developing simulations and practical experience of the isotope $^{43}\text{Ca}^+$. Until recently our group has worked with the most common calcium isotope, $^{40}\text{Ca}^+$, which has no hyperfine structure and so is simple to work with. As mentioned above, $^{43}\text{Ca}^+$ has hyperfine structure and so allows qubits with long coherence times [58]. We thus expect to do many of our future experiments with this isotope. So far our $^{43}\text{Ca}^+$ work has been limited to coherence-time measurement [58, 97] and sympathetic cooling [93].

Chapter 2 describes the apparatus that we have used – the trap itself, the control system, lasers, signal generators and imaging system. I also present supplementary experiments that measure the extinction provided by our optical switches, and observation of unwanted polarisation variability in one of our beams.

Chapter 3 presents rate-equations simulations of $^{43}\text{Ca}^+$. The background theory, atomic data and computational details are presented, along with comparisons between theory and experiment. I calculate certain off-resonant excitation processes that are relevant to our experiments.

Chapter 4 describes high-fidelity readout of $^{43}\text{Ca}^+$, with simulations and experiments.

Chapter 5 describes an attempt to perform an entangling quantum gate between one $^{40}\text{Ca}^+$ ion and one $^{43}\text{Ca}^+$ ion. This has potential value as part of a readout-free quantum error-correction protocol. Unfortunately our attempt was unsuccessful, and the rest of the chapter describes various noise problems with our apparatus.

Chapter 6 presents theoretical and experimental work on dynamical decoupling. Dynamical decoupling is an extension of the basic spin-echo sequence that has recently
received much interest as a method of increasing the phase-coherence times of qubits.

Chapter 7 concludes and describes prospects for future work.
Chapter 2

Apparatus

Our experiments can be summarised as manipulating ions, and recording the results. The ions themselves are singly-ionised calcium ions (Ca\textsuperscript{+}, often written as Ca-II). They are suspended by electric fields in ultra-high vacuum. Manipulations are performed with up to ten lasers (and their attendant optics), microwaves and radio waves. Results are recorded by collecting light from the ions with a series of lenses, and detecting the light with a charge-coupled device (CCD) camera or photomultiplier tube (PMT). The lasers, detection system etc. are all outside the stainless-steel vacuum chamber; the chamber has windows and feedthroughs to allow light and electrical signals in and out. A personal computer (augmented with specialist scientific electronics) controls the experiment and saves the resulting data.

I shall start by introducing the calcium ion itself, and then go on to describe the ion trap and the rest of the apparatus.

2.1 Calcium

2.1.1 Notation

$P_{3/2,-1/2}$ specifies the ($M_J = -1/2$) Zeeman state of $P_{3/2}$ in $^{40}\text{Ca}^+$. 

$P_{1/2}^{1,+4}$ means the ($F = 4$, $M_F = +4$) hyperfine state of $P_{1/2}$ in $^{43}\text{Ca}^+$. 

$P_{1/2}^4$ means the entire ($F = 4$) hyperfine manifold of $P_{1/2}$ in $^{43}\text{Ca}^+$. 

$P_{3/2,3,4}^{3/2}$ refers collectively to the ($F = 2, F = 3, F = 4$) hyperfine manifolds of $P_{3/2}$ in $^{43}\text{Ca}^+$. 

I will refer to “levels”, by which I mean the fine-structure levels such as $4P_{1/2}$ and $3D_{5/2}$; “manifolds”, by which I mean the hyperfine-structure levels such as $4P_{1/2}$ or
3D$^{1/2}$; and “states”, by which I mean states of specific magnetic quantum number such as 4P$^{1+1}$ or 3D$_{5/2}$, $-3/2$.

### 2.1.2 Levels and Transitions

![Figure 2.1: The low lying energy levels of a Ca$^+$ ion that are used in our experiments. Lifetimes ($\tau$) of the levels \cite{14, 55, 98} and branching ratios (Br) of the transitions \cite{20} are labeled. 4S$^{1/2}$ is labeled with the hyperfine splitting (for $^{43}$Ca$^+$) or the Zeeman splitting per gauss (for $^{40}$Ca$^+$).](image)

Figure 2.1 shows the energy levels and transitions of a calcium ion. They fall into three broad groups depending on what we use them for:

**S$_{1/2}$** We use qubits which are stored in ground states of the ion. In $^{40}$Ca$^+$, the two Zeeman substates of S$_{1/2}$ are the qubit states $|\uparrow\rangle$ and $|\downarrow\rangle$. In $^{43}$Ca$^+$, the hyperfine interaction splits S$_{1/2}$ into two manifolds separated by 3.23 GHz. We can use any of the pairs (S$^{4,+4}_{1/2}$, S$^{3,+3}_{1/2}$), (S$^{4,-4}_{1/2}$, S$^{3,-3}_{1/2}$) or (S$^{4,0}_{1/2}$, S$^{3,0}_{1/2}$) as a qubit. The latter choice provides a “clock” qubit whose frequency is insensitive to the magnetic field to first order, allowing quantum information to be stored for long periods with high
2.2. TRAPPING IONS

The experiments described in this thesis were performed using a linear Paul trap. Paul traps confine ions using an oscillating electric quadrupole field (usually at radio frequencies, RF) – in the linear version, this field is produced by four long electrodes arranged in a square (Figure 2.2). Each electrode is at the same RF phase as its diagonally opposite partner; the pairs are in antiphase with each other. Averaged over a cycle of the field, an ion feels a harmonic pseudopotential well centred on the null point of the field. The RF null of a linear Paul trap is a line parallel to the electrodes – this defines the trap axis \( z \), and the RF confines the ion only in the perpendicular, radial directions.

Higher-order multipoles can also be used as ion traps [99].
Two endcap electrodes are placed at the ends of the trap, separated by 7.2 mm. The endcaps are raised to a positive voltage (if, as in our case, the ion is positively charged) producing a potential well that confines the ion in the $z$ direction. The radial ($\omega_r$) and axial ($\omega_z$) secular frequencies of the ion (i.e. the frequencies of the harmonic pseudopotential wells) can be set separately within a wide range, although an ion of a given charge:mass ratio will only be stably trapped for a certain range of voltages and RF frequencies \cite{100,101}.

Stray static electric fields are usually present and cause the equilibrium position of the ion to be not quite at the RF null point. It hence feels an oscillating force from the RF field, causing “micromotion” at the RF frequency that could be severely detrimental to high fidelity quantum operations\footnote{In theory, because micromotion is coherent with the RF drive, the laser frequencies could be modulated to track the Doppler shift. Micromotion also manifests as sidebands on the laser transition and a change in Rabi frequency, both of which can be measured and taken into account, or even be used deliberately \cite{102,66}. But if more than one ion is trapped, micromotion can cause unwanted motional...}. We balance out those stray fields using a further set...
2.2. TRAPPING IONS

of electrodes placed in a square outside, and parallel to, the RF electrodes. DC voltages are applied to these to push the ion back into the RF null. In fact, we only need to use the top two electrodes, the bottom pair being grounded (or used as a microwave antenna, see Section 2.5.3). The procedure for setting the compensation voltages is described in section 5.3.1.

The RF frequency is generated by a Colpitts oscillator with a fixed frequency of 6.4 MHz, with no further resonator or amplifier. It has two equal-amplitude outputs, 180° out-of-phase, that drive the two pairs of RF electrodes. This arrangement is atypical; linear Paul traps are often driven by oscillators with a single RF output, connected to one diagonal pair of electrodes with the other pair grounded. Our oscillator’s amplitude can be varied manually (but not controlled by computer) up to \( \approx 170 \text{ V}_{\text{pk-pk}} \). The voltages on the endcaps and the top two compensation electrodes are independently variable by computer up to \( \approx 700 \text{ V} \), limited by breakdown of the vacuum feedthrough; typical values 250-700 V for endcaps, < 100 V for compensation electrodes.

When various ion traps are compared [103, Figure 8 in preprint], the heating rate of the ions is found to be approximately inversely proportional to the 4th power of the trap size – usually defined as the smallest distance between an ion and any electrode [104, 105]. In this trap the RF electrodes are closest to the ions, and the distance is 1.22 mm (Figure 2.2).

2.2.1 Tickling

The secular frequencies of an ion are most conveniently measured by “tickling”. We apply an oscillating voltage to an endcap (to measure axial frequencies) or DC compensation electrode (to measure radial frequencies), and scan its frequency while monitoring the ion’s fluorescence. When the applied frequency is close to a motional frequency, the ion will be driven into large oscillations that modify the ion’s fluorescence signal (or that are visible with the camera). The quality factor of these oscillations is high (\( Q \sim 2000 \)) so they can be measured precisely (to \( \pm \sim 0.2 \text{ kHz} \)), but also care must be taken to avoid driving the ion out of the trap. For the axial mode (the centre-of-mass mode, if there is more than one ion), the resonance is just visible for tickle voltages \( \sim 0.2 \text{ V}_{\text{pk-pk}} \); radial modes are just visible at \( \sim 1 \text{ V}_{\text{pk-pk}} \). Much larger amplitudes are used if the frequency is unknown in advance, so that the resonance becomes visible in a coarse scan.
The radial pseudopotential is often assumed to be symmetrical, but we have been able to measure two slightly different radial frequencies as shown in Figure 2.3. This can happen due to accidental asymmetries in the construction of the trap, or stray nonuniform DC electric fields. Non-degenerate radial frequencies are actually necessary: if they were degenerate, then the principal axes of the radial modes can be in any orientation. Applying a Doppler cooling laser beam can define these axes perpendicular and parallel to the beam\(^3\). The ion can then remain hot in the direction perpendicular to the beam. Ion trap designers often choose the radial modes to be non-degenerate, and to have principal axes at 45° to the Doppler cooling beam. This forces the ion’s radial vibrations to precess, and so both modes are cooled\(^{[12]}\).

![Graph](image)

Figure 2.3: Radial secular frequencies of a single \(^{40}\)Ca\(^+\) as a function of trap RF amplitude. Dotted lines indicate 50% confidence intervals of the linear fits. The micromotion compensation was readjusted for every data point. The endcap voltages were constant at 240 V and 238 V producing an axial frequency of 470 kHz for all the RF voltages.

\(^3\)More precisely, parallel to the projection of the beam onto the trap’s \(x - y\) plane.
2.2. TRAPPING IONS

2.2.2 Loading

Near the trap is an oven, consisting of a thin-walled stainless-steel tube, loosely packed with calcium granules and with a small hole in the side pointing towards the centre of the trap. To load ions into the trap the tube is first heated by passing current (between 4 and 5 amps) through it; it heats up and sprays calcium atoms towards the trap. Two lasers, at 423 nm and 389 nm, are used to ionise some of the atoms in a two-photon process. The 423 nm beam (from a grating-stabilised external-cavity diode laser) excites the atoms on the $4s^2 \, ^1S_0 \rightarrow 4s4p \, ^1P_1$ transition. The natural width is 35 MHz, and we take care to cross the atomic and laser beams at right angles to minimise Doppler broadening: we observe the transition with a full-width half-maximum (FWHM) of 76 MHz. The smallest isotope shift of this transition (between Calcium-43 and Calcium-44) is 160 MHz, so it is possible to excite predominantly one desired isotope. From $4s4p \, ^1P_1$ an atom will be ionised by a photon of wavelength less than 389.8 nm; we provide this light with an unstabilised 388.9 nm diode laser (with no external cavity). If an atom is ionised near enough to the centre of the trap, and if correctly tuned Doppler-cooling beams are applied, it will be caught.

$^{40}\text{Ca}^+$, having 97% natural abundance, is relatively easy to load. $^{43}\text{Ca}^+$ is much more challenging because it makes up only 0.135% of natural calcium. We use much higher intensity 389 nm light than for $^{40}\text{Ca}^+$, and higher oven temperatures. We can also ensure that only $^{43}\text{Ca}^+$ ions are cooled by tuning the 397 nm Doppler laser just red of the $S^1_{1/2} \rightarrow P^1_{1/2}$ hyperfine component of the transition, which is blue-detuned from all other stable isotopes as shown in Figure 2.4 (the Doppler cooling laser must have 3.22 GHz sidebands when working with $^{43}\text{Ca}^+$; one sideband is red of all the other isotopes in this situation, but its intensity is less than the carrier and so the net effect is still to heat unwanted isotopes so they are not trapped). Full details of our loading method can be found in Reference [106].

For the $^{40}\text{Ca}^+ - ^{43}\text{Ca}^+$ experiments of Chapter 5, we would first load the $^{43}\text{Ca}^+$. We then retuned the ionisation and cooling lasers for $^{40}\text{Ca}^+$, reducing the laser powers and oven temperature so that the loading rate was $\sim 1$ per minute, allowing us to load a single ion.

While the oven is on, the magnetic field at the ion is altered (by $\sim 0.05$ G), presumably because the hot metal becomes magnetised by ambient fields or by the oven
Figure 2.4: The isotope shifts $\Delta$ of the 397 nm transitions in the stable isotopes of calcium, relative to $^{40}\text{Ca}^+$, are shown by the dotted lines and labeled by their mass numbers. For $^{43}\text{Ca}^+$ the four hyperfine components are shown as solid lines, labeled with $F_{S_{1/2}} : F_{P_{1/2}}$. Taken from [106].

current itself. When the oven is turned off, the field drifts exponentially back to its original value within about 2 hours. A 0.05 G field Zeeman-shifts a $^{40}\text{Ca}^+$ ground-state qubit by 140 kHz, so we must wait for the field to settle before attempting experiments that depend on frequency stability [74, 97].

2.2.3 Vacuum

The trap is housed in a stainless-steel vacuum chamber, maintained at $\approx 1.0 \times 10^{-11}\text{torr} = 8 \times 10^{-14}\text{Pa}$ by an ion pump and a getter pump. The pressure is approximate; it is measured by an ion gauge, and such values are at the lower limit of its sensitivity.

Ions can be kept in the trap for several days (once for over a month), the most common loss mechanism being a Doppler-cooling laser hopping to a mode that is blue-detuned, and hence heating the ion. In contrast, a micro-fabricated trap tested by our group achieved calcium ion lifetimes of only a few minutes, probably because the pressure was relatively high ($\approx 1 \times 10^{-9}\text{torr}$) [94, Section 6.3].

2.3 Computer Control

The experiment is controlled by a computer program called PC. It is written in Turbo Pascal and runs under MS-DOS – the group has taken this approach rather than, say, Labview under Windows, because it allows us to turn the computer’s interrupts off during an experimental sequence. This makes the timing reliable enough that the computer can control the experiment in real time, with $\sim 0.1\mu\text{s}$ precision or better.

PC, together with various interface cards connected to the computer, has the following capabilities:
• It records photons that are detected by the PMT, counting how many fall within definable-length time bins.

• It records analogue quantities such as photodiode measurements of laser powers.

• It sets and scans Digital-to-Analogue Converters (DACs) that control the trap DC electrodes, laser frequencies, etc.

• It has “pseudo-DACs” for digitally controlling the frequencies and phases of our high-precision synthesisers (for Raman or microwave transitions), using RS-232 serial ports.

• When necessary, it monitors the 50 Hz mains signal so that sequences can be triggered at the same phase of the AC (to reduce magnetic field uncertainty, see Section 6.4.1).

• When necessary, it monitors correlations between the trap RF and photon arrival times, to allow micromotion compensation (see Section 5.3.1).

• It switches on/off laser beams via Acousto-Optic Modulators (AOMs) and shutters (Section 2.4.5), and also microwaves and RF for magnetic resonance, in both cases working through the Laser Control Unit described below.

• It switches on/off the oven, photoionisation beams and trap RF, for loading ions.

It has two main modes. The default is a continuous display of the PMT count rate, photodiode readings and vacuum-system pressure. Lasers and other devices can be switched and scanned manually. A “DAC scan” uses this mode while automatically scanning a DAC over a pre-defined range, typically used to locate quickly the resonant frequency for a laser.

In the second mode, the computer runs timed sequences. A “sequence” is a series of instructions that mostly define laser or microwave/RF pulses, but can also change DACs. A sequence typically initialises the ion(s) in the desired qubit state, performs some quantum manipulations of the qubit(s), and finally performs a shelving read-out (see Chapter 4) of the final qubit state(s). A sequence is repeated with identical settings, usually between 200 and 1000 times, to obtain an estimate of the probability of the ion(s) being shelved. This produces one data point. The computer changes something in the sequence (either a DAC setting or a pulse time) according to the pre-defined scan range,
records the next point, and so on. The points collectively make up a “scan”. After each sequence, the computer plots the number of photons counted and the photodiode readings; this makes it easy for the experimenter to spot ion decrystallisations (see Section 5.2.1) or laser frequency hops. In that case the scan can be paused while the problem is fixed. At the end of the scan the data are saved.

A variant of the timed-sequence mode is “whizzo-interactive” mode. This allows the sequence to be edited between each point, for optimising parameters or quickly comparing different sequences.

### 2.3.1 Laser Control Unit

The Laser Control Unit (LCU) was designed and built by Ben Keitch \[97\]. It is the interface between the computer and the physical devices, such as the switches that pass or block the RF power to the AOMs. Most of the devices use standard 5 V TTL voltage pulses, which the LCU supplies using buffer amplifiers to accommodate devices with 50 Ω input impedances. It provides accurate synchronisation of the pulses, with the pulse times settable to 0.1 \(\mu\)s resolution. It also has a mechanical switch for each of the 16 channels, for convenient manual override.

### 2.4 Lasers

One of the advantages of using Ca\(^+\) is that we can use diode lasers to produce all the necessary wavelengths, without frequency doubling. Short-wavelength laser diodes (397 nm, 393 nm and 423 nm) have short lifetimes compared to those producing infra-red (IR) light (in the ten years since the experiment was begun, we have had two of our seven blue diodes fail, but none of the three IR diodes). They are not currently manufactured, but when stocks run out it will be possible to produce those frequencies by frequency-doubling light from IR laser diodes (indeed, this is necessary if beams of more than \(\sim 15\) mW are required).

### 2.4.1 Summary of Lasers

Table 2.1 summarises our lasers. First I state whether the laser is a commercial Toptica system or was built by the group, and whether it has a diffraction grating to provide an extended laser cavity. Then I give the nominal maximum power output of the diode,
2.4. LASERS

after the grating if there is one (the output power of a diode is limited by its ability to withstand the total optical power inside it, so if some light is reflected back into the diode its own power output must be reduced). I briefly describe its uses, and state what type of lock (if any) is used. Lasers are locked to temperature-stabilised, external reference cavities, with $\leq 1$ MHz/hr drift rates.

2.4.2 Beam Geometry and Polarisations

The geometry of the beams themselves, as they reach the ions, is shown in Figure 2.5. The four beams shown together in one line (397Doppler, 397Probe, 866 and 854) are superposed using polarising beamsplitter (PBS) cubes and a dichroic mirror. $R_{63}$ and $R_V$ are also superposed with a PBS cube; so is 397Vertical combined with the photionisation beams (which come from the same optical fibre). Each of the circularly polarised beams has a $\lambda/4$ waveplate to allow them to drive $\sigma^+$ or $\sigma^-$ transitions, or can be made linearly polarised to drive both.

The magnetic field $B$ is shown as it would be set for experiments with $^{40}\text{Ca}^+$ – carefully aligned with the 850 nm beam for high $\sigma$ polarisation purity at the ion, which is needed for the EIT readout process in that isotope (summarised at the start of Chapter 4). Readout of $^{43}\text{Ca}^+$ is actually improved if the 850 nm beam is slightly off the magnetic field direction (Chapter 4), and so for experiments with this isotope we align $B$ with the 397$\sigma$ state-preparation beam.

The vertical beams (423, 389 and 397Vertical, which is only used to detect vertical micromotion) enter the chamber through the same window that the imaging system looks through. A small black-paper flag is placed just below the imaging system’s objective lens, to prevent reflections of these beams entering the imaging system.

2.4.3 Diagnostics

2.4.3.1 Frequency Diagnostics

Every laser has a little light (20 $\mu$W to 2000 $\mu$W) split off from the beam into its own multimode optical fibre (except the 389, which is not monitored because its frequency is unimportant; the 423 and 850 lasers share a fibre with one beam blocked at any time). The fibres are connected to a HighFinesse WS/7 wavemeter via an eight-channel fibre switcher, both under the control of a Labview computer program written by David
### Table 2.1: Summary of the lasers used in the experiment.

<table>
<thead>
<tr>
<th>Name, Wavelength / nm</th>
<th>Model</th>
<th>Grating?</th>
<th>Power / mW</th>
<th>Uses and Notes</th>
<th>Lock (see Section 2.4.4)</th>
</tr>
</thead>
<tbody>
<tr>
<td>423</td>
<td>Toptica DL100</td>
<td>Yes</td>
<td>15</td>
<td>Isotope-selective excitation for photoionisation.</td>
<td>None</td>
</tr>
<tr>
<td>389</td>
<td>Home-made</td>
<td>No</td>
<td>2</td>
<td>Non-selective second stage of photoionisation.</td>
<td>None</td>
</tr>
<tr>
<td>397D40</td>
<td>Toptica DL100</td>
<td>Yes</td>
<td>15</td>
<td>Provides beams for Doppler cooling, state preparation and continuous Raman cooling of $^{40}\text{Ca}^+$ (which uses the beams 397$\sigma$ and 397Probe).</td>
<td>PDH lock via EOM</td>
</tr>
<tr>
<td>397D43</td>
<td>Toptica DL100</td>
<td>Yes</td>
<td>15</td>
<td>Provides beams for Doppler cooling and state preparation of $^{43}\text{Ca}^+$.</td>
<td>PDH lock via current modulation, with fast current feedback</td>
</tr>
<tr>
<td>866</td>
<td>Home-made</td>
<td>Yes</td>
<td>50</td>
<td>Repumps from D$_{3/2}$.</td>
<td>Side-of-fringe lock</td>
</tr>
<tr>
<td>397 Master/Slave</td>
<td>Toptica DL100</td>
<td>Yes</td>
<td>30</td>
<td>Produces the beams R$<em>\parallel$, R$</em>{63}$ and R$_V$, used for Raman transitions in $^{40}\text{Ca}^+$ (Rabi flopping, pulsed sideband cooling) and for the travelling standing wave of Chapter 5. See Section 2.4.6.2 for details.</td>
<td>None</td>
</tr>
<tr>
<td>393</td>
<td>Toptica DL100</td>
<td>Yes</td>
<td>5</td>
<td>Shelves ions during readout.</td>
<td>PDH lock via EOM</td>
</tr>
<tr>
<td>854Old</td>
<td>Home-made</td>
<td>Yes</td>
<td>25</td>
<td>Deshelves the ions, returning them to the ground level from D$_{5/2}$ after readout is complete. The grating of this laser was replaced due to falling power output, but has performed extremely poorly (it can only be tuned a small amount before modehopping).</td>
<td>None</td>
</tr>
<tr>
<td>854New</td>
<td>Toptica DL100</td>
<td>Yes</td>
<td>45</td>
<td>Temporary replacement for 854Old. This beam is delivered by optical fibre from the laboratory next-door.</td>
<td>None</td>
</tr>
<tr>
<td>850</td>
<td>Home-made</td>
<td>Yes</td>
<td>100</td>
<td>Used for readout. For $^{40}\text{Ca}^+$, it creates a dark resonance so only one of the qubit states is shelved. For $^{43}\text{Ca}^+$, it repumps the ion if it falls into D$<em>{3/2}$ rather than D$</em>{5/2}$. See Chapter 4 and Section 2.7.2.</td>
<td>Side-of-fringe lock</td>
</tr>
</tbody>
</table>
2.4. LASERS

![Diagram of laser beams]

At 26° to the vertical

Figure 2.5: A diagram of the laser beams as they enter the hexagonal vacuum chamber, showing the trap axis ($z$) and magnetic field direction (B).

Allcock [107]. The system rapidly ($\sim 10$ Hz) switches between the beams (the user can choose the set of lasers to monitor), and displays their wavenumbers. Some light is also sent to a pair of optical spectrum analysers, one for IR beams and one for the UV; a dichroic mirror ensures that light is sent to the correct analyser. The program displays the analyser trace for each beam, which can reveal multimode behaviour before the laser loses lock; it also displays the error signals from the laser locks. An alarm on each channel alerts the user when a laser loses lock or mode hops.

2.4.3.2 Intensity Diagnostics

Most beams can have their powers and spot sizes measured. A glass microscope slide picks off a small fraction of the beam and reflects it (via a beamsplitter) onto a camera and a photodiode. The camera is placed the same distance along the beam as the trap is; so it records the same beam size that the ion sees. We can thus monitor the power of the beams, and calculate their intensities. The Raman beams, and 854New, do not pass through a pickoff; the Raman beam intensities must be measured using the ion’s light shift.

The camera is also a useful check of beam alignment.
2.4.4 Locking

We need many of our lasers to have better frequency stability than they achieve passively. In all these cases we lock each laser to its own Low-Drift Etalon (made by the National Physical Laboratory, NPL). The mirrors in these cavities have “W” reflective coatings – achieving high reflectivity for both our IR and UV wavelengths (giving finesse of $\approx 30 - 520$, depending on the required linewidth). Their free spectral range (the frequency separation of cavity resonances) is 1.5 GHz.

For a side-of-fringe lock, the transmitted power through the cavity is monitored. That power has a narrow peak when the beam is resonant with the cavity. Feedback electronics are engaged to keep the laser at the frequency corresponding to about halfway up this peak – the point of maximum gradient providing narrowest laser linewidth.

A Pound-Drever-Hall (PDH) lock [97, 108] is more complicated but more robust than side-of-fringe. It is not affected by a change in the power of the laser, as side-of-fringe locks are vulnerable to. A PDH lock has a higher “capture range” of frequencies, so that a laser that makes a sudden jump (up to $\sim 100$ MHz) will be brought back to its set point rather than break out of lock. Sidebands are put on the beam by modulating the laser current, or by using an Electro Optic Modulator (EOM), and the locking signal is reflected from the cavity.

In both cases, the locking electronics feed back and adjust the frequency of the laser. All the locked lasers are grating stabilised, in the Littrow configuration. The beam straight out of the diode hits a diffraction grating at an angle chosen to be the first order diffraction angle for the desired wavelength. The first order diffracted beam is thus reflected back into the diode, the grating acting as one mirror of the laser cavity. The zeroth order is the laser’s output beam. Coarse frequency tuning is by rotating the grating in the horizontal direction. Fine frequency tuning is by translating the grating towards (away from) the laser to shorten (lengthen) the laser cavity and shorten (lengthen) the wavelength. A piezo-electric actuator can perform this fine tuning, and this is one way in which the lock controls the laser frequency. It also adjusts the current supply to the laser diode, providing faster feedback (and hence narrower linewidth) as well as reducing the probability that the laser hops to a different mode.

The 397D43 has an extra current feedback path to a field effect transistor (FET) that can alter the diode supply current extremely fast (5 MHz bandwidth). This greatly
reduces the laser jitter as deduced from the PDH error signal – from \( \pm 10 \text{MHz} \) to \( \pm 0.4 \text{MHz} \). Testing using ion fluorescence, however, was unable to detect any difference in linewidth from using the FET feedback, and suggested that the linewidth was always \( \lesssim 5 \text{MHz} \).

The reference etalons have one mirror which can be translated with piezos. We can thus change the resonant frequency of the cavity, and hence scan the laser: provided it is scanned slowly compared with the lock bandwidth, the locked laser will follow the cavity.

### 2.4.5 Switching and Fine Frequency Control

Beams are switched on and off by Acousto-Optic Modulators (AOMs). These are made from crystals whose refractive index changes significantly when the material is compressed. An acoustic wave (typically 80 MHz or 200 MHz) is passed through the crystal (as a travelling wave, rather than a standing wave) to create a travelling diffraction grating. When the wave is being driven, the \( \pm 1 \text{st-order} \) diffracted beams are Doppler shifted by \( \pm \) the drive frequency. The input beam is carefully aligned to maximise the strength of the chosen diffracted beam, and that beam then continues to the ion. The zeroth order (and any others that may be present) is usually blocked; but sometimes the zeroth order continues to the input of the next AOM (such as the 397 nm \( \sigma \) and Doppler AOMs) or a diagnostic (854Old).

Even when an AOM is nominally switched off, the diffracted beam is not perfectly extinguished. Two possible reasons include imperfect extinction of the RF drive, and scattering from the AOM crystal. The former is believed to be dominant. Section 2.7 describes some experiments that investigated AOM extinction.

For the Raman beams (\( R_{\parallel}, R_{63} \) and \( R_{V} \)), and 397Probe, the switching AOMs are also used to control the frequency. This is because the relative frequencies of the Raman beams must be variable, as well as the frequency difference between 397Probe and \( 397\sigma \) (which are used for continuous Raman cooling of \( ^{40}\text{Ca}^+ \), but will not be called “Raman beams” in this thesis). Usually, changing the frequency of an AOM causes the deflection angle to change; we prevent this by placing a lens after each of these AOMs (imaging the middle of the AOM onto the ion). The 397Probe AOM is powered by a commercial IntraAction DE series AOM driver; this has a frequency modulation input that is driven by a DAC from PC. The Raman beams are driven by versatile,
high-precision synthesers via amplifiers.

2.4.6 Laser-Specific Details

2.4.6.1 397D40 and 397D43

The lasers 397D43 and 397D40 can be used to produce four different beams: 397Doppler, 397σ, 397Probe and 397Vertical. Their optics is therefore more complex than the other beams (Figure 2.6), and so will be explained here.

![Diagram showing the 397 nm beams.](image)

Both lasers, as well as having a diffraction grating as part of their laser cavity, have a second grating to reduce the amount of amplified spontaneous emission (ASE) that reaches the ion (otherwise these lasers would produce enough light at 393 nm to shelf the ion \(\sim\) once per second [100]). Additionally, for 397D43 this grating splits off beams for the PDH lock and the frequency diagnostics. The beam from 397D40 passes twice through a “Master” AOM to improve the extinction (to better than 1 : 30 000 = \(-45\) dB [109, Table 3.3]); however each pass only deflects \(\approx\) 60% of the power. The beam from 397D43 is switched using a mechanical shutter that gives perfect transmission and extinction; however it requires careful timing when used in a timed sequence experiment (see Section 2.7.1.2).

The beams then meet at a 50% beamsplitter cube. One output leads to the 397σ and
397 Doppler AOMs, the zeroth order of the former is the input to the latter because we almost never need to use those beams at the same time. The other beamsplitter output leads to the 397 Probe AOM. The probe and Doppler beams are combined at a PBS cube. The probe beam is transmitted because it is horizontally polarised. The Doppler beam can be reflected or transmitted to any desired degree using the $\lambda/2$ waveplate, allowing the use of the vertical beam when it is needed for micromotion compensation.

### 2.4.6.2 397 Master/Slave

The Master is a grating-stabilised 15 mW laser whose light is injected into the front of the Slave diode. The Slave has no grating, but coherently amplifies the light from the Master. The pair combines the low linewidth of grating-stabilisation with the high power possible from a diode with no external cavity.

The individual beams it produces ($R_\parallel$, $R_{63}$ and $R_V$) are each switched with single-pass AOMs.

### 2.4.6.3 393

The 393 nm laser is switched by a double-pass AOM. There is a 1938 MHz EOM for simultaneous shelving of $^{43}\text{Ca}^+$ and $^{40}\text{Ca}^+$ (see Section 5.1.2).

### 2.4.6.4 866

The 866 nm laser is switched by a double-pass AOM, and has a second diffraction grating to greatly reduce the effect of ASE [55].

The 866 nm transitions of $^{40}\text{Ca}^+$ and $^{43}\text{Ca}^+$ are separated by an isotope shift of 3464 MHz, which is close to the $S_{1/2}$ hyperfine shift of $^{43}\text{Ca}^+$ (3226 MHz). This allows us to drive a second EOM from the 3220 MHz oscillator that powers the 397D43 EOM; and since the 866 nm transition of $^{43}\text{Ca}^+$ is spread over 770 MHz of hyperfine shift, we can obtain a reasonable fluorescence rate from both isotopes without retuning the laser. This is vital for doing readout from both ions during a 40-43 experiment.

### 2.4.6.5 854 Old and 854 New

854 Old is switched by a single-pass AOM. For sensitive experiments (such as the readout experiments of Chapter 4) a shutter can be used as well. 854 New is switched by a double-pass AOM.
2.4.6.6 850

The 850 nm laser is switched by a single-pass AOM. The laser and AOM are on a different optical table to the vacuum system, with the light being transferred by a polarisation-maintaining optical fibre. In Section 2.7.1.1 I describe a measurement of the extinction produced by the AOM when the beam is switched off, and Section 2.7.2 describes how the optical fibre produces periodic changes in the polarisation of the beam (which translates to power variability at the ion, because PBS cubes are used to polarise the beam after the fibre).

2.5 Coherent Manipulation

There are three main methods we can use to perform coherent single qubit operations. These are the Raman beams (in $^{40}\text{Ca}^+$), magnetic resonance at $\sim 5 \text{ MHz}$ (in $^{40}\text{Ca}^+$) and microwaves at $\sim 3.2 \text{ GHz}$ (in $^{43}\text{Ca}^+$).

We directly apply qubit rotations only if their axes are perpendicular to the $z$ axis – including $\sigma_x$ and $\sigma_y$ Pauli operators, for instance, but not phase shifts about the $z$ axis. Instead of applying a phase gate, we change the phase of the radiation that drives the coherent manipulations. The $x$ and $y$ axes are essentially arbitrary, being fixed by the phase of the first coherent pulse applied to the ion.

2.5.1 Magnetic Resonance

For us, “magnetic resonance” refers to driving the $S_{1/2,+1/2} \leftrightarrow S_{1/2,-1/2}$ magnetic dipole transition in $^{40}\text{Ca}^+$ with an oscillating magnetic field. The Zeeman splitting is $2.8 \text{ MHz/G}$, which gives $4.8 \text{ MHz}$ at $1.7 \text{ G}$. The field is produced by amplifying a synthesizer output with a Frankonia FLL 25 amplifier, emitting up to $25 \text{ W} = 44 \text{ dBm}$. The amplifier output drives a 40-turn coil which is mounted just outside the large imaging window of the vacuum chamber. The coil has two layers of 20 turns each, sits around the imaging system tube and is conical in shape to allow the vertical laser beams to pass outside it. Its resonance can be tuned from $4.1 \text{ MHz}$ to $4.9 \text{ MHz}$ using a variable capacitor in series with the coil; the resonance width is $\sim 250 \text{ kHz}$ [110]. The amplifier is particularly robust and is not affected if the RF load is a short- or open-circuit, so we do not impedance-match the coil to $50 \Omega$.

In practice the maximum power is limited by breakdown of the (air-spaced) variable
2.5. COHERENT MANIPULATION

 capacitor, and because other pieces of equipment in the laboratory (such as laser locks) start to pick up the radio signal at high powers. The highest Rabi frequency is \( \approx 5 \text{ kHz} \) (\( \pi \)-time of 100 \( \mu \text{s} \)). Such slow Rabi-flopping means that single-qubit gates are highly susceptible to magnetic field drift.

2.5.2 Raman Transitions

We achieve faster Rabi flops by driving Raman transitions between the Zeeman states. Raman transitions use two far-detuned 397 nm laser beams, whose frequency difference equals the Zeeman splitting. It is vital that the beams are coherent with each other, so we derive them both from the 397 Master/Slave laser. In this case the beams do not excite the ion to \( P_{1/2} \); instead, by a process called adiabatic elimination, coherent Rabi oscillations are driven between the two ground states [74].

The 397 Master/Slave laser is typically set to a wavenumber \( \approx 25190.3 \text{ cm}^{-1} \), a detuning of \( \approx 40 \text{ GHz} \) below the 397 nm resonance. The beams \( R_{63} \), \( R_V \) and \( R_{||} \) usually have powers from 100 \( \mu \text{W} \) to 600 \( \mu \text{W} \) each, depending on the desired Rabi frequency for the current experiment.

We used to use \( R_{63} \) and \( R_{||} \) for Raman transitions. The difference wavevector of these beams lies along the trap \( z \) axis – deliberately, so that they can be used for Raman cooling. But this coupling with the ions’ motion means that at high temperatures, the fidelity of Rabi oscillations is reduced (even if the difference frequency is tuned to the carrier transition rather than a motional sideband).

For the work of Chapter 5 we changed to using the beams \( R_{63} \) and \( R_V \). They co-propagate so we can drive qubit transitions without affecting or being affected by the ion’s motion. Beam powers of 540 \( \mu \text{W} \) gave a Rabi frequency of 200 kHz (a \( \pi \)-time of 2.6 \( \mu \text{s} \)).

2.5.3 Microwave Transitions

In \( ^{43}\text{Ca}^+ \), the magnetic dipole transition between the qubit states (the hyperfine levels of \( S_{1/2} \)) are approximately 3.2 GHz, in the microwave region of the spectrum. Dr. Keitch [97] studied the best way of driving these transitions. He tested four types of antennae mounted outside the vacuum chamber, including a magnetic loop, a \( \lambda/2 \) dipole and a cylindrical horn antenna. The horn was the best of these, and was successfully used to detect the resonance of an ion. However, superior results were obtained when the
microwave signal was applied to one of the trap’s DC compensation electrodes (in the vacuum chamber, of course) – the Rabi frequency increased by a factor of $\sim 100$ due to more efficient coupling from the antenna to the ion.

No effort was made to match impedance between the antenna and the $50\,\Omega$ output of the amplifier. The power reflected to the amplifier is $7\,\text{dB}$ (a factor of 5) lower than the power emitted, and it is not known how much of this reflection is from the electrode itself and how much is from the vacuum feedthrough. The amplifier is a Minicircuits ZVE-8G that puts out nearly $29\,\text{dBm} \approx 750\,\text{mW}$, and we can drive Rabi oscillations at up to $18\,\text{kHz}$ ($\pi$-time of $30\,\mu\text{s}$).

2.5.4 Synthesiser Network

In Figure 2.7 I show the arrangement of switches and synthesisers that control the coherent qubit operations. For the operations that demand the greatest flexibility and frequency stability from their signal generators, we use Agilent ESG synthesisers. These are either from the ESG-A series (E4422B) or the ESG-AP series (E4426B), the major difference being that the APs have higher spectral purity. They all operate from $250\,\text{kHz}$ to $4\,\text{GHz}$, and have a wide range of control options. In particular, we use three methods of controlling their output – manual (the front panel); digital, (RS-232 interface via the serial/COM port on PC); and analogue (TTL on/off as well as modulation of amplitude, phase, frequency, etc.). We use the digital interface to precisely set the synthesiser’s frequency or phase from PC, but this is too slow to use within a timed-sequence and so is limited to being changed between data points. Analogue control is fast enough to use within a sequence (typical modulation bandwidths up to $1\,\text{MHz}$), for instance to change the phase between the two $\frac{\pi}{2}$-pulses of a Ramsey experiment.

We ensure long-term stability by using a rubidium frequency reference (Stanford Instruments FS725), whose frequency has an Allan variance of $< 2 \times 10^{-12}$ over $100\,\text{s}$. It produces a $10\,\text{MHz}$ output that is used as the master clock by all our Agilent synthesizers.

Certain operations do not need such high specification synthesisers. Specifically, when we perform pulsed Raman sideband cooling we drive one of the Raman beams with Marconi 2019A signal generators. We set them manually to the desired frequency for a stretch or centre-of-mass red sideband pulse, and do not need modulation or computer control.
2.5. COHERENT MANIPULATION

Figure 2.7: The network of synthesizers and switches as used for the experiments of Chapter 5. $f_Z \approx 4.7 \text{MHz}$ is the Zeeman splitting of the $^{40}\text{Ca}^+$ qubit states; $f_H \approx 3.2 \text{GHz}$ is the splitting of the $^{43}\text{Ca}^+$ qubit states; $f_{str}$ and $f_{CoM}$ are the frequencies of the stretch and centre-of-mass motional modes; $\delta_W$ is the detuning of the “wobble” gate pulse; and $\delta$ represents the detuning that may be applied during a scan over a Raman or microwave resonance. The possible modulations are: pulse modulation (PM), a TTL switch internal to the synthesizer; analogue phase modulation ($\Phi M$); and digital control of phase and frequency by RS-232 (COM).
2.6 Imaging System

We have two reasons for observing the ions. We must be able to count how many ions are in the trap (and whether they are the desired isotope), and we must be able to measure the state of the ion(s). We typically use different instruments for each purpose – a camera is used to image the centre of the trap, allowing us to easily see individual fluorescing ions; and a PMT counts UV photons scattered by the ions, allowing high fidelity readout (as in Chapter 4 and in Myerson et al. [82]). Both devices receive light from the ions via the same imaging system. In normal operation, light is collected by a large aperture objective lens and travels up the imaging system’s light-tight tube to the PMT. There is a pinhole just in front of the PMT to reduce background counts – the lens(es) focuses an image of the ions onto this pinhole for maximum transmission. A beamsplitter (power transmission 18% at 397 nm) can be rotated into place to reflect most of the light to the camera, with the ions being imaged on the camera’s CCD.

Originally the objective focused the ions’ image several centimetres below the beamsplitter. Here there was a movable aperture (700 µm × 870 µm[100]) and a shutter. The shutter could be closed to protect the camera and PMT from bright light in the days of electron-bombardment ionisation; it is obsolete now photoionisation is used. Then there were three additional lenses before the beamsplitter, camera and PMT, which focused the light onto the instruments. Coloured-glass blue band-pass filters were used to further reduce background light. Donald [100] calculated the collection efficiency to be 0.13(2)%, and measured it (by comparing the maximum count rate from a fluorescing $^{40}$Ca$^+$ with a 3-level system rate-equations model) to be 0.11%, a figure confirmed by later work.

The imaging system was significantly simplified partway through this work (2nd April 2008) to improve the collection efficiency – each lens and filter absorbed or reflected some of the ion fluorescence we try to observe, so removing them would increase the photon count rate and make readout faster and more accurate. The movable aperture and shutter were also removed. Both versions used the same objective lens (Nikon ED PLAN 1.5x SM2-U, a compound lens with $\approx 70$ mm focal length (although the nominal value is 65 mm [100]). The system now contains only one lens (the objective), no wavelength filters and just one spatial filter (the PMT pinhole).
Also, the objective lens was moved downwards by 4 mm\(^4\), which both increases the light collection angle (and hence the collection efficiency, by \(\approx 13\%\)) and moves the ions’ primary image upwards. The geometrical collection efficiency \(\epsilon_g\) of the objective is, according to the lens specifications, given by the radius \(r_a = 17\) mm of its effective aperture and the distance from the bottom of the lens cowling to the ion \(r_d = 66(2)\) mm. Then we have

\[
\epsilon_g = \frac{\pi r_a^2}{4\pi r_d^2} = 0.0167(20) \tag{2.1}
\]

which is indistinguishable from the value in \([100]\). I have estimated the uncertainty as being the difference between the equivalently-calculated value in Ref. \([100]\) (0.016) and a value measured in that work by using a known, variable aperture (0.018(2)). It is now the primary image that is focused onto the camera CCD and PMT pinhole.

Figures 2.8 and 2.9 respectively show the old and new imaging systems.

I measured the transmission, at 397 nm, of the lenses and glass filters removed from the imaging system. A power meter was used to measure the power of a beam before and after an element, or set of elements. When using the lenses, care was taken that the transmitted spot was placed in the same position, with approximately the same size, as the laser spot measured before the lens. Results are shown in table 2.6.

<table>
<thead>
<tr>
<th>Optical element (refer to Figure 2.8)</th>
<th>Power transmission at 397 nm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Filter BG38</td>
<td>77.2(3)%</td>
</tr>
<tr>
<td>Filter BG37</td>
<td>83(2)%</td>
</tr>
<tr>
<td>Lens 50PS25</td>
<td>87.5(3)%</td>
</tr>
<tr>
<td>Lens 50DQ16</td>
<td>86.6(3)%</td>
</tr>
<tr>
<td>Lens 100DQ25</td>
<td>65.8(3)%</td>
</tr>
</tbody>
</table>

Combinations of the optical elements were also measured, suggesting that the filter and two lenses in the PMT (camera) light path transmitted only 63(1)\% (45(1)\%) of the light from a fluorescing ion. Previously the lenses’ transmission had been measured as 92\% each at 397 nm \([100]\).

We can estimate the total efficiency of the new imaging system by multiplying together:

\(^4\)The lens was moved down by 4 mm relative to its position just before the rebuilding; but it is only \(\approx 1\) mm lower than shown in \([100]\) and Figure 2.8.
Figure 2.8: The imaging system as used until 24th March 2008. This diagram is by Charles Donald [100]. All dimensions in mm.
Figure 2.9: The imaging system as used after 2nd April 2008. All dimensions in mm. Dimensions taken from or deduced from Donald [100] are shown in orange and sans-serif font; those in serif font and dark red were measured by the current author.
CHAPTER 2. APPARATUS

\[
\begin{array}{|c|c|}
\hline
\text{Transmission of window} & 0.92 \\
\text{Transmission of objective lens} & 0.73 \\
\text{Quantum efficiency of the PMT} & 0.16 \\
\hline
\text{Total efficiency } \epsilon_t & 0.18(3)\% \\
\hline
\end{array}
\]

5\% uncertainty was assumed in all the quantities except \( \epsilon_g \). Fluorescence measurements confirm that \( \epsilon_t \approx 0.2\% \).

2.7 Ancillary Experiments

Some experiments to measure the performance of specific parts of our apparatus.

2.7.1 AOM Extinction

2.7.1.1 RF Extinction of 850 nm AOM

Once, we noticed that the 850 nm laser was spuriously shelving an ion, even though the beam was off at the AOM. This beam is controlled by a 200 MHz AOM, driven by a Voltage Controlled Oscillator (VCO) that passes through an RF switch and an amplifier before being fed into the AOM. The VCO also contains an internal switch – both switches are controlled by TTL pulses from the same LCU channel. When the power supply to the amplifier was turned off, the shelving stopped. This inspired us to measure the system more carefully.

We connected the amplifier output, through 30 dB of attenuation, into an RF spectrum analyser. The internal (external) switch provided \(-40\) dB (\(-60\) dB) of attenuation when switched off individually – although the pair together only have a total of \(-70\) dB. This could be caused by the VCO radiating some RF that is picked up by the amplifier without having to pass through either switch.

A laser power meter was placed after the 850 nm’s optical fibre. The following table shows the results. The leakage when the beam is switched off by the TTL switches alone, is \(1 : 2{,}500{,}000 = -64\) dB (slightly less attenuation than the RF, presumably because the AOM is saturated with RF while in operation).
VCO Amplifier Switches Blocked

<table>
<thead>
<tr>
<th>power</th>
<th>power</th>
<th>TTL</th>
<th>with card</th>
<th>Power</th>
</tr>
</thead>
<tbody>
<tr>
<td>on</td>
<td>on</td>
<td>on</td>
<td>no</td>
<td>3.62 mW</td>
</tr>
<tr>
<td>on</td>
<td>on</td>
<td>off</td>
<td>no</td>
<td>1.5 nW</td>
</tr>
<tr>
<td>off</td>
<td>off</td>
<td>off</td>
<td>no</td>
<td>(\approx 0.8) nW</td>
</tr>
<tr>
<td>off</td>
<td>off</td>
<td>off</td>
<td>yes</td>
<td>(\approx 0.1) nW</td>
</tr>
</tbody>
</table>

The 1.5 nW could have been the cause of the shelving. However, the problem did not recur so we did not attempt to improve the extinction.

### 2.7.1.2 Extinction of 397 nm beams

The beams produced by the 397D40 laser have two stages of extinction: the beam goes through a double-pass “Master” AOM, then is split into the Doppler, \(\sigma\) and probe beams each of which has its own, independently switched, single pass AOM. A double-pass AOM is not expected to be as effective at blocking a beam as two separate AOMs, because of RF leakage effects as described in the previous section. However, this arrangement reduces leakage of resonant 397 nm light enough to allow coherence times up to \(\approx 1\) s [97].

The 397D43 laser does not have a “Master” AOM – only the individual AOMs in the three product beams. So to prevent leakage, a mechanical shutter is placed in the beam path. This provides near-total extinction of the beam. However, the experimental sequence must be carefully timed around it because it is prone to bouncing (blocking the beam when it should be open, or vice-versa) and has a variable delay 1-4 ms between receiving the open/close signal and acting.

For some of the readout experiments (see Section 4.3) a similar shutter was used in the 854 nm beam. Figure 2.10 shows the control TTL signal sent to this shutter, and the power of the beam as measured by a pick-off photodiode. Notice the wide time variability of the shutter. The 397D43 shutter is similarly variable.

This variability makes shutters awkward to use in sequences. If long coherence times are required (such as in the two-qubit gate experiments of Chapter 5 or the dynamic decoupling experiments of Chapter 6) then the shutter is essential to perfectly block the beam between the state-preparation and fluorescence-detection stages of the sequence. Otherwise photons can leak through an AOM and change the state of the ion. But shorter experiments, or those that don’t need very high fidelity, can be con-
Figure 2.10: Screenshot from a mixed-channel oscilloscope that shows the pulse sequence and beam powers as measured by pickoff photodiodes. The upper red line is the control TTL signal “∼854S” sent to the 854 nm shutter (logic low means “open”). The lower red region shows the 854 nm beam power (down means higher power). For the power measurement, the scope was set to “persist” so that previous traces stayed on the screen – that gives the lighter red area, while the darker line is the instantaneous reading. Note where the shutter has previously bounced partially closed (circled in red). For scale, the green vertical dashed lines are separated by 20 ms, the repetition period of the sequence.

Conveniently performed without the shutter. Unlike the 854 nm and 850 nm beams, the 397 nm Doppler AOM (and all the other 397 nm AOMs, except the Raman beams) are driven by commercial AOM drivers. These devices have inputs for on/off (via TTL), analogue frequency modulation (FM) and analogue amplitude modulation (AM) (as well as amplitude and frequency offset knobs), all of which can be used to block a beam.

For instance, the microwave frequency scans of Section 6.4.1 (such as Figure 6.11) were performed with the 397D43 shutter fixed open. The scans feature 500 µs-long microwave π-pulses, and the result of each is a resonance “dip” with a certain contrast. If a photon scatters off the ion during the pulse, the ion’s state will be randomised for that run of the sequence, reducing the average contrast of the scan. When the 397 beam was switched using TTL on/off alone, the contrast was very low (reducing the precision
and accuracy with which the resonance could be located). I connected the AM and FM controls to DACs so that the experimental control computer could change them during the sequence.

**FM** The driver was originally set to 84.44 MHz. The FM input accepts voltages in the range \( \pm 500 \text{ mV} \). I set the offset so that the driver gave 84.44 MHz at FM +500 mV; then −500 mV produced 109.2 MHz, a shift of 24.8 MHz. The AOM itself has a bandwidth of 20 MHz (−3 dB width), so this shift should significantly reduce the power of the deflected beam. With the TTL on, the FM alone reduced the beam power by a factor of 20. The 397 nm transition has a linewidth of 22 MHz, so the shift also detunes the leaked light. With just TTL on/off the microwave scan contrast was \( \sim 7\% \); also using the FM to detune the AOM during the sensitive part of the sequence gave contrast of 43%; using the shutter gave 77%. This shows progressive reduction in the amount of leakage light. To detune the AOM takes \( \approx 300 \mu\text{s} \), and to retune to resonance takes \( \approx 600 \mu\text{s} \) (because of a low pass filter in the signal path; the AOM driver itself has a specified slew time of 1 \( \mu\text{s} \) for the full frequency range).

**AM** The amplitude modulation (which takes inputs between 0 V and 1 V) takes only \( \approx 6 \mu\text{s} \) to rise or fall its full range, limited by the set scan rate of the DAC. It can attenuate the beam to a level undetectable by the pickoff photodiode (a factor of at least 450). Experiments were performed on a different day to those described above.

<table>
<thead>
<tr>
<th>Attenuation Method(s)</th>
<th>Contrast</th>
</tr>
</thead>
<tbody>
<tr>
<td>TTL on/off only</td>
<td>&lt;5%</td>
</tr>
<tr>
<td>TTL and FM</td>
<td>49%</td>
</tr>
<tr>
<td>TTL and AM</td>
<td>42%</td>
</tr>
<tr>
<td>TTL, AM and FM</td>
<td>50%</td>
</tr>
</tbody>
</table>

So we see that using both methods together is just a small improvement over FM or AM alone, perhaps because there is significant scattering from the AOM crystal even when there is no power input.
2.7.2 850 Polarisation

The 850 nm laser is on a different optical table from the vacuum system, with an optical fibre carrying light between the tables. The fibre was designed for use at 876 nm [111] and is monomode and (nominally) polarisation preserving. However, during our work on readout (Chapter 1), we discovered that the polarisation of light coming from the fibre varies on a timescale of minutes.

We found that the total power out of the fibre was constant to 0.2%; only the polarisation varied. But since there was a PBS cube between the fibre output and the trap, the power seen by the ion did vary, by $\sim 20\%$ as shown in Figure 2.11. The polarisation of the light entering the fibre was linear, and stable to $\sim 5\text{ mrad}$, so the variation must be caused by the fibre.

Figure 2.11 also shows the results of an optical pumping experiment, making a $^{40}\text{Ca}^+$ ion fluoresce with the 397Doppler, 854 and 850 beams. The 850 was set to $\sigma-$polarisation by setting the $\lambda/4$ waveplate, shown in Figure 2.12 to $+45^\circ$; both other beams were linearly polarised as usual. The count rate from the ion was seen to vary over a timescale of minutes, from $\sim 15$ to $\sim 400$ counts per second (cps) above background, with higher counts at lower recorded power. At linear 850 polarisation (i.e. equal $\sigma-$ and $\sigma+$), the count rate was 16 000 cps.

A rate equations simulation showed that 400 cps can be caused by an extremely low 850 intensity, $0.015I_0$. The total power was $18\ 000\ I_0$ at the times of highest fluorescence, suggesting that the polarisation impurity is $\sim 8 \times 10^{-7}$. This is surprisingly good given that PBS cubes typically transmit $\sim 10^{-3}$ of the incident light of the “wrong” polarisation [112, Page 679]. By measuring the large PBS, we estimate that it transmits 0.8% of the incident vertically polarised light.

A second, “small” PBS cube was added to the beam path as shown in Figure 2.12. The optical pumping experiment was repeated: with the waveplate at $+45^\circ$ the fluorescence was 60 cps independent of the 850 beam power (figures 2.13). When we set the waveplate to $-45^\circ$, for $\sigma+$ polarisation, the pumping was worse (about 320 cps) and the count rate was correlated with the Red PD reading (figures 2.14). However the count rate increased when the PD reading increased which suggests that this might be purely due to 850 intensity variation at the ion rather than the polarisation changing at the ion, with the polarisation impurity coming from the waveplate.
We guessed that the variation might have been caused by the lab’s air conditioning. This had been installed the previous year, to stabilise the temperature to $\approx 1^\circ C$. The cooling unit is discretely controlled (on/off) rather than continuous, a situation sometimes called “bang-bang control”. One air vent had been installed directly above the fibre, and so the fibre was subjected to periodic changes in temperature as the system switched between blowing out cold or room-temperature air. However the fibre is protected by a plastic tube for its entire length, which provides a little insulation.

No data-logging thermometer was available; but we did have a thermocouple interface unit with an “alarm” output that opens and closes a relay at an adjustable temperature. When connected to the ADC this gives a high voltage for a temperature above $18^\circ C$, and a low voltage below $18^\circ C$. Placing the thermocouple tip just below the air vent that blows over the 850 fibre, this gives a convenient record of whether the air conditioning cooler is on or off. Air is constantly blown from the vent whether or not it is being cooled: when cooling was on (off), the thermocouple registered as low as $16^\circ C$.
Figure 2.12: Layout of the 850 nm beam path for optical pumping experiments.

(up to 22°C).

The small PBS was removed to leave only the large. The power of the 850 beam (transmitted by the large PBS) was monitored. Comparing the variation in the power with the status of the air cooling clearly shows a connection. Figure 2.15 shows the power as a function of time; notice how the variation is faster during the short cold periods than during the long warm periods. This is what would be expected if the fibre’s temperature is oscillating about a constant value, with each swing causing a change in the birefringence of the fibre that causes $\approx 2$ oscillations of the polarisation.

Figure 2.16 performs a wavelet transform of this data, which shows the correlation even more clearly. A wavelet transform takes a signal (such as the 850 power) and shows how the frequency content of the signal varies with time (as opposed to a Fourier transform, that only shows the frequency content averaged over the whole length of the signal). The transform steps along the signal, and at each step attempts to fit a wavelet (a short length of a wave containing up to $\sim 5$ oscillations, such as a sine under a Gaussian envelope) to the data. If the fit has a large amplitude, the transform has a high value (shown darker grey in figure 2.16). Then the wavelet is stretched a little and the process is repeated, effectively searching for regions of the signal with a slightly lower frequency than the first scan; and so on. The resulting transform is two-dimensional, at each point showing the strength of a particular frequency component at a particular time.

For our later readout experiments (Chapter 4), we re-installed the small PBS to improve the polarisation purity of the 850. We wrapped foam insulation around the
Figure 2.13: Ion fluorescence and 850 nm intensity during an optical pumping experiment with two PBS cubes. 850 polarisation is $\sigma^-$ ($\lambda/4$ waveplate at $+45^\circ$). The horizontal dashed line indicates the background count rate of 109.3(5) cps. The fluorescence has been smoothed with a moving average filter (covering 24 0.8332 s bins). Note the inverted scale for the intensity. Figures 2.13 and 2.14 have the same (but shifted) axes scales for comparison.

... fibre where it passed closest to the vent, but power oscillation still occurred. Simulations showed the readout process to be insensitive to the 850 intensity, so it was not worth drastically re-routing the fibre to eliminate the oscillations. It is possible that slightly adjusting the polarisation of light into the fibre (perhaps making it a better match to the fibre’s polarisation-maintaining axis) may reduce the variation. However, in the laboratory next door Gergely Imreh has observed a similar phenomenon in a polarisation-maintaining fiber at 866 nm despite carefully optimising the input polarisation [113].
Figure 2.14: Ion fluorescence and 850 nm intensity during an optical pumping experiment with two PBS cubes. 850 polarisation is $\sigma^+$ ($\lambda/4$ waveplate at $-45^\circ$). The background count rate is 111(2) cps. The fluorescence has been smoothed with a moving average filter (covering 24 0.8332 s bins). Note the inverted scale for the intensity. Figures 2.13 and 2.14 have the same (but shifted) axes scales for comparison.
Figure 2.15: 850 beam power measured with only the “large” PBS. The red shaded areas show when the thermocouple has detected cold air from the vents.
Figure 2.16: The 850 power data from figure 2.15 has been wavelet-transformed. The horizontal axis is time; the vertical axis is period-of-oscillation in arbitrary units, lower frequency is at the top. The contour plot shows, for each point in time, the magnitude of each frequency present at that time, where darker is stronger. When the cooling is on (red hatched areas), the 850 power is varying at higher frequency than when the cooling is off.
Chapter 3

Rate Equations

Although our group has worked with $^{40}\text{Ca}^+$ since 1999, it had relatively little experience with the isotope $^{43}\text{Ca}^+$. Its hyperfine structure leads to significant extra complexity, and some experimental problems. For instance, the maximum observable fluorescence rate from $^{43}\text{Ca}^+$ is typically only a fifth of that achievable with $^{40}\text{Ca}^+$. Using $^{43}\text{Ca}^+$ promises significant benefits though: it can be used to provide clock-state hyperfine qubits (Section 1.1.3.1) that are resistant to dephasing from magnetic field noise. And it allows a highly accurate readout process (Chapter 4).

Being able to simulate the states and transitions of $^{43}\text{Ca}^+$ should help us to solve the problems and to exploit the benefits of this isotope. Rate equations are a simple, fast way to model an atom, and although we shall see that they are occasionally poor matches to the experiment, they will be vital for the readout optimisations of Chapter 4. This is not actually our first $^{43}\text{Ca}^+$ rate equations program – Simon Webster has also written one [110]. My version is more general, more flexible and more developed.

In this chapter I describe the theory behind my rate equations model, and some of the simulations performed with it. I will extensively use the notation described in Section 2.1.1.

3.1 Basic Atomic Theory

3.1.1 Rate Equations

Consider an ion with $N$ energy states, interacting with zero or more laser beams. In this case, each state is a specific $M_J$ or $M_F$ substate. Let the populations of these states (the probability of the ion being in that state at any one time) be $n_1, n_2, \ldots, n_N$, written as
a column vector \( n \). The rate of change of the populations is given by

\[
\dot{n} = M n
\]  

(3.1)

where \( M \) is a matrix containing the spontaneous and stimulated transition rates (per atom). Equation (3.1) is the matrix form of the rate equations. Note that this model ignores coherent effects – for instance it cannot model superpositions of states.

If we write the stimulated rate from level \( j \) to level \( i \) as \( R_{j \rightarrow i} \), and the spontaneous rate as \( \Gamma_{j \rightarrow i} \), we see we must have

\[
M_{ij} = \Gamma_{j \rightarrow i} + R_{j \rightarrow i}
\]  

(3.2)

\[
M_{jj} = -\sum_k (\Gamma_{j \rightarrow k} + R_{j \rightarrow k})
\]  

(3.3)

We wish to calculate how the state populations \( n \) change over time, and find what steady-state they eventually settle into.

For constant \( M \) (i.e. the beams’ intensity, polarisation and detuning do not vary), and knowing the initial population state \( n(0) \), equation (3.1) can be directly integrated to find the state populations at time \( t \).

\[
n(t) = e^{Mt}n(0)
\]  

(3.4)

The steady-state population in the limit \( t \to \infty \) should be independent of \( n(0) \). Again we assume that \( M \) is constant. Simply solving equation (3.1) for \( \dot{n} = 0 \) will not work, because the total population is not defined. We add the constraint that the total population is 1 (we are certain that the ion is in exactly one of these states),

\[
\sum_i n_i = 1,
\]  

(3.5)

by replacing each element of the first row of \( M \) with 1s:

\[
M'_{ij} = \begin{cases} 
M_{ij} & i \neq 1 \\
1 & i = 1 
\end{cases}
\]  

(3.6)

and solving

\[
M'n = b
\]  

(3.7)

where

\[
b = \begin{pmatrix} 
1 \\
0 \\
0 \\
\vdots \\
0 
\end{pmatrix}
\]  

(3.8)
Counter-intuitively, no information is lost by this replacement. This is because every column of $\mathbf{M}$ sums to zero (equations (3.2) and (3.3)). Equivalently, it is rank-deficient, having only $N - 1$ linearly independent rows instead of $N$. In principle, the replacement is not strictly necessary; solving

$$
\mathbf{Mn} = \begin{pmatrix}
0 \\
0 \\
0 \\
\vdots \\
0
\end{pmatrix}
$$

(3.9)

would give us $\mathbf{n}$ up to a constant factor, which can easily be set so that $\mathbf{n}$ sums to 1 as required. In practice we would likely obtain only the trivial solution $\mathbf{n} = \mathbf{0}$, because finite precision arithmetic makes it unlikely that $\mathbf{M}$ is precisely singular. The choice of making the replacement on the first row of $\mathbf{M}$ is arbitrary; any row $k$ will do, provided that $\mathbf{b}$ matches:

$$
\mathbf{b}_i = \begin{cases} 
0 & i \neq k \\
1 & i = k
\end{cases}
$$

(3.10)

Our solution to (3.7) is

$$
\mathbf{n} = \mathbf{M}^{-1} \mathbf{b}.
$$

(3.11)

Clearly, $\mathbf{M}'$ must be non-singular for this to work. In particular, $\mathbf{M}'$ will be singular if any two (or more) columns are identical, which happens if at least two columns of $\mathbf{M}$ were all zero. Physically, this means that there were at least two states with no stimulated or spontaneous transitions leading out of them (“dark” states). Using the matrix inverse is actually an inefficient and numerically inaccurate way to solve this; instead we use MATLAB’s \texttt{mldivide} function, also written “\textbackslash”, which is faster and more accurate

$$
\mathbf{n} = \mathbf{M}' \textbackslash \mathbf{b}.
$$

(3.12)

### 3.1.2 Forming $\mathbf{M}$

We can decompose $\mathbf{M}$ into two matrices: $\mathbf{M}^{\text{spont}}$ (which is upper-triangular if the levels are ordered in increasing order of energy) and $\mathbf{M}^{\text{stim}}$ which is symmetric.

$$
\mathbf{M}_{ij}^{\text{spont}} = \begin{cases} 
\Gamma_{j \rightarrow i} & j > i \\
-\sum_k \Gamma_{j \rightarrow k} = \Gamma_j & j = i \\
0 & j < i
\end{cases}
$$

(3.13)
\[ M_{ij}^{stim} = \begin{cases} R_{j \rightarrow i} = R_{i \rightarrow j} = R_{ij} & j \neq i \\ - \sum_k R_{j \rightarrow k} & j = i \end{cases} \]  

(3.14)

\subsection*{3.1.2.1 Electric Dipole Transitions (E1)}

The Einstein A coefficient \( A_{ji} \) is defined as the total probability per unit time of an atom in a specific state \( j \) making a transition to any of the \( (2J_i + 1) \) states of the energy level \( i \). \( A_{ji} \) depends on the quantum numbers \( n, L \) and \( J \) of the two levels (but not on the \( M \) value of state \( j \), due to isotropy). However we are interested in transitions where both the initial and final magnetic sub-states are specific. The selection rules and matrix elements depend on Clebsch-Gordon coefficients, here represented using 3-j symbols ([definitions and tables can be found in Cowan [114], Chapter 5 and Appendix C]). Letting \( j \) and \( i \) represent specific states, the spontaneous transition rate is [110]

\[ \Gamma_{j \rightarrow i} = A_{ij} (2J_j + 1) \left( \begin{array}{cc} J_i & 1 \\ -M_{J,i} & q M_{J,j} \end{array} \right)^2 \]  

(3.15)

where \( q = M_{J,i} - M_{J,j} \) represents the polarisation of the emitted photon: 0 for a photon linearly polarised parallel to the \( z \)-axis (\( \pi \)); +1 for a photon circularly polarised clockwise (as seen from the positive \( z \) direction, for a photon emitted in that direction) (\( \sigma^+ \)); −1 for anticlockwise circular polarisation (\( \sigma^- \)). The 3-j symbol is zero unless its bottom row sums to zero – this selects for conservation of angular momentum.

When discussing transitions between hyperfine levels, rather than fine structure levels, an additional factor involving a 6-j symbol is needed [114, Appendix D]. We need to include the nuclear spin \( I \) in the formula (\( I = 7/2 \) for calcium-43), and work with \( F = J + I \) as the ion’s total spin operator. The result is [110]

\[ \Gamma_{j \rightarrow i} = A_{ij} (2J_j + 1)(2F_i + 1)(2F_j + 1) \times \left( \begin{array}{cc} F_i & 1 \\ -M_{F,i} & q M_{F,j} \end{array} \right)^2 \left\{ \begin{array}{cc} J_i & I \\ F_j & 1 \end{array} \right\}^2 \]  

(3.16)

My MATLAB routines calculate the 3-j and 6-j symbols using “threej.m” and “sixj.m” (both written by Simon Webster). The 3-j and 6-j symbols are highly symmetrical in their inputs: for example the 3-j symbol is invariant under any cyclic permutation of its columns, and the 6-j symbol is invariant under any permutation of its columns.
3.1. BASIC ATOMIC THEORY

The total decay rate out of state $j$ is

$$\Gamma_j = \sum_i \Gamma_{j \rightarrow i}. \quad (3.17)$$

This also gives the width of the transition. If we apply a laser beam to the atom, detuned by $\delta$ from the resonant frequency of the transition, the stimulated transition rate is given by

$$R_{i \rightarrow j} = \frac{\Gamma_j^2 \Gamma_{j \rightarrow i}}{4\delta^2 + \Gamma_j^2} \frac{I}{I_0}, \quad (3.18)$$

where $I_0 = \frac{\hbar \omega_{ij}^2 \Gamma_j}{6\pi c^2}$ \quad (3.19)

is the saturation intensity of the transition $^{110}$. $I_0$ is different for every fine-structure transition, but the context will make it obvious which $I_0$ is being used.

3.1.2.2 Electric Multipole Transitions

The decay of the D levels of Ca$^+$ is electric-dipole-forbidden ($\Delta l = 2$). Instead, they decay by electric quadrupole transitions, E2. The equivalents of equation (3.16) for E2 (or higher) transitions are much rarer in textbooks than the dipole version, but Cowan $^{114}$ gives us all the tools we need to work them out.

First, define the notation

$$[x] \equiv 2x + 1 \quad (3.20)$$

$$[x, y, \ldots] \equiv (2x + 1)(2y + 1) \cdots. \quad (3.21)$$

We will also use the notation $C^{(k)}$ to refer to an “irreducible tensor operator of (integral) rank $k$”. This means it has $2k+1$ components $C_q^{(k)}$ (for $q = -k, 1-k, \ldots, k$) each of which transforms like the spherical harmonic $Y_{kq}(\theta, \phi)$ when acted upon by other operators. An example would be the renormalised spherical harmonics

$$C_q^{(k)}(\theta, \phi) \equiv \sqrt{4\pi/[k]} \ Y_{kq}(\theta, \phi) \quad (3.22)$$

which can be used to rewrite other operators as irreducible tensor operators. For in-

---

$^{1}$Note that there are several conventions for the saturation intensity, differing by constant factors. My definition is such that, for a cycling transition on resonance, one saturation intensity gives equal stimulated and spontaneous transition rates ($R_{i \rightarrow j} = \Gamma_{i \rightarrow j}$).
stance, a vector operator

\[
\mathbf{r} = \begin{pmatrix}
  r_x \\
  r_y \\
  r_z 
\end{pmatrix} = \begin{pmatrix}
  r \sin(\theta) \cos(\phi) \\
  r \sin(\theta) \sin(\phi) \\
  r \cos(\theta)
\end{pmatrix}
\] (3.23)

becomes \[ Section 11-3 \]

\[ r^{(1)} = r C^{(1)} \] (3.24)

where

\[
\begin{align*}
  r^{(1)}_1 &= -\frac{1}{\sqrt{2}}(r_x + ir_y) = -\frac{r}{\sqrt{2}} \sin(\theta)e^{i\phi} \\
  r^{(1)}_0 &= r_z = r \cos(\theta) \\
  r^{(1)}_{-1} &= \frac{1}{\sqrt{2}}(r_x - ir_y) = \frac{r}{\sqrt{2}} \sin(\theta)e^{-i\phi}
\end{align*}
\] (3.25)

are its components. If we assume \( \mathbf{r} \) is the position operator of the outer electron of \( \text{Ca}^+ \), we immediately see that the electric dipole operator is also an irreducible tensor operator

\[ P^{(1)} = -e r^{(1)} = -e r C^{(1)} \] (3.26)

as is the electric quadrupole operator

\[ P^{(2)} = -e r^{(2)} = -e r^2 C^{(2)} \] (3.27)

We will need the Wigner-Eckart Theorem: let \( T^{(k)} \) be any irreducible tensor operator acting in a space spanned by basis functions \( |\alpha jm\rangle \). These are eigenstates of \( \mathbf{J}^2 \) with value \( j(j+1) \), and \( J_z \) with value \( m \), with \( \alpha \) representing all other quantum numbers. Then commutation relations between \( J_{\pm} \) and \( T^{(k)}_q \) imply that \[ Section 11-4 \]

\[ \langle \alpha jm | T^{(k)}_q | \alpha' j' m' \rangle = (-1)^{j-m} \begin{pmatrix} j & k & j' \\ -m & q & m' \end{pmatrix} \langle \alpha j | T^{(k)} | \alpha' j' \rangle \] (3.28)

where \( \langle \alpha j | T^{(k)} | \alpha' j' \rangle \) is a reduced matrix element and contains the rest of the physics such as wavefunction overlap.

Now consider the product of two tensor operators, \( T^{(k_1)} \) and \( W^{(k_2)} \). Let

\[ V^{(K)}_Q \equiv (T^{(k_1)} \times W^{(k_2)})^{(K)}_Q \] (3.29)
3.1. BASIC ATOMIC THEORY

*\( (x\) is the tensor product). \( V_Q^{(K)}\) acts in a space \( |\alpha jm\rangle\). However, \( T \) and \( W \) need only act in subspaces of \( |\alpha jm\rangle\), spanned by \( |\alpha j_m m\rangle\) and \( |\alpha w j_w m_w\rangle\) respectively. Cowan [114 Section 11-5] shows that

\[
\langle \alpha_t j_t \alpha_w j_w | V^{(K)} | \alpha_{t'} j_{t'} \alpha_{w'} j_{w'} \rangle \\
\equiv \langle \alpha_t j_t \alpha_w j_w | (T^{(k_t)} \times W^{(k_w)})^{(K)} | \alpha_{t'} j_{t'} \alpha_{w'} j_{w'} \rangle \\
= \sqrt{[j, j', K]} \langle \alpha_t j_t | T^{(k_t)} | \alpha_{t'} j_{t'} \rangle \langle \alpha_w j_w | W^{(k_w)} | \alpha_{w'} j_{w'} \rangle \\
\quad \left\{ \begin{array}{c}
j_t & j_w & j \ 
j_{t'} & j_{w'} & j' \ 
k_t & k_w & K \end{array} \right\} (3.30)
\]

where a 9-j symbol has been introduced at the end.

How does this help us? Well, soon we will identify \( T \) and \( W \) as the (externally imposed) electric multipole operators acting on the electrons and nucleus, respectively; \( j \) is \( F \), \( j_t \) is \( J \) and \( j_w \) is \( I \). But as an excellent approximation, we can ignore the direct effect of the light field on the nucleus. We can thus set \( W \) to be the identity, in which case \( k_w = 0 \) and

\[
\langle \alpha_w j_w | W^{(k_w)} | \alpha_{w'} j_{w'} \rangle \\
= \langle \alpha_w j_w | 1 | \alpha_{w'} j_{w'} \rangle \\
= \sqrt{[j_w]} \delta_{\alpha_w, \alpha_{w'}} \delta_{j_w j_{w'}} (3.31)
\]

and thus

\[
\langle \alpha_t j_t \alpha_w j_w | V^{(K)} | \alpha_{t'} j_{t'} \alpha_{w'} j_{w'} \rangle \\
= \delta_{\alpha_w, \alpha_{w'}} \delta_{j_w j_{w'}} (-1)^{j_t + j_w + j' + K} \sqrt{[j, j']} \left\{ \begin{array}{c}
j_t & j_w & j \ 
j_{t'} & j_{w'} & j' \ 
k & K & K' \end{array} \right\} \langle \alpha_t j_t | T^{(K)} | \alpha_{t'} j_{t'} \rangle. (3.32)
\]

The probability per unit time of an electric \( \zeta \)-pole (E\( \zeta \)) spontaneous decay from \( |\gamma' J' I' F' M'_F\rangle\) to \( |\gamma J I F M_F\rangle\) is (by analogy with [114 Section 15-2], and see also [115 Page 439])

\[
\alpha_{E\zeta} = \text{Constant}_\zeta \times \omega^{2\zeta+2} \sum_q \left| \langle \gamma J I F M_F | P_q^{(\zeta)} | \gamma' J' I' F' M'_F \rangle \right|^2. (3.33)
\]

\( \gamma \) stands for any other atomic properties that change in the transition, such as the principal quantum number. The constant includes only fundamental constants. Apply the Wigner-Eckart Theorem [328], identifying \( j = F, m = M_F \) and all other variables
as $\alpha$:

$$a_{E\zeta} = \text{Constant}_{\zeta} \times \omega^{2\zeta+2} \sum_{q} \left( \begin{array}{ccc} F & \zeta & F' \\ -M_F & q & M'_F \end{array} \right)^2 \times \left| \langle \gamma J I F \| P^{(\zeta)} \| \gamma' J' I F' \rangle \right|^2.$$ (3.34)

Now we can use equation (3.32). Identify $j = F$, $j_t = J$, $j_w = I$, $V^{(K)} = T^{(K)} = P^{(\zeta)}$; set $j_w = j'_w$, and $\alpha_w = \alpha'_w$ because the light doesn’t couple to the nuclear spin; and we obtain

$$a_{E\zeta} = \text{Constant}_{\zeta} \times \omega^{2\zeta+2} \sum_{q} \left( \begin{array}{ccc} F & \zeta & F' \\ -M_F & q & M'_F \end{array} \right)^2 \times \left\{ \begin{array}{ccc} J & I & F \\ F' & \zeta & J' \end{array} \right\}^2 \left| \langle \gamma J \| P^{(\zeta)} \| \gamma' J' \rangle \right|^2.$$ (3.35)

It turns out that

$$\left| \langle \gamma J \| P^{(\zeta)} \| \gamma' J' \rangle \right|^2 \times \text{Constant}_{\zeta} \times \omega^{2\zeta+2} = [J']A$$ (3.36)

where $A$ is the relevant Einstein A Coefficient. So

$$a_{E\zeta} = \sum_{q} \left( \begin{array}{ccc} F & \zeta & F' \\ -M_F & q & M'_F \end{array} \right)^2 \left\{ \begin{array}{ccc} J & I & F \\ F' & \zeta & J' \end{array} \right\}^2 A$$ (3.37)

which, setting $\zeta \rightarrow 2$, is the formula I use in my programs.

### 3.1.2.3 Magnetic Dipole Transitions (M1)

While a complete treatment of this subject would also consider magnetic dipole (and perhaps magnetic multipole) transitions, they are not necessary for calculations with Ca$^+$. Sahoo et al. [15] calculated the lifetimes of the 3D levels of Ca$^+$ using relativistic coupled-cluster theory. M1 transitions are allowed from D$^3/2 \rightarrow$ S$^1/2$ and from D$^5/2 \rightarrow$ D$^3/2$, but in both cases they make only very small contributions to the levels' lifetimes. For the former transition the M1 reduced matrix element is only $10^{-4}$ times the strength of the E2 element; and the D$^5/2 \rightarrow$ D$^3/2$ M1 transition is suppressed because of the small energy difference and the $\omega^3$ factor in the transition rate (its Einstein A coefficient is calculated to be only $2.4 \times 10^{-6}$ s$^{-1}$ [116]). In Ba$^+$, though, the D$^5/2 \rightarrow$ D$^3/2$ reduces the lifetime of D$^5/2$ by 16% compared to the E2 decay alone.
3.1.3 Hyperfine Energy Shifts

Because the rate of a stimulated transition depends on the laser detuning $\delta$, it is important to be able to accurately calculate the energy spacing of all the states. In $^{40}\text{Ca}^+$ (which has zero nuclear spin $I$), the spacings are determined by the fine structure of the ion, and the Zeeman shifts of individual states. $^{43}\text{Ca}^+$ is the only stable isotope of calcium with non-zero nuclear spin: $I = 7/2$. We will only be concerned with two ways that the electrons’ wavefunctions can interact with the nucleus – the nucleus’s magnetic dipole moment and its electric quadrupole moment.

The effect of those moments is given by Woodgate [119, Second Edition, Section 9.5]:

Let $K = F(F + 1) - J(J + 1) - I(I + 1)$

Then $\Delta E = \frac{A_{L,J}}{2}K + \frac{B_{L,J}}{4} \frac{3K(K + 1) - 2I(I + 1)J(J + 1)}{I(2I - 1)J(2J - 1)}$ (3.39)

where $A_{L,J}$ and $B_{L,J}$ are the hyperfine structure constants for the magnetic dipole and electric quadrupole interactions respectively, and depend only on $L$ and $J$ (for a given isotope). $B_{L,J} = 0$ for $J < 1$ or $I < 1$. $\Delta E$ is the energy shift of a state relative to the centre-of-gravity of a level. That is,

$$\sum_{F,M_F} \Delta E_{L,J,F,M_F} = 0 \quad \forall L, J.$$ (3.40)

$A_{L,J}$ is not to be confused with an Einstein A coefficient! These energy shifts are plotted in Appendix A.

The Zeeman energy shift due to an external magnetic field $B$ is given by

$$\Delta E_Z = g_F M_F \mu_B B$$

$$= g_J \left( \frac{F(F + 1) + J(J + 1) - I(I + 1)}{2F(F + 1)} \right) M_F \mu_B B$$

$$= \left( \frac{3J(J + 1) + S(S + 1) - L(L + 1)}{2J(J + 1)} \right) \times \left( \frac{F(F + 1) + J(J + 1) - I(I + 1)}{2F(F + 1)} \right) M_F \mu_B B.$$ (3.43)

This neglects the direct interaction between the nuclear moments and $B$; and is valid only in the limit of low magnetic field when $\Delta E_Z \ll \Delta E$. This condition is generally fulfilled

---

2The nucleus’s electric dipole moment, and other odd electric moments and even magnetic moments, are very close to zero. They would be precisely zero if either parity-reversal or time-reversal symmetries held exactly; Weak interactions violate these symmetries but the effect is still unmeasurably small [117, Section 2.2.8], even to specialised experiments [118].
in the experiments and simulations in this work. The exception is the $D_{5/2}$ level, where the Zeeman shifts become non-linear even for our typical fields of $\sim 2 \times 10^{-4}$ T; however my programs still use the linear model because the precise splittings are unimportant for this work. Note that the formula (3.43) is still valid for isotopes with no nuclear spin – the second bracketed term in the product becomes 1 when $I = 0$ and $F \equiv J$. Quantum electrodynamic effects lead to $g_J$ deviating from $\left(\frac{3J(J+1)+S(S+1)-L(L+1)}{2J(J+1)}\right)$, and for some levels these have been measured to high precision as shown in Table 3.1. I do not use these measurements and simply use the formula (3.43).

3.2 The Transitions Suite

“Transitions” is my suite of MATLAB functions. Their main purpose was to allow rate-equations simulations of $^{43}\text{Ca}^+$, although they include routines to calculate intermediate-field Zeeman shifts and light shifts. They are written to be relatively general: simply by changing one settings file, they can simulate other alkaline earth ions (e.g. Sr$^+$), neutral alkaline atoms (e.g. Rb) or other similar one-electron systems. Note however that capability for M1 transitions may need to be added to work with species such as Ba$^+$ (Section 3.1.2.3). The programs will not necessarily work with multi-electron systems such as neutral alkaline earth atoms – this is because I have assumed the electron’s spin $S$ is $\frac{1}{2}$ throughout. I have also assumed that the fine-structure splitting is always small enough that levels with the same value of $n$ and $L$, but different $J$s, are adjacent when the levels are ordered by energy.

The detailed implementation of the model is described in the users’ manual in Appendix B.

3.3 Atomic Constants

These are some of the relevant atomic data for Ca$^+$. Here I list the most precise values I could find at the time of writing; early simulations may have been performed with less precise numbers.

**Nuclear Spin** This is zero for all isotopes except $^{43}\text{Ca}^+$, which has $I = \frac{7}{2}$.
3.3. ATOMIC CONSTANTS

Levels Each fine-structure level is listed separately and manually. They are identified by their principal quantum number $n$, orbital angular momentum $L$ and total angular momentum $J$. $n$ is not used in any calculations: its purpose is only to distinguish between different levels with the same $L$ and $J$, if such a situation were ever needed. For each such level is recorded its hyperfine $A$ and $B$ coefficients. These are obviously non-zero only for $^{43}\text{Ca}^+$, and are recorded in Table 3.1. I also include gyromagnetic factors $g_J$, if they have been measured, for reference only (currently my program calculates them from the quantum numbers using Equation (3.43)).

<table>
<thead>
<tr>
<th>Level</th>
<th>$A$ / MHz</th>
<th>$B$ / MHz</th>
<th>Ref.</th>
<th>$g_J$</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>4S$_{1/2}$</td>
<td>$-806.402\ 071\ 60(8)$</td>
<td>0</td>
<td>[120]</td>
<td>2.002 256 64(9)</td>
<td>[17]</td>
</tr>
<tr>
<td>4P$_{1/2}$</td>
<td>$-145.4(1)$</td>
<td>0</td>
<td>[16]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4P$_{3/2}$</td>
<td>$-31.0(2)$</td>
<td>$-6.9(1.7)$</td>
<td>[16]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3D$_{3/2}$</td>
<td>$-47.3(2)$</td>
<td>$-3.7(1.9)$</td>
<td>[16]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3D$_{5/2}$</td>
<td>$-3.8(6)$</td>
<td>$-3.9(6.0)$</td>
<td>[16]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3D$_{5/2}$</td>
<td>$-3.893\ 1(2)$</td>
<td>$-4.241(4)$</td>
<td>[121, 122]</td>
<td>1.200 334 0(3)</td>
<td>[123]</td>
</tr>
</tbody>
</table>

Table 3.1: The hyperfine structure constants for $^{43}\text{Ca}^+$, and gyromagnetic ratios for $\text{Ca}^+$ in general. The more precise values for $D_{5/2}$ were published after many of the results in this thesis were calculated.

Transitions Transitions between hyperfine- or fine-structure-split levels are ignored (there is no $P_{3/2} \rightarrow P_{1/2}$ for instance). Each transition we want to include is labeled by the $n$, $L$ and $J$ values of the upper and lower levels, and for each I include its Einstein $A$ coefficient, the wavelength and the isotope shift between the same transition in $^{43}\text{Ca}^+$ and $^{40}\text{Ca}^+$. The same array is used to store the saturation intensity of the transition, although this is calculated by the setup function rather than specified as a parameter. The wavelength and isotope shift are stored in this array for reference and ease of access, although they are not directly used in calculations. Table 3.2 shows the data.
<table>
<thead>
<tr>
<th>Transition</th>
<th>Wavenumber / cm$^{-1}$</th>
<th>Wavelength / nm</th>
<th>Frequency / THz</th>
<th>Ref.</th>
<th>Isotope Shift / MHz</th>
<th>Ref.</th>
<th>Einstein A Coefficient / s$^{-1}$</th>
<th>Ref.</th>
<th>Saturation / W m$^{-2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$4S_{1/2} \rightarrow 4P_{1/2}$</td>
<td>25 191.519 87(6)</td>
<td>396.958 978 8(9)</td>
<td>755.222 766 2(17)</td>
<td>[21]</td>
<td>688(17)</td>
<td>[106]</td>
<td>132 × 10$^6$</td>
<td></td>
<td>933.82</td>
</tr>
<tr>
<td>$4S_{1/2} \rightarrow 4P_{3/2}$</td>
<td>25 414.415 62(2)</td>
<td>393.477 471 6(3)</td>
<td>761.905 012 7(5)</td>
<td>[124]</td>
<td>692(19)</td>
<td>[106]</td>
<td>135.0(4) × 10$^6$</td>
<td>[20]</td>
<td>987.58</td>
</tr>
<tr>
<td>$3D_{3/2} \rightarrow 4P_{1/2}$</td>
<td>11 541.32</td>
<td>866.452</td>
<td>346.000</td>
<td>[125]</td>
<td>-3464.3(3.0)</td>
<td>[16]</td>
<td>8.4 × 10$^6$</td>
<td></td>
<td>89.798</td>
</tr>
<tr>
<td>$3D_{3/2} \rightarrow 4P_{3/2}$</td>
<td>11 764.21</td>
<td>850.036</td>
<td>352.682</td>
<td>[125]</td>
<td>-3462.4(2.6)</td>
<td>[16]</td>
<td>0.955(6) × 10$^6$</td>
<td>[20]</td>
<td>97.954</td>
</tr>
<tr>
<td>$3D_{5/2} \rightarrow 4P_{3/2}$</td>
<td>11 703.52</td>
<td>854.444</td>
<td>350.863</td>
<td>[125]</td>
<td>-3465.4(3.7)</td>
<td>[16]</td>
<td>8.48(4) × 10$^6$</td>
<td>[20]</td>
<td>96.446</td>
</tr>
<tr>
<td>$4S_{1/2} \rightarrow 3D_{5/2}$</td>
<td>137 10.889 610 718 40(3)</td>
<td>729.347 276 793 955(2)</td>
<td>411.042 129 776 393 2(10)</td>
<td>[123]</td>
<td>4134.713(5)</td>
<td>[121]</td>
<td>0.856(5)</td>
<td>[55]</td>
<td>9.181 × 10$^{-7}$</td>
</tr>
<tr>
<td>$4S_{1/2} \rightarrow 3D_{3/2}$</td>
<td>13 650.19</td>
<td>732.591</td>
<td>409.222</td>
<td>[125]</td>
<td></td>
<td></td>
<td>0.850(8)</td>
<td>[58]</td>
<td>8.818 × 10$^{-7}$</td>
</tr>
</tbody>
</table>

Table 3.2: Properties of the transitions between energy levels in $^{40}$Ca$^+$. The isotope shift is $\nu_{\text{Centre of Gravity, Ca-43}} - \nu_{\text{Ca-40}}$. 
3.4 Simulations of Ion Fluorescence in $^{43}\text{Ca}^+$

The rate at which we observe 397 nm photons scattered by a calcium ion is directly proportional to the probability that the ion is in $P_{1/2}$. Specifically,

$$\text{Count Rate} = \text{Pop}_{P_{1/2}} \times \Gamma_{P_{1/2}\rightarrow S_{1/2}} \times \text{Collection Efficiency} \quad (3.44)$$

where $\text{Pop}_X$, the population of level $X$, is the probability of the ion being in that level. Of course, we also count photons that are emitted by decays from $P_{3/2}$, although these are generally so rare that we can ignore them. The collection efficiency of the imaging system was $1.1 \times 10^{-3}$ before 24th March 2008, and $\approx 2 \times 10^{-3}$ after 2nd April.

A basic estimate of the maximum possible $\text{Pop}_{P_{1/2}}$ can be made by noticing that when a two-level system is completely saturated, it spends equal time in both states. In general, a completely saturated system spends equal time in every state, and so

$$\text{Pop}_X = \frac{\text{Number of states in level } X}{\text{Total number of states}} = \frac{2J_X + 1}{\sum_i (2J_i + 1)} \quad (3.45)$$

where the denominators are summed only over states that the ion is likely to inhabit; for example if neither the 393 nm nor 850 nm beams are on, the ion will never be in $P_{3/2}$ nor $D_{5/2}$ and so those states are not added to the denominator. It can be shown that these ratios do not depend on the nuclear spin – they are not affected by hyperfine structure.

For an ion fully saturated with 397 nm and 866 nm light (neither beam being pure $\sigma$ or $\pi$ polarised, so there are no optical pumping effects and all states are connected), the expected populations are

$$\text{Pop}_{S_{1/2}} : \text{Pop}_{P_{1/2}} : \text{Pop}_{D_{3/2}} = \frac{1}{2} : \frac{1}{2} : 4$$

The expected maximum count rate is therefore

$$\frac{1}{4} \times 132 \times 10^6 \text{s}^{-1} \times 0.0011 = 36,000 \text{ Counts per second} = 36,000 \text{ cps.} \quad (3.46)$$

We achieve this with $^{40}\text{Ca}^+$, for 397 nm intensity $\sim 12 I_0$ and 866 nm intensity $\sim 62 I_0$.

But with $^{43}\text{Ca}^+$ we usually observe many fewer counts; for instance 6800 cps for $I_{397} = 14 I_0$ and $I_{866} = 170 I_0$, corresponding to $\text{Pop}_P = 0.047$. A goal of my rate equations programs was to investigate why this is.
An early question is whether the lasers are tuned to the correct frequency. The 397 nm Doppler cooling laser must excite out of both the $S_{3/2}^1$ and $S_{3/2}^4$ hyperfine manifolds. These are so far apart (3226 MHz compared to the 397 nm transition’s natural linewidth of 22 MHz, Figure 2.1) that the fluorescence rate will almost vanish unless sidebands are added to the beam, e.g. with an EOM. There are several choices for the beam’s detuning and modulation. The carrier can address any one of the four transitions, and a sideband can address either of the two transitions that excite from the other $S_{1/2}$ manifold (the other sideband is wasted). A rate equations fluorescence calculation is shown in Figure 3.1 that simulates each of these eight choices. I assume parameters (laser intensity, polarisation, sideband power distribution etc.) similar to the experiment that found $P_{1/2} = 0.047$ – that result is marked on the graph for reference. The simulation shows the $P_{1/2}$ population as a function of 866 nm detuning – the experiment was also a scan of this laser, and the 4.7% result was the peak of this scan.

It can be seen that the simulation achieves $P$ populations above 7%, somewhat higher than the experiment. Note that the count rate should increase slightly if we tuned the 397 nm carrier and sideband to $S_{1/2}^4 \rightarrow P_{3/2}^3$ and $S_{1/2}^3 \rightarrow P_{1/2}^3$. But the $S_{1/2}^4 \rightarrow P_{1/2}^3$ transition is less than 600 MHz blue of the $S_{1/2}^4 \rightarrow P_{1/2}^4$ line, so having a laser component at that frequency would run a slightly higher risk of Doppler-heating the ion. We thus prefer to use $S_{1/2}^1 \rightarrow P_{1/2}^4$ and $S_{1/2}^3 \rightarrow P_{1/2}^4$ as marked on the plot.

Depending on the $P_{1/2}$ $F$-manifold(s) to which the 397 excites, the 866 will need to repump from different $D_{3/2}$ manifolds at different rates (for instance, if the 397 does not excite to $P_{1/2}^3$ then the ion will rarely fall into $D_{3/2}^2$). Since the 866 hyperfine components vary in strength (see Figure A.2 but note that that figure uses the opposite labelling convention to Figure 3.1), the optimal 866 detuning depends on the choice of 397 frequencies.

The experiment required the ion to be continuously Doppler cooled by the lasers, so the 397 nm carrier was red-detuned from resonance by approximately 12 MHz and the sideband by 6 MHz. Feeding this into the simulation does indeed reduce $P_{1/2}$, but not enough to match the experiment. The problem can be seen by comparing the simulation with the actual data from the experimental scan, in Figure 3.3. We immediately see three sharp dips in the experimental data: dark resonances. Dark resonances (also known as electromagnetically induced transparency or coherent population trapping) occur in a three-level system when the two laser beams have the same detuning (as
3.4. SIMULATIONS OF ION FLUORESCENCE IN $^{43}$CA$^+$

Figure 3.1: Rate equations simulation of ion fluorescence as a function of 866 nm beam detuning, for a variety of detunings and sideband modulations of the 397 nm beam. $I_{397} = 14 I_0$; Sideband:Carrier:Sideband intensity splitting = 13:74:13; $I_{866} = 170 I_0$; both beams are equally split between $\sigma^-$ and $\sigma^+$ polarisations. This attempts to replicate the experiment that produced maximum PopP of 4.7%; in the experiment the carrier was tuned to $S_{1/2} \rightarrow P_{1/2}$, sideband to $S_{3/2} \rightarrow P_{3/2}$ (starred on plot). Here the 397 nm components are set to be exactly resonant with the stated transitions. Solid/dotted lines of the same colour show 397 choices that address the same transitions, but with sidband and carrier swapped. Vertical lines show positions of the hyperfine components of $D_{3/2} \rightarrow P_{1/2}$, labeled $F_{\text{lower}} \rightarrow F_{\text{upper}}$. 

---

[Note: The figure contains a graph with various lines and labels indicating transitions and intensities.]
shown in Figure 3.2. One of the resulting dressed states contains only $S_{1/2}$ and $D_{3/2}$ and does not scatter photons. The ion then falls into the dark state by optical pumping.

Figure 3.2: Three-level system representing the 397 nm and 866 nm transitions. A dark resonance occurs when the detunings are equal: $\delta_b = \delta_r$.

Optical pumping to dark states can occur even when the two-beam resonance condition is not met. The most obvious situation is when pure circularly polarised (say, $\sigma^+$) 397 nm light is applied to $^{43}\text{Ca}^+$. No such transition exists from the state $S_{1/2}^{4+,4}$ so that state is dark and the ion will be optically pumped into it, no matter what is happening on the 866 nm transition. If the laser is changed to any other polarisation, there exists a superposition of Zeeman-states that is dark, and again the ion will eventually fall into that state. In our experiment we apply a magnetic field to the ions. This field lifts the degeneracy of the states, so the dark state is no longer stable and the ion precesses out of it. However, the precession is relatively slow and so the fluorescence rate is still reduced.

Dark states and resonances cannot in general be calculated using rate equations, because they depend on coherent interactions between states and light fields that rate equations do not include. Including coherences leads to the Bloch equations. Berkeland and Boshier have used Bloch equations to study dark states, and methods for destabilising them [127]. They consider modulations $\delta$ being applied to the system either by magnetic field (in which $\delta$ is the Zeeman shift between states) or by modulation of the polarisation of the laser ($\delta$ is the product of the modulation frequency and the amplitude of the phase shift imparted between the polarisation components). Typically they found that the fluorescence rate was maximised when $\delta$ was about half the Rabi frequency $\Omega$ of a laser-stimulated transition; $\delta \ll \Omega$ allowed the system to spend too
Figure 3.3: Rate equations simulation and experimental measurement of ion fluorescence as a function of 866 nm beam detuning. Parameters of simulation and experiment: $I_{397} = 14 I_0$; Sideband:Carrier:Sideband intensity splitting = 13:74:13; $I_{866} = 170 I_0$; both beams are equally split between $\sigma^-$ and $\sigma^+$ polarisations; carrier was tuned 12 MHz red of $S_{1/2} \rightarrow P_{1/2}$, sideband 6 MHz to red of $S_{1/2} \rightarrow P_{1/2}$. The data (coloured lines) came from four scans, two in reverse direction (high frequency to low frequency); the different scans are shown in different colours to demonstrate the results are repeatable. The simulation is the black solid line. Predicted positions of dark resonances are marked as vertical dashed lines (the middle one, at -257 MHz, was used to determine the offset on the experimental frequency scale and match it to the simulation).
much time in the dark state for strong fluorescence, and $\delta \gg \Omega$ corresponded to the laser being too far detuned. However, in systems with large angular momenta (such as $^{43}\text{Ca}^+$) the fluorescence rate is relatively independent of $\delta$ [127, Section IV.C.].

In the experiment above, the Rabi frequencies of both the 397 nm and 866 nm transitions were $\sim 20$ MHz, compared to Zeeman shifts of 0.6 MHz in $S_{1/2}$, 0.2 MHz in $P_{1/2}$ and $\sim 0.6$ MHz in $D_{3/2}$. Although we are in the regime of $\delta \ll \Omega$ we have been unable to improve $^{43}\text{Ca}^+$ count rates by reducing either laser intensity, presumably an effect of the large number of states. In $^{40}\text{Ca}^+$, however, count rate is maximised for an 866 nm intensity of $\sim 30 I_0$. $^{40}\text{Ca}^+$ has the additional benefit that the 397 nm transition is $J_i \rightarrow J_j$ for $J_i = J_j$ and $J_i$ being a half-integer – in this case there are no dark states except for pure $\sigma$ polarisation [127].

The first-order Zeeman splitting of a manifold vanishes when $F(F + 1) + J(J + 1) = I(I + 1)$ (3.43). In $^{43}\text{Ca}^+$ this happens when $F = 3$ and $J = 3/2$. $\delta$ is thus extremely small for $D_{3/2}$, and we may worry that this allows a dark state to easily form. A crude simulation can be performed in rate equations, simply by setting the $D_{3/2} \rightarrow P_{1/2}$ transition rate to zero. We do not eliminate $D_{3/2} \rightarrow P_{4/2}$; there is no dark state for any polarisation when the upper level has higher angular momentum than the lower. Figure 3.4 repeats Figure 3.3 with just this change, and we see that total elimination is overly pessimistic. In practice the existence of the $D_{3/2} \rightarrow P_{1/2}$ transition partially prevents the dark state becoming established.

Attempts have been made to follow the other recommendation of Berkeland and Boshier [127]; polarisation modulation. A second 866 nm beam, and a second 397 nm beam, both derived from separate lasers, were focussed on the ion with different polarisations and frequencies to the usual beams. The effect should have been for the ion to feel a light field of constantly changing polarisation, destabilising the dark states and increasing fluorescence. However, no improvement was found. The Innsbuck group has also noted that $^{43}\text{Ca}^+$ produces fewer counts than $^{40}\text{Ca}^+$ [128]. Their 866 nm beam has three frequency components, at 145 MHz and 390 MHz above the lowest component; then they split the beam into two, and direct them to the ion at perpendicular directions [129]. It is claimed that this increases the fluorescence, although no further details are given.
3.4. SIMULATIONS OF ION FLUORESCENCE IN $^{43}\text{Ca}^+$

Figure 3.4: A repeat of Figure 3.3 except that the dashed curve shows the result of setting the $D_{3/2} \rightarrow P_{1/2}$ transition rate to zero.

3.4.1 Bloch Equations

Derek Stacey is currently constructing a detailed Bloch equations model of $^{43}\text{Ca}^+$. Our group has previously used Bloch equations to study $^{40}\text{Ca}^+$ [108], but the odd isotope is considerably more challenging. There are 64 states in total in $S_{1/2}$, $P_{1/2}$ and $D_{3/2}$, and a rate equations model needs to work with 64-by-64 matrices for this system. Bloch equations use the density matrix of the system, that is itself a 64-by-64 matrix; the transitions thus (in principle) involve matrices with $64^4 = 16777216$ elements. Many fewer are needed in practice because the transitions matrix is highly sparse; if the situation is simplified to include no $\pi$ polarised light, there are 17286 non-vanishing matrix elements [130]. This is a tractable computer calculation. The simulation has been tested against fluorescence data I recorded from the ion – an example is shown in Figure 3.5.

A long-standing idea for improving the fluorescence is to add sidebands to the 866 nm beam, allowing it to bridge some of the hyperfine structure in that transition. When this was tried the result was highly dependent on the 866 nm detuning, having a forest
Figure 3.5: Rate equations and Bloch equations simulations, and experimental measurement, of ion fluorescence as a function of 866 nm beam detuning. The Bloch equations curve was fitted to the data in a least-squares sense, the fitted parameters being: $I_{397} = 3.66 I_0$; Sideband:Carrier:Sideband intensity splitting = 1:16.1:1; $I_{866} = 197 I_0$; both beams are equally split between $\sigma^-$ and $\sigma^+$ polarisations. The 397 was red detuned by 22 MHz. The experiment was performed deliberately with low 397 nm power so that the bright resonances (a coherent effect that allows the fluorescence to be higher than rate equations predict) would be prominent, as a test of the simulation.

of two-photon dark resonances. This would make for unstable fluorescence, especially as dark resonances are often associated with Doppler heating if the frequencies lie on the wrong slope of the resonance. Bloch equations simulations would more easily allow us to find the best parameters. Unfortunately the equations become more complicated with 866 nm sidebands. They invalidate an implicit assumption in the Bloch equations: that each transition is excited by no more than one laser frequency, and that the polarisation remains constant (397 nm sidebands are no problem, because they are so far apart that they stimulate at negligible rates on the other transition). When this condition holds, the Bloch equations can be written as a set of simultaneous, linear, first-order differential equations with constant coefficients – an efficiently solvable system. When
3.4. SIMULATIONS OF ION FLUORESCENCE IN $^{43}\text{Ca}^+$

the condition is invalid, the Bloch equations include exponential terms that prevent this efficient solution (brute force integration is still possible, but currently computationally infeasible for $^{43}\text{Ca}^+$). Stacey \cite{131} shows that we can often make an additional approximation: if the frequency difference between the components is much greater than the rate at which the populations and coherences vary, the troublesome exponential terms average to zero and can be ignored. Thus the equations are once again linear, first-order and efficiently solvable. This approach has been shown to accurately match experiments with $^{40}\text{Ca}^+$ \cite{131}; the more complicated $^{43}\text{Ca}^+$ program is under construction.

$^{43}\text{Ca}^+$ has been studied with Bloch equations before: Kajita et al. \cite{132} use them to study Doppler cooling (including motional effects) and preparation of the clock state $S_{4,0}$. They worked with only 25 states ($S_{3/2}$, $S_{1/2}$ and $P_{1/2}$) but three 397 nm lasers ($S_{1/2} \rightarrow P_{1/2}$ $\pi$-polarised; $S_{1/2} \rightarrow P_{1/2}$ $\pi$-polarised; and $S_{1/2} \rightarrow P_{1/2}$ $\sigma \pm$-polarised), the lasers being independently tunable. Their equations do not seem to make the simplifying assumptions that we do to make them efficiently solvable; instead they add in terms for the Doppler shift and light pressure, and solve the equations with a Runge-Kutte method. They showed that an ion could be cooled from 110 mK down to 700 $\mu$K (equivalent to fifteen quanta in a 1 MHz one-dimensional trap) in 200 $\mu$s.

3.4.2 397 nm, 850 nm and 854 nm Fluorescence

For an ion fully saturated with 397 nm, 850 nm and 854 nm light (none of the beams being pure $\sigma$ or $\pi$ polarised), we can expect to achieve nearly double the fluorescence rate achieved with 397 nm and 866 nm (ignoring coherent effects). This is because the ion spends most of its time equally spread between $S_{1/2}$ and $P_{1/2}$, so it scatters UV photons at a rate a little below $\frac{1}{2} \times 132 \times 10^6 \text{s}^{-1} \times 0.0011 = 72 000 \text{cps}$. $\text{Pop}_P$ is not quite half because every 15.7 (on average) spontaneous decays, the ion decays from $P_{1/2}$ to $D_{3/2}$; the saturated $D_{3/2}$-$D_{3/2}$-$P_{3/2}$ system spends only $\frac{2}{7}$ of its time in $P_{3/2}$, so emits UV photons at a relatively low rate.

For $^{40}\text{Ca}^+$, modelling this in rate equations reveals $\text{Pop}_P$ to be 47.9%, giving a count rate of 70 000 cps (taking into account that the 393 nm decay is slightly faster than 397 nm). In an experiment we observed up to 50 400 cps, which approximately agrees with a simulation ($I_{397} = 8.4 I_0$, $I_{850} = 5720 I_0$, $I_{854} = 61 I_0$ based on measurements; detunings assumed to be zero except for 397 nm which is assumed to be 12 MHz red-detuned; polarizations taken to be equal $\sigma \pm$; predicts 50 700 cps).
Unlike fluorescence with 397 nm and 866 nm beams, the 397-850-854 scheme provides a good approximation to a two-level system on the 397 nm transition. Our group has recently used this observation to simplify measurements of heating rates in a surface trap built by David Allcock [133]. It might also allow us to increase the Doppler-cooling rate in future experiments, although it can not be used for improved fluorescence state-detection because there is no “shelf” in this scheme.

3.5 Simulations of Far Off-Resonance

As seen above, rate equations neglect many important coherent effects. Nevertheless, there are many situations where they are useful, e.g. in the case of far-off resonant lasers. Below, we outline some examples.

3.5.1 Effect on $^{43}\text{Ca}^+$ of 397 nm radiation tuned to $^{40}\text{Ca}^+$

One idea for a $^{43}\text{Ca}^+$ quantum computer is to sympathetically cool that ion with $^{40}\text{Ca}^+$. To perform Raman sideband cooling we need a resonant repumping 397 nm beam; by using a $^{40}\text{Ca}^+$ “coolant” ion rather than a $^{43}\text{Ca}^+$ coolant, this beam is well detuned from resonance with the $^{43}\text{Ca}^+$ “logic” ions that are actually being used to store quantum information. Decoherence of the qubits is thus low. We have performed experiments to demonstrate that this works; details are in Home et al. [93].

The contribution of rate equations is to calculate the rate at which $^{43}\text{Ca}^+$ scatters photons in this repumping beam. One of the experiments was to measure the phase acquired by a $^{43}\text{Ca}^+$ clock-state qubit while this detuned repump beam was applied to it (the beam was turned on for a pulse during the gap of a Ramsey sequence, and the duration of the pulse was varied (See inset, Figure 3.6)). Cosine fringes were observed, with an amplitude that decayed over time and a baseline that rose over time. The fringe frequency revealed the light shift caused by the beam, and hence its intensity was found by comparing it to a calculation I made using a Hamiltonian-diagonalisation method. Then a rate equations simulation was set up using this information. The initial population was approximately equally spread over the substates of $S_{3/2}^3$, by optical pumping with a resonant, unpolarised 397 nm beam tuned to $S_{1/2}^1 \rightarrow P_{1/2}^1$. The repumping beam was then applied, at its calculated intensity and detuned by the isotope shift between $^{40}\text{Ca}^+$ and $^{43}\text{Ca}^+$. The model’s result was the population of $S_{1/2}^1$, just as in the
3.5. SIMULATIONS OF FAR OFF-RESONANCE

After multiplying the simulation by a constant (that approximately accounts for the fact that the real ion only spends \( \sim \frac{13}{14} \) of its time in \( S_{3/2} \) during the Ramsey gap), we obtained a reasonable match to the rising baseline fitted to the data as shown in Figure 3.6. This helps confirm our analysis of noise sources in the experiment.

![Figure 3.6: A Ramsey experiment using the \( S_{3/2}^0 \) and \( S_{3/2}^1 \) states of \( ^{43}\text{Ca}^+ \). The data points have been fitted with a cosine that includes amplitude decay and a rising baseline. The dashed line is the rate-equations simulation of the rising baseline. This figure is from Home et al. [93].](image)

3.5.2 Shelving Effect on \( ^{40}\text{Ca}^+ \) of 397 nm and 866 nm Light

In Myerson et al. [82] we describe a detailed investigation of high-fidelity readout for an optical qubit in \( ^{40}\text{Ca}^+ \). An optical qubit has qubit states separated by energies of the order of visible photons – in this case the levels \( S_{1/2} \) and \( D_{5/2} \) were used (usually the two Zeeman states of \( S_{1/2} \) are used as the qubit; one of those states is transferred to \( D_{5/2} \) as part of readout, mapping it to the optical qubit). When the ion is illuminated by 397 nm and 866 nm light, the ion fluoresces if it is in \( S_{1/2} \) and not if it is in \( D_{5/2} \). The study involved the demonstration and theory of time-resolved photon counting, and using those counts to infer as accurately as possible the state of the qubit. When a number of counts are obtained from the PMT, the state of the ion may be misidentified for various reasons. A major problem is the finite lifetime of the \( D_{5/2} \) shelf – if it decays near the start of the counting period, the ion will scatter many photons and the “bright” state will be incorrectly inferred. Alternatively an ion, originally in the bright state, might be
shelved into $D_{3/2}$ by the 397 nm (acting off-resonantly on the 393 nm transition) or the 866 nm (acting off-resonantly on the 850 nm transition). This will spuriously lead to a “dark” result.

I used rate equations to estimate the rate of these bright→dark processes. By default transitions does not include such far off-resonant effects. For instance, a 397 nm beam in the model can only excite $S_{1/2} \rightarrow P_{1/2}$; never the 393 nm transition $S_{1/2} \rightarrow P_{3/2}$. To calculate the effect of 397 nm beam on the 393 nm transition, we must add a 393 nm beam to the model and set its detuning to be 223 cm$^{-1}$ to the red.

I set up such a simulation with laser intensities relevant to the experiment ($I_{397} = 7.6 I_0$; $I_{866} = 6.3 I_0$), both with equal $\sigma^+$ and $\sigma^-$ components. The off-resonant actions of the beams on the 393 nm or 850 nm transitions could be included individually or together; I also allowed the 866 nm beam to off-resonantly excite the 854 nm transition, desheling the ion (although as shown below, this has negligible effect compared to the spontaneous decay rate). The ion started in $S_{1/2, -1/2}$, and the state populations as a function of time were calculated. The shelving rates are shown in Table 3.3. The shelving rates are constant for pulse times from about 1 $\mu$s to 0.1 s, but are only approximately linear with laser intensity (because they depend on the populations of the $S_{1/2}$ or $D_{3/2}$ levels, as well as the transition rate per unit population).

<table>
<thead>
<tr>
<th>Beam / nm</th>
<th>Intensity / $I_0$</th>
<th>Shelving Rate at Given Intensity / s$^{-1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>397</td>
<td>7.6</td>
<td>$2.6 \times 10^{-5}$</td>
</tr>
<tr>
<td>866</td>
<td>6.3</td>
<td>$1.7 \times 10^{-7}$</td>
</tr>
<tr>
<td>Both</td>
<td></td>
<td>$2.6 \times 10^{-5}$</td>
</tr>
</tbody>
</table>

Table 3.3: Shelving rates due to off-resonant excitation by 397 nm and 866 nm light. Intensities are given in terms of saturation intensities of the 397 nm and 866 nm transitions that the lasers are resonant with, rather than of the 393 nm or 850 nm transitions.

Alice Burrell (née Myerson) and David Lucas measured this experimentally. The fluorescence of a $^{40}$Ca$^+$ was monitored for several hours (with 397 nm and 866 nm lasers applied). Several times the count rate suddenly dropped for $\sim 1$ s – if all these events corresponded to the ion being shelved to $D_{5/2}$, their frequency would reveal the off-resonant shelving rate as in the simulation. However, the ion may become invisible for reasons other than shelving; for instance a collision with a gas molecule might give it a large amount of energy. Doppler cooling is inefficient for such hot ions, leading
3.5. SIMULATIONS OF FAR OFF-RESONANCE

to (and because of) a very low photon scattering rate. These events could sometimes be distinguished from shelving events because the fluorescence rises gradually as the ion cools down; in contrast an ion decaying from the shelf will become bright again suddenly. It is impossible to tell heating events from shelving events with certainty. But the shelving rate is estimated to be of order $6 \times 10^{-4} \text{s}^{-1}$.

The experimental value is larger than my simulation, with several possible explanations. A laser diode emits some light as amplified spontaneous emission (ASE). This can have a large wavelength spread, $\pm \sim 5 \text{nm}$, and so could excite off-resonant transitions more rapidly than a monochromatic beam. Collisions with gas molecules could impart enough energy to the ion to change its internal energy level (potentially shelving it), even if the collision is not energetic enough to affect the ion’s motion. This rate is difficult to estimate because pressure gauges are extremely unreliable at ultra-high vacuums such as in our vacuum chamber.

3.5.3 Deshelving Effect on $^{40}\text{Ca}^+$ of 850 nm and 866 nm Light

An ion in the $D_{5/2}$ shelf is transferred out of it with 854 nm light. This transition can be off-resonantly excited by either the 866 nm or 850 nm lasers. I do a similar simulation to the previous section. A $^{40}\text{Ca}^+$ ion is prepared in a state in $D_{5/2}$, and a beam on the 854 nm transition (but far detuned to correspond to an 866 nm or 850 nm laser) is added to the model. The state populations are monitored as a function of time, and the deshelving rates recorded in Table 3.4. As noted above, the spontaneous decay of the $D_{5/2}$ level dominates the simulation at low laser intensities (the rate is $0.856(5) \text{s}^{-1}$). I set to zero the Einstein A coefficients of the two quadrupole decays from $D_{5/2}$ and $D_{3/2}$ to leave only the stimulated rate. This was more convenient than subtracting the spontaneous rate away from the simulation, but gave the same results to the given precision. The results are slightly different for the different $M_J$ state in which the ion was prepared, because of the Clebsch-Gordan coefficients. The deshelving rate is linear with intensity over many orders of magnitude.

3.5.3.1 $^{43}\text{Ca}^+$

An experiment was performed with a $^{43}\text{Ca}^+$ ion to measure this rate. The ion was shelved with probability 99%, followed by a gap of 2 ms. An 850 nm beam was pulsed on during that gap, and the time of the pulse was variable. After the gap came the
Table 3.4: Desheling rates due to off-resonant excitation by 850 nm and 866 nm light. Intensities are given in terms of saturation intensities of the 866 nm and 850 nm transitions that the lasers are resonant with, rather than of the 854 nm transition.

<table>
<thead>
<tr>
<th>Beam / nm</th>
<th>Desheling Rate per Unit Intensity / $s^{-1}I_0^{-1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>866</td>
<td>$1.3 \times 10^{-5}$</td>
</tr>
<tr>
<td>866</td>
<td>$7.6 \times 10^{-6}$</td>
</tr>
<tr>
<td>866</td>
<td>$5.1 \times 10^{-6}$</td>
</tr>
<tr>
<td>850</td>
<td>$9.8 \times 10^{-5}$</td>
</tr>
<tr>
<td>850</td>
<td>$5.9 \times 10^{-5}$</td>
</tr>
<tr>
<td>850</td>
<td>$3.9 \times 10^{-5}$</td>
</tr>
</tbody>
</table>

usual fluorescence detection stage. For each value of the pulse time, the sequence was run 1000 times. The whole experiment was performed twice; once with the 850 nm beam $\sigma^-$ polarised, and once with it equally $\sigma^+$ and $\sigma^-$. The pulse time was scanned 0 ms to $\approx 2$ ms. The probability of finding the ion shelved fell linearly in both cases (presumably this was really an exponential decay, but this was not evident from the data). The decay rates were 73(3) $s^{-1}$ and 70(6) $s^{-1}$ respectively: no noticeable difference.

Comparing this experiment to simulation is made more difficult because there is a relatively large uncertainty for the intensity of the 850 nm beam. Measurement of beam power and spot size imply that these experiments had intensities of $10^{900}I_0$ and $9800I_0$. But an attempt to find the intensity directly, by comparing fluorescence scans with a Bloch equations model, implies $16500I_0$ and $14800I_0$.

Using the last of these numbers, the 850 nm beam is calculated to deshelve the ion at a rate of $1.2s^{-1}(2s^{-1}$ including the natural $D_{5/2}$ decay). This is clearly much less than the experimental result; we attribute the excess deshelving rate in the experiment to ASE. It would take only $8 \times 10^{-6}I_0$ of resonant 854 nm light to give the experimental decay rate. Figure 3.7 shows the experiment and the simulation.

The ASE could be greatly attenuated with a second diffraction grating in the beam path. In a previous experiment to measure the lifetime of $D_{5/2}$ in $^{40}$Ca$^+$, a second grating and iris were added to the 866 nm laser which reduced the effect of ASE at 854 nm by five orders of magnitude.
3.6 Simulations of Optical Pumping into $^{43}\text{Ca}^+$ Clock States

Another application of rate equations was to simulate state preparation by optical pumping in $^{43}\text{Ca}^+$. In most of our current experiments this means using circularly polarised 397 nm light, beamed parallel to the magnetic field to produce pure $\sigma-$ ($\sigma+$) polarised transitions at the ion, optically pumping the ion into $S_{1/2}^{4-4}$ ($S_{1/2}^{4,+4}$). The prepared state will not be pure if the beam is not parallel to the magnetic field or if it is not purely circularly polarised.

Currently we cannot prepare the $M_F = 0$ clock states. For experiments with a field-insensitive qubit [58] we made do by preparing all of the $S_{1/2}^3$ states with approximately equal probability, by switching off the 3.2 GHz EOM to leave $S_{1/2}^{4} \rightarrow P_{1/2}^{4}$ ($\sigma\pm$ polarisation) as the only 397 nm beam.

Figure 3.7: The decay of the $D_{5/2}$ level stimulated by off-resonant 850 nm light. The simulation, using $I_{850} = 14800 I_0$ split equally between $\sigma\pm$, shows a much lower decay rate than the experiments, suggesting the effect of ASE. The dotted lines are weighted linear fits to the experimental data. The simulation has been normalised to an initial population of 0.984.

Figure: The decay of the $D_{5/2}$ level stimulated by off-resonant 850 nm light. The simulation, using $I_{850} = 14800 I_0$ split equally between $\sigma\pm$, shows a much lower decay rate than the experiments, suggesting the effect of ASE. The dotted lines are weighted linear fits to the experimental data. The simulation has been normalised to an initial population of 0.984.

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But $M_F = 0$ states can be prepared with a linearly polarised beam whose electric field component is parallel to the applied magnetic field at the ion (the beam itself must be at right angles to the magnetic field, a direction that is impossible in our current experiment). This is because transitions with $\Delta F = 0$ and $M_{F,i} = 0 \rightarrow M_{F,j} = 0$ are forbidden, so applying $S_{1/2}^i \rightarrow P_{1/2}^i$ and $S_{1/2}^i \rightarrow P_{1/2}^i$ beams will cause population to build up in the dark state $S_{1/2}^0$. Unfortunately, whereas preparing $S_{1/2}^{\pm4}$ is limited entirely by the purity of the circularly polarised pumping beam, preparing a clock state is fundamentally limited by the fact that $S_{1/2}^{4,0} \rightarrow P_{1/2}^{3,0}$ is not forbidden.

In Figure 3.8 I show the results of simulations of this process. A variety of 397 nm intensities were chosen, each split equally between the two frequencies, tuned to resonance and perfectly $\pi$ polarised. The 866 nm intensity was fixed at 100 $I_0$ (this does not significantly affect the final result), split equally $\sigma \pm$. State-preparation pulses, lasting for a particular time, were simulated for a range of 866 nm detunings, and the highest $S_{1/2}^{4,0}$ population was recorded. The pulse time was also scanned. Figure 3.8 thus shows the best state preparation for a given time and 397 nm intensity.

![Diagram](image)

Figure 3.8: Simulation of optical pumping into $S_{1/2}^{4,0}$. At each point, the detuning of the 866 nm beam was optimised to the nearest 5 MHz.

Moderate fidelity is possible moderately rapidly; 98% in $\sim 20 \mu s$. But even an
unfeasibly slow pulse (0.1 s) can achieve only 98.93%. It is possible that this could be increased by varying other parameters, although a great improvement seems unlikely. Kajita et al. studied this form of optical pumping using their limited Bloch equations model [132] (and see Section 3.4.1). They state 98.2% as the maximum $S_{1/2}^{43}$ population, although it is unclear whether this is a rigorous limit or simply the best value found by their search.
Chapter 4

Readout

“Readout” refers to the process of measuring the state of a qubit. This is obviously necessary to extract results from a quantum computer, but it has more general significance too. The standard method of quantum error correction requires some qubits to be measured at each correction step (allowing a classical computer to diagnose what error, if any, occurred, and choose single qubit gates to correct the error). If the measurement is not of high enough fidelity, the correction will fail and errors will accumulate in the calculation. Measurement does not have to be as accurate as two-qubit logic gates, because many more gates are performed than measurements. For instance Steane estimates 2-qubit gate error probability \( \lesssim 10^{-4} \) for a large-scale quantum computer, while allowing 1-qubit gates and measurements to be ten times worse [134].

There is also work on one-way, or measurement-based, quantum computing [86]. An array of qubits would be mutually entangled in the computer’s initialisation phase, and the calculation would proceed only by measurements and single-qubit gates. The maximum allowable measurement error for fault-tolerant computation is thought to be \( \sim 10^{-3} \) in this model [135].

Measurement of trapped-ion qubits almost always involves forcing the ion to fluoresce if-and-only-if it is in a particular qubit state.[4] The other state remains dark. The ion is observed with a PMT or a camera, and the number of photons collected reveals the original state. The simplest discriminant is to count for a fixed time, and if more photons are detected than some fixed threshold, the ion is declared bright. General limits on the accuracy of such a method have been investigated, and more efficient discriminants

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[4] The proposed ionisation method of Stock and James [86] (mentioned in Section [4.1.3.1]) is an exception.
have been developed that take account of the photon arrival times; see Myerson et al. and references therein.

Some ion trap groups (such as Innsbruck) work with optical qubits – qubit states separated by large energy gaps, the upper level being metastable and out of the usual Doppler cooling transitions (in Ca$^+$ the levels would be S$_{1/2}$ and D$_{5/2}$). In this case the qubit states are intrinsically bright and dark. The upper level is often called a “shelf”.

A qubit stored in a hyperfine-split ground level may allow similarly straightforward readout; if the splitting is large and a cycling transition is available for the bright state. Where those conditions do not apply, or with Zeeman-split ground-level qubits, the qubit states must be mapped to bright and dark states. Usually this means selectively transferring ions in one qubit state to a shelf level; for instance the Innsbruck group implements electron shelving from $^{43}$Ca$^+$ hyperfine qubits using $\pi$-pulses on the S$_{1/2}$ → D$_{5/2}$ quadrupole transition.

Such a quadrupole laser is technologically demanding, so instead our group uses a 393 nm beam to shelve Ca$^+$. This excites an ion in the ground level to P$_{3/2}$, from whence it can decay to D$_{5/2}$. The branching ratio to the shelf is only 6.2% (Table 3.2) and the ion will most likely fall back to S$_{1/2}$; but after several photons have been scattered the S$_{1/2}$ population will be negligible.

In $^{40}$Ca$^+$ the shelving is made state-selective by use of polarisation (Figure 4.1). Suppose we want to shelve only from S$_{1/2, +1/2}$. We polarise the 393 nm beam $\sigma^+$, making S$_{1/2, +1/2} \rightarrow$ P$_{3/2, +3/2}$ a cycling transition (the ion will not decay into the other qubit state). To prevent the other qubit state S$_{1/2, -1/2}$ being shelved, a very intense 850 nm $\sigma^-$ beam is shone onto the ion. When its detuning is correct, the 850 nm beam creates a dark resonance with the 393 nm beam – but only for S$_{1/2, -1/2} \rightarrow$ P$_{3/2, +1/2}$ because the 850 nm $\sigma^-$ beam does not interact with P$_{3/2, +3/2}$. This is called Electromagnetically-Induced Transparency (EIT). Excitation from S$_{1/2, -1/2}$ is thus prevented, and we have our state-selective shelving mechanism. We achieve up to 90% fidelity with this method. See Matt McDonnell’s thesis for a full discussion.

In $^{43}$Ca$^+$ we have devised and implemented a state-selective shelving method that is both more accurate than EIT shelving of $^{40}$Ca$^+$, and more resilient against imperfections such as drift of laser detuning, impure polarisation, large linewidth etc.
Figure 4.1: An illustration of EIT readout of $^{40}\text{Ca}^+$, to accompany the explanation in the text. Dashed lines indicate spontaneous decay. The decays $P_{3/2, +3/2} \rightarrow D_{1/2, +3/2}$ and $P_{5/2, +3/2} \rightarrow D_{5/2, +1/2}$ are not shown (for clarity), but will reduce the shelving fidelity as discussed for $^{43}\text{Ca}^+$ (the 850 provides some repumping).

4.0.1 Notation

I will assume throughout this section that $|1\rangle$ is the qubit state to be shelved, and $|0\rangle$ the state to be left in the ground level.

Our measure of the accuracy of a readout process will be the fidelity $\mathcal{F}$, equal to $1 - \epsilon$ where $\epsilon$ is the average error. $\mathcal{F}$ is the probability of measuring the state correctly, assuming that $|1\rangle$ and $|0\rangle$ are equally likely to occur. Let $\epsilon_{|0\rangle}$ be the probability that we shelve the ion when it was in state $|0\rangle$, and $\epsilon_{|1\rangle}$ the probability that is was not shelved when it was in state $|1\rangle$. Then

$$\epsilon = \frac{1}{2} \left( \epsilon_{|0\rangle} + \epsilon_{|1\rangle} \right).$$

(4.1)

Note that $\mathcal{F} = \epsilon = \frac{1}{2}$ corresponds to entirely useless readout (such as if the result is completely random for both states; or if the ion is always shelved from both states). In the theory section of this chapter, I will use these terms purely for errors in the
shelving phase of readout. However in the experimental section I will use them more loosely to refer to the whole readout process, including errors with state-preparation and fluorescence-detection.

4.1 Shelving $^{43}$Ca$^+$

We choose qubit state $|1\rangle$ to be in the $S_{1/2}^4$ manifold, and $|0\rangle$ to be in $S_{1/2}^3$. We usually use the “stretch” states $S_{1/2}^{4,+4}$ and $S_{1/2}^{3,+3}$ as qubit states in experiments, because $S_{1/2}^{4,+4}$ is easy to prepare by optical pumping. The 3.2 GHz hyperfine splitting between the qubit states allows us to selectively excite one of them – the other is far off resonance. We use $S_{1/2}^4 \rightarrow P_{5/2}^0$ as the shelving transition because $P_{3/2}^5$ cannot decay to the other qubit state $S_{1/2}^3$.

At best, this shelving method still has $\epsilon_{|1\rangle} = 0.1012(6)$. This is because $P_{3/2}^3$ can also decay to $D_{3/2}^5$. The probability of eventually shelving to $D_{3/2}^5$ is

$$\frac{\text{Br}(P_{3/2}^3 \rightarrow D_{3/2}^5)}{\text{Br}(P_{3/2}^3 \rightarrow D_{3/2}^5) + \text{Br}(P_{3/2}^3 \rightarrow D_{3/2}^4)} = \frac{0.0587(2)}{0.0587(2) + 0.00661(4)} = 0.8988(6)$$

(4.2)

where $\text{Br}(P_{3/2}^3 \rightarrow D_X)$ is the overall branching ratio [20]. We seek to improve $\epsilon_{|1\rangle}$ by re-climbing most of the population in $D_{3/2}$, using light at 850 nm. Figure 4.2 shows the states involved.

The probability of each state $D_{3/2}$ can become populated after a pure $\sigma+ 393$ nm pulse: $D_{3/2}^{5,+5}$, $D_{3/2}^{5,+4}$ and $D_{3/2}^{4,+4}$; with 60%, 12% and 28% of the $D_{3/2}$ population respectively. 850 nm $\sigma+$ light will reclaim the population in $M_F = +4$ through $P_{3/2}^{5,+5}$ – the ion is thus unable to fall back into the $|0\rangle$ qubit state. Once $D_{3/2}^{M_F = +4}$ are empty, 850 nm $\pi$ polarised light can be safely applied to reclaim $D_{3/2}^{5,+5}$ through $P_{3/2}^{5,+5}$ (to get pure $\pi$ polarised light the laser beam must be at right angles to the magnetic field; unfortunately our apparatus does not have a window in the right place, so we cannot use this step in practice). $\sigma-$
Figure 4.2: The transitions involved in shelving from a stretched state in $^{43}\text{Ca}^+$. Note that 23.0 MHz is the linewidth of the 393 nm transition (and the 850 nm and 854 nm transitions), rather than the decay rate on that transition (which is $2\pi \times 23.0$ MHz $\times \text{Br}(P_{3/2}^{5/2} \rightarrow S_{1/2}^{3/2}) = 2\pi \times 21.5$ MHz).

Polarised 850 nm light must be avoided, otherwise the ion could be excited through some state that isn’t $P_{3/2}^{5/2}$, ultimately allowing it to fall into $S_{1/2}^{3}$ where it will appear to be $|0\rangle$.

The three pulses 393 nm $\sigma^+$, 850 nm $\sigma^+$ and 850 nm $\pi$ are repeated as many times as desired, at each step reducing the unshelved population by a factor of (ideally) ten. It is most efficient to finish with a final 393 nm pulse. The sequence can thus be described as

$$(393\sigma^+, 850\sigma^+, 850\pi)^n, 393\sigma^+$$  \hspace{1cm} (4.3)

where we need to determine a suitable number of repeats $n$.

### 4.1.2 Single Pulse Shelving

We discovered experimentally that we could achieve high-fidelity shelving with a single pulse of 393 nm and 850 nm light together, when the 850 nm beam was at a small angle to
the magnetic field direction. Even if the 850 nm beam were perfectly circularly polarised, it would still be able to excite $\pi$ transitions.

To show this, it is convenient to decompose the light field at the ion into components that drive $\pi$, $\sigma^+$ and $\sigma^-$ transitions. The intensity of each component ($I_{\pi}$, $I_{\sigma^+}$, $I_{\sigma^-}$) is the absolute square of the amplitude of the oscillating electric field projected onto that component (i.e. $I_{\pi} \propto E_z^2$, $I_{\sigma^+} \propto |E_x + iE_y|^2$, $I_{\sigma^-} \propto |E_x - iE_y|^2$). For a right-circularly polarised beam, propagating at an angle $\theta$ to the magnetic field (which is along the $z$ axis), we have

$$I_{\pi} = I \frac{(\sin \theta)^2}{2}, \quad I_{\sigma^+} = I \frac{(1 + \cos \theta)^2}{4}, \quad I_{\sigma^-} = I \frac{(1 - \cos \theta)^2}{4} \quad (4.4)$$

(from Webster [110, Section 4.5.1] or by considering Jones vectors and rotation matrices [137]). If the beam is linearly polarised in the plane made by the beam itself and the magnetic field direction, we have

$$I_{\pi} = I \sin^2 \theta, \quad I_{\sigma^+} = I \frac{(1 + \cos \theta)^2}{2}, \quad I_{\sigma^-} = I \frac{(1 - \cos \theta)^2}{2}; \quad (4.5)$$

if it is linearly polarised perpendicular to that plane then

$$I_{\pi} = 0, \quad I_{\sigma^+} = \frac{I}{2}, \quad I_{\sigma^-} = \frac{I}{2}. \quad (4.6)$$

In the case of our 850 nm circularly polarised beam, we take the small-$\theta$ approximation to Equations (4.4), and find

$$I_{\pi} \approx I \frac{\theta^2}{2}, \quad I_{\sigma^+} \approx I \left(1 - \frac{\theta^2}{2}\right), \quad I_{\sigma^-} \approx I \frac{\theta^4}{16} \quad (4.7)$$

showing that the rate of $\pi$ transitions increases much faster than the rate of unwanted $\sigma^-$ transitions as $\theta$ increases. As seen in Figure 2.3, the 850 nm beam is nominally at 2.3° to the magnetic field direction so

$$I_{\pi} : I_{\sigma^+} : I_{\sigma^-} = 8.1 \times 10^{-4} : 0.99919 : 1.6 \times 10^{-7}. \quad (4.8)$$

This does not include any $\sigma^-$ light introduced through imperfect circular polarisation of the beam itself.

### 4.2 Optimisation Simulations

Having decided broadly on the pulse sequence, we need to choose the intensities and durations of each pulse, and the number of repeats $n$. I set up rate equations simulations
of such a sequence as MATLAB functions. The functions take the pulse lengths and intensities as inputs, and calculate \( \log_{10}(|\epsilon_0| + |\epsilon_1|) = \log_{10}(2\epsilon) \) that that sequence would achieve. The functions are then used in one of MATLAB’s built-in optimisation functions, that attempts to minimise \( \epsilon \) (I take the logarithm to try to encourage the optimisers to continue working even when the error \( \epsilon \) is already very small). I constrain the shelving sequence to take a fixed total amount of time.

To reduce the number of dimensions to the multi-pulse problem, I generally assume all pulses of the same type are the same length and intensity. So the parameters to optimise are \( t_{393}, t_{850\sigma^+} \) (\( t_{850\pi} \) is then the remaining time).

The 393 nm frequency is of course tuned to \( S_{1/2}^{1/2} \rightarrow P_{3/2}^5 \), and the 850 nm to \( D_{3/2}^5 \rightarrow P_{3/2}^5 \).

There is a bit more choice for the 850\( \sigma^+ \) beam because it must reclaim from both \( D_{3/2}^5 \) and \( D_{3/2}^4 \) – I have chosen to include a frequency component at both \( D_{3/2}^5 \rightarrow P_{3/2}^5 \) and \( D_{3/2}^4 \rightarrow P_{3/2}^5 \). Each of these components (separated by 160 MHz) has an independently adjustable intensity. Experimentally it would be a little easier (and probably just as effective) to use a single beam tuned between those two transitions, but this setup is simpler to simulate, and possibly a more stable optimisation problem.

I have not included any far-off-resonant effects for speed and simplicity. However, deshelving caused by the 850 nm beam (Section 3.5.3) would be an extra source of error. The optimal 850 intensities turn out to be \( \lesssim 10^4 I_0 \), which in the worst case would add \( \sim 7 \times 10^{-5} \) to \( \epsilon_{11} \) – just a small adjustment to my final results. This neglects possible ASE in the 850 nm beam; ASE could be significantly reduced by adding a second diffraction grating to that beam path [100].

### 4.2.1 Optimisation Methods

There are numerous ways to optimise a general function. I investigated several methods to find the most effective. The obvious way is to use an algorithm with constraints, and set the constraints to be “sum of pulse lengths is equal to total time”. This is reinforced by the MATLAB documentation, which states, [138] Page 4-47] “Fewer function evaluations are usually taken when a problem has more constraints and bound limitations because the optimization makes better decisions regarding step size and regions of feasibility than in the unconstrained case. It is, therefore, good practice to bound and constrain problems, where possible, to promote fast convergence to a solution.” I use MATLAB’s \texttt{fmincon} for this, and in the figures below it is labeled “Constrained”.
There are other options though, and I tried a variety of methods over the course of the project. One can use penalty functions to prevent unphysical values being used. For instance, none of my optimisable parameters should be negative. I set my simulation function to check that all the parameters it is passed are positive. If not, it returns the absolute value of the most negative parameter: a positive number that “pushes” the optimiser back into the feasible region (normally the function returns a negative result because I take the logarithm of a quantity $\leq 1$). In the figures below, this method is labeled “Penalty”.

John D’Errico [139, Section 19] suggests, “The simple trick is to use a transformation of variables. Allow the optimizer to leave your variable unconstrained, but then inside the objective function you perform a transformation of the variable. If a variable must be positive, then square it. If it must lie in a closed interval, then use a sine transformation to transform an unbounded variable into one which is implicitly bounded.” I implemented this by optimising $I_{393}'$, $t_{393}'$ and $t_{850\sigma^+}$, where

$$
\begin{align*}
I_{393} &= I_{393}'^2, \\
I_{393} &= t_{393} = \frac{t_t}{n+1} \left( \frac{\arctan(t_{393}')}{\pi} + \frac{1}{2} \right), \\
t_{850\sigma^+} &= \frac{t_t - (n+1)t_{393}}{n} \left( \frac{\arctan(t_{850\sigma^+}')}{\pi} + \frac{1}{2} \right).
\end{align*}
$$

(4.9)

We need not transform $t_{850\pi}$, because it is still just the remainder of $t_t$. The upshot is that the primed optimisation parameters can freely vary from $-\infty$ to $\infty$, and they get transformed into times that fill up $t_t$ before the simulation runs. In the figures below, this method is labeled “Transformed”.

An alternative idea is to split up the optimisation. I created a subfunction that optimises the 393 nm intensity given a sequence with pulse times. This is a simple, robust 1D optimisation. This subfunction is then taken as the input function to a routine that optimises the pulse times. In the figures below, this method is labeled “SOTI” for Separate Optimisation of Time and Intensity.

Figure 4.3 shows the optimised shelving fidelity predicted by the different methods, and Table 4.1 shows how long they took. SOTI is by far the slowest yet is not the best performer; the Penalty function method finds the highest Fidelities. The method with Transformed variables performed worst. However, in other simulations different methods seem to do best. In particular, the simulations of Section 4.2.2 used the Transformed method. Its speed allowed a wide variety of starting guesses to be tried, the best result being chosen later. Two of MATLAB’s optimisation routines were used in series (the
Figure 4.3: Rate equations optimisation simulation of a shelving sequence 
\((393\sigma^+, 850\sigma^+, 850\pi)^n, 393\sigma^+)\). Four different approaches to optimisation have
been used, as described in Section 4.2.1. The 393 nm laser is tuned to \(S_{1/2}^{4,+4} \rightarrow P_{3/2}^{5,+5}\); 850 nm \(\sigma^+\) is tuned to \(D_{3/2}^{4,+4} \rightarrow P_{3/2}^{5,+5}\); 850 nm \(\pi\) is tuned to \(D_{3/2}^{5,+5} \rightarrow P_{3/2}^{5,+5}\). The two
850 nm beams are each assumed to have 1000 \(I_0\) intensity. Total time \(t_t = 100\mu s\).

<table>
<thead>
<tr>
<th>Optimisation Method</th>
<th>Time Taken / minutes:seconds</th>
</tr>
</thead>
<tbody>
<tr>
<td>SOTI</td>
<td>56:46</td>
</tr>
<tr>
<td>Penalty</td>
<td>9:00</td>
</tr>
<tr>
<td>Transformed</td>
<td>4:52</td>
</tr>
<tr>
<td>Constrained</td>
<td>6:45</td>
</tr>
</tbody>
</table>

Table 4.1: Computational time taken for the optimisations of Figure 4.3. Performed on
a 3 GHz Intel Pentium 4 CPU with 1 GB RAM.

first providing an initial guess to the second), which seemed to give better results than
using either routine singly.

Figure 4.5 shows that the optimised parameters can vary a lot even for similar final
fidelities. One possibility is that the optimiser halts too early because the fidelity is
highly insensitive to some parameters (Section 4.2.3). The tolerances on the routines
Figure 4.4: Probabilities of shelving from individual qubit states, for the simulations of Figure 4.3.

Figure 4.5: The optimised parameters for the simulations of Figure 4.3. The pulse times have been multiplied by the number of pulses in the sequence, so the graph indicates the total time in the sequence devoted to that laser.
had been set to $10^{-10}$ to try to prevent this. We may expect the optimised parameters to vary smoothly as $n$ increases, but this is true only for Penalty; we may guess that this indicates reliability. Again, however, in other simulations SOTI produced the smoothest results.

### 4.2.2 Optimum Fidelity as a Function of Time

#### 4.2.2.1 Multi-pulse

Choosing $n = 16$ as a large number of repeats (under the assumption that higher fidelity is obtained by dividing the total allowed time into more pulses), I tried to find the very highest fidelity possible for a given total shelving time. Figure 4.6 shows the result. The peak is at 100 $\mu$s total, achieving a fidelity of 99.968%. The decay from the $D_{5/2}$ shelf means that we do not benefit from taking any longer over the shelving. But we also suffer if the total time is made much shorter – the 393 nm intensity must then be raised to compensate, the effective linewidth increases by power broadening, the excitation rate from $S_{1/2}$ increases and hence $\epsilon_{|0\rangle}$ increases (though $\epsilon_{|1\rangle}$ falls again as $t_t$ is reduced below $\sim 1 \mu$s). We can see this in Figure 4.7 that shows $\epsilon_{|0\rangle}$ and $(1-\epsilon_{|1\rangle})$ separately, and Figure 4.8 that shows the optimal laser intensities. Figure 4.9 shows the pulse times, in the form of the fraction of the total shelving time $t_t$ for which that pulse is active. At 100 $\mu$s these parameters are shown in Table 4.2.

<table>
<thead>
<tr>
<th>Laser</th>
<th>Intensity / $I_0$</th>
<th>Fraction of $t_t$</th>
<th>Pulse Time / $\mu$s</th>
</tr>
</thead>
<tbody>
<tr>
<td>$850_{\pi^{+} 5\rightarrow 5}$</td>
<td>3100</td>
<td>0.03091</td>
<td>1.932e-7</td>
</tr>
<tr>
<td>$850_{\pi^{+} 4\rightarrow 5}$</td>
<td>4400</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$850_{\pi 5\rightarrow 5}$</td>
<td>59</td>
<td>0.02734</td>
<td>1.709e-7</td>
</tr>
<tr>
<td>$393_{\pi^{+}}$</td>
<td>0.014</td>
<td>0.9418</td>
<td>5.54e-6</td>
</tr>
</tbody>
</table>

Table 4.2: Multi-pulse sequence parameters for the best shelving achieved in these simulations. Fidelity 99.968% at $t_t = 100 \mu$s using the sequence $((393_{\pi^{+}}, 850_{\pi^{+}}, 850_{\pi})^{16}, 393_{\pi^{+}})$.

The requirement for sidebands in the 850 nm beam may seem awkward. I repeated the simulation leaving out the $850_{\pi^{+} 4\rightarrow 5}$ beam (i.e. assuming monochromatic 850 nm light on the $5 \rightarrow 5$ line), and achieved very similar results (see Table 4.3). The peak fidelity is just $10^{-5} \%$ (absolute) lower than the full version, and occurs 10 $\mu$s later.
Figure 4.6: Multipulse shelving simulation with $n = 16$, from stretch states, showing only the highest fidelity at each value of total time $t_t$.

Figure 4.7: Shelving errors from each qubit state, for the simulations of Figure 4.6.
4.2. OPTIMISATION SIMULATIONS

Figure 4.8: Optimal intensities for the simulations of Figure 4.6.

Figure 4.9: Optimal pulse times for the simulations of Figure 4.6.
The parameters plots Figures 4.8 and 4.9 are extremely noisy, demonstrating how bad the optimiser is. In Figure 4.10 I show the fidelities that the optimiser achieved when starting with various different guesses – Figure 4.6 is simply the best of these. The starting guesses are fixed (I do not use the previous best solution as the guess for the next point) and the found solution jumps as $t_t$ increases. This is presumably because the basin of attraction\(^2\) has a complex shape that depends on $t_t$, and thus a starting guess lies in different basins for different values of $t_t$. For many of the following graphs, I was able to isolate a particular starting guess that consistently gave the best results for almost the whole range of times; with the optimal parameter graphs also being smooth. But this wasn’t true here. One possible reason why this set of simulations was so bad is that it featured so many parameters: two independent times and four intensities. Optimisation does become more difficult in higher dimensions. Another idea is that the fidelity is relatively insensitive to the parameters in this simulation – the optimiser tries to descend a gradient, and if the function is too flat the optimiser may stop too early.

At very short total times, the shelving is apparently improved by leaving out some pulses altogether. Each coloured line on Figures 4.11-4.14 shows the optimal fidelities and parameters for the sequence $((393\sigma+, 850\sigma+, 850\pi)^{16}, 393\sigma+)$, with some of the beams being left out. As well as the result if all beams are allowed, we see $(393\sigma+)$ alone; $((393\sigma+, 850\pi)^{16}, 393\sigma+)$; and $((393\sigma+, 850\sigma+)^{16}, 393\sigma+)$. Notice how $393\sigma+$ alone is best at times $< 0.6\mu s$; $393$ and $850\pi$ are best in the range $0.6\mu s < t_t < 1.4\mu s$; and using all the beams is best for $t_t > 1.4\mu s$. The naïve explanation is that, at short times, maximising $t_{393}$ (and thus allowing the $393$ intensity to be reduced) yields a greater fidelity than using some of the time to repump from $D_{3/2}$. However, we also find this effect when shelving with a single pulse, so this might not be the correct explanation. Another reason is suggested below.

It is not necessarily best to use $n = 16$ repeats. In Figures 4.15-4.18 I show the optimal results achieved for $n = 16, 8, 4, 2$ and 1. We see that, while large $n$ gives the best fidelity overall, for short total times it is better to have a smaller number of repeats.

---

\(^2\)When trying to find the roots (or extrema) of a function, using some iterative numerical method, the basin of attraction of root $x_i$ is the set of starting guesses $\{x_{0,i}\}$ such that the successive approximations $x_{0,i}, x_{1,i}, x_{2,i}, \ldots$ converge to $x_i$. Many beautiful fractals are based on basins of attraction for, for instance, Newton’s method of root finding. See, for instance, Gleick [?] or almost any other book about chaos and fractals.
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Figure 4.10: Multipulse shelving simulation with \( n = 16 \), from stretch states, showing the optimised fidelity of all starting guesses.

For instance, \( n = 8 \) is marginally best (of the sequences tested) for \( 2 \mu s < t < 7 \mu s \). This could be because a sequence with smaller \( n \) has a higher ratio of 393 nm pulses to 850 nm (because of the final 393 nm pulse), possibly allowing more time overall to be devoted to the 393 nm beam and hence lower 393 nm intensity and higher fidelity.

It might also be due to the absolute duration of the pulses. For a 16-repeat sequence of \( 1 \mu s \) total time, the average pulse length is just 20 ns. \( P_{3/2} \) has a lifetime of 7.4 ns, so there may not be enough time for it to fully decay during every pulse. This could reduce fidelity; for instance if \( P_{3/2} \) was significantly occupied at the start of an 850 nm pulse, the 850 could cause a net transfer to \( D_{3/2} \), rather than from it. Dividing the time into fewer pulses may help ensure that \( P_{3/2} \) is almost empty at the end of each pulse. A similar explanation might explain why, for a fixed 16 repeats, the best shelving at short times omits one or both of the 850 pulses.

For short, intense pulses, the rate equations model may be insufficient, because in reality the dynamics would be dominated by Rabi oscillations. It would be possible to add Rabi oscillations to the model to investigate this regime, without needing full Bloch equations, at the probable expense of more difficult optimisation (Rabi oscillations may
Figure 4.11: Multipulse shelving simulation with $n = 16$, from stretch states, showing optimised shelving fidelity.

Figure 4.12: Shelving errors from each qubit state, for the simulations of Figure 4.11.
4.2. OPTIMISATION SIMULATIONS

Figure 4.13: Optimal intensities for the simulations of Figure 4.11.

Figure 4.14: Optimal pulse times for the simulations of Figure 4.11.
lead to numerous local minima).

### 4.2.2.2 Single Pulse, Multiple 850 nm Beams

For the single pulse shelving method, I first assumed exactly the same laser situation as in the previous section (three 850 nm beams, each with its intensity independently optimised). But all four beams are switched on together during a pulse of length \( t_t \). Figures 4.19-4.21 show the results.

We see that although the overall best fidelity is very slightly lower than for multipulse shelving (99.965% rather than 99.968%) the biggest difference is that the fidelity takes more than twice as long to reach the 99.9% level (8.4 \( \mu s \) rather than 3.5 \( \mu s \)). This could be because the 850\( \pi \) beam is on while there is still significant population in \( D_{3/2}^{(4,5),+4} \), exciting some population to \( P_{3/2} \) states that are *not* \( P_{3/2}^{5,+,5} \), whence it can ultimately fall back to \(|0\rangle\) and be lost. The optimiser has to choose the 850\( \pi \) intensity to compromise between that process, and leaving population in \( D_{3/2}^{5,+,5} \); while in the pulsed method the intensity can be made much stronger.

Figures 4.8 and 4.21 show that all the 850 beams are stronger in the pulsed method than in the single pulse method. Remember that very high-intensity 850 beams *equalise* the populations of \( P_{3/2} \) and \( D_{3/2} \), and so could reduce the population of \( P_{3/2} \) and hence the shelving rate. This might also explain why, at short times, it is best to leave some of the 850 beams off altogether.

### 4.2.2.3 Single Pulse, Single 850 nm Beam

Here I simulate another single-pulse shelving method (850 and 393 on at the same time). This time I use a single, monochromatic, circularly polarised 850 nm beam at angle \( \theta \) to the magnetic field direction – this is the situation in our experiment as described in Section 4.1.2. Our experiment has \( \theta = 2.3(1)° \). For the simulation I take a range of angles, starting at 90° and halving each time: 90°, 45°, 22.5°, 11.25°, 5.625°, 2.8125°, 1.40625°, 0.703125° and 0.3515625°. However, I used 2.3° rather than 2.8125° for better comparison with the experiment. Optimisation is relatively easy now because there are only three quantities to optimise: the 393 nm and 850 nm intensities, and the frequency of the 850 nm beam. I optimised the frequency manually, running the optimisation repeatedly while scanning the frequency and taking more closely-spaced points where the results looked good. The automatic optimiser might have found only local optima.
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Figure 4.15: Multipulse shelving simulation with various $n$, from stretch states, showing optimised shelving fidelity.

Figure 4.16: Shelving errors from each qubit state, for the simulations of Figure 4.15.
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Figure 4.17: Optimal intensities for the simulations of Figure 4.15.

Figure 4.18: Optimal pulse times for the simulations of Figure 4.15.
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Figure 4.19: Single pulse shelving simulation, from stretch states, showing optimised shelving fidelity.

Figures 4.22-4.25 show the frequency scan for every second 850 angle. The frequencies of the hyperfine components of the 850 nm transition have also been marked on, and labeled with the notation: $D_{3/2}^{F=7} \rightarrow P_{3/2}^{F=7}$. (note this is the opposite direction to the notation of Appendix A). Each coloured line shows the scan for a particular total shelving time. The optimal frequency for each time is marked with a filled symbol. A few scans had their maxima at detunings well outside the range shown; they can be seen in Figure 4.28.

We see an interesting trend. At $\theta = 90^\circ$ (the polarisation ratio at the ion is $I_\pi : I_{\sigma^+} : I_{\sigma^-} = \frac{1}{2} : \frac{1}{4} : \frac{1}{4}$), the best shelving occurs near the $D^{4}_{3/2} \rightarrow P^{5}_{3/2}$ component, and the worst is near $D^{4}_{3/2} \rightarrow P^{5}_{3/2}$ (except at the shortest times). At $22.5^\circ$ we see deep valleys at $D^{4}_{3/2} \rightarrow P^{4}_{3/2}$, $D^{4}_{3/2} \rightarrow P^{3}_{3/2}$ and $D^{5}_{3/2} \rightarrow P^{4}_{3/2}$. As the angle narrows further, and the beam becomes more purely $\sigma^+$ polarised at the ion, the $D^{5}_{3/2} \rightarrow P^{5}_{3/2}$ component becomes more and more favourable. Below $1.406^\circ$ there is little further change.

The last observation is easiest to explain: the $\pi$ component of the light becomes weaker as $\theta$ falls, so to effectively repump from $D^{5}_{3/2}$ the beam must be tuned more closely to $D^{5}_{3/2} \rightarrow P^{5}_{3/2}$. As $\theta$ becomes larger the $\pi$ component becomes stronger and
Figure 4.20: Shelving errors from each qubit state, for the simulations of Figure 4.19.

Figure 4.21: Optimal intensities for the simulations of Figure 4.19.
4.2. OPTIMISATION SIMULATIONS

Figure 4.22: Single pulse shelving simulation with monochromatic 850 beam at an angle \( \theta \) to the magnetic field, showing optimised shelving fidelity as a function of 850 frequency for \( \theta = 90^\circ \). Maximum fidelity at each value of \( t_1 \) is indicated by a symbol. Vertical lines show positions of the hyperfine components of \( \text{D}_{3/2} \rightarrow \text{P}_{3/2} \), labeled \( F_{\text{lower}} \rightarrow F_{\text{upper}} \).

Figure 4.23: \( \theta = 22.5^\circ \). See caption to figure 4.22.
Figure 4.24: $\theta = 5.625^\circ$. See caption to figure 4.22.

Figure 4.25: $\theta = 1.40625^\circ$. See caption to figure 4.22.
accurate tuning becomes unnecessary, and the $\sigma-$ component is also becoming stronger. $D_{3/2}^4 \rightarrow P_{3/2}^3$ and $D_{3/2}^5 \rightarrow P_{3/2}^4$ have strong $\sigma-$ components from $D_{3/2}^{4,+4}$ and $D_{3/2}^{5,(+4,+5)}$ which the 850 beam had best avoid, else the shelving process loses its selection-rule protection from falling back to $|0\rangle$. Similarly $D_{3/2}^4 \rightarrow P_{3/2}^4$ has a strong $\pi$ component from $D_{3/2}^{4,+4}$ that should be avoided. This explains the valleys in the 22.5° plot. It is not clear why the $D_{3/2}^4 \rightarrow P_{3/2}^5$ transition is favoured for $\theta = 90^\circ$, but becomes a valley at smaller angles.

The overall optimised fidelities, shelving errors and parameters are shown in Figures 4.26-4.28. At 2.3° we should be able to shelve at 99.962% fidelity in 300 $\mu$s, at an entirely reasonable 850 intensity of 190 $I_0$ (the optimal 393 intensity is 0.004 $I_0$). By chance, our experimental beam is close to the optimal angle. For smaller angles, shelving becomes much slower (limited by the low power in the $\pi$ component). Notice that there are places where the optimal 850 detuning (and 850 intensity) become extremely large; however the best shelving at a given angle always occurs at such a time that it avoids those anomalies.

Figure 4.26: Single pulse shelving simulation with monochromatic 850 beam at an angle $\theta$ to the magnetic field, showing optimised shelving fidelity.
Figure 4.27: Shelving errors from each qubit state, for the simulations of Figure 4.26.

Figure 4.28: Optimal intensities and 850 frequency for the simulations of Figure 4.26.
4.2.2.4 Clock States

Future experiments with $^{43}\text{Ca}^+$ will mostly use the $M_F = 0$ clock states, because they have a much lower susceptibility to magnetic field fluctuations than stretched states. When using our shelving procedure from $S_{1/2}^0$, we can no longer rely on using the approximate cycling transitions through $P_{5/2}^5$, so we lose much of the protection against decays to $|0\rangle$. There is some protection due to the 160 MHz hyperfine splitting between $P_{3/2}^5$ and $P_{3/2}^4$: the 393 nm beam is tuned to excite to $P_{3/2}^5$, and selection rules then forbid a direct decay to $S_{1/2}^1$. Figures 4.29–4.32 and 4.33–4.35 are the equivalents of Figures 4.11–4.14 and 4.19–4.21 for shelving from a clock state qubit. The 16-pulse and single-pulse methods both reach a fidelity of 99.64% – an error that is ten times that for shelving from stretch states. This is almost entirely due to a rise in $\epsilon_{|1\rangle}$ rather than $\epsilon_{|0\rangle}$, because unwanted decays to $|0\rangle$ are more likely than with stretch-state shelving.

There might be possible improvements – perhaps allowing extra beams with the polarisations I have so far ignored. But in practice, it might be better to use four microwave or Raman pulses to coherently transfer from clock state to stretch state; $S_{1/2}^{4,0}$ to $S_{1/2}^{4,4}$ [128, Section III.C.2-3]. This becomes worthwhile if the transfer pulses each have average error $8 \times 10^{-4}$. General fault tolerance demands single-qubit gates with errors of order $10^{-3}$ or better, and the same technology could almost certainly perform this function too. However these transfer pulses would not be insensitive to magnetic field fluctuations, and so would be more prone to error than operations between the clock states.

4.2.2.5 Summary

Figure 4.36 compares the multipulse, single-pulse and 850-at-angle methods, summarising Figures 4.15, 4.19 and 4.26. Table 4.3 collects together some of the best optimised results from this section.

4.2.3 Fidelity as a Function of Parameters

It is important to consider how the shelving fidelity is affected by perturbations in the sequence. I have chosen the best of all the preceding simulations as an example, because the perturbations should have a greater relative effect at higher fidelities. As a reminder, this is the pulse sequence $((393\sigma^+, \ 850\sigma^+, \ 850\pi)^{16}, \ 393\sigma^+)$, that achieved a fidelity
Figure 4.29: Multipulse shelving simulation with $n = 16$, from clock states ($S_{3/2}^{1,0}$ and $S_{3/2}^{3,0}$), showing optimised shelving fidelity.

Figure 4.30: Shelving errors from each qubit state, for the simulations of Figure 4.29.
4.2. OPTIMISATION SIMULATIONS

Figure 4.31: Optimal intensities for the simulations of Figure 4.29.

Figure 4.32: Optimal pulse times for the simulations of Figure 4.29.
of 99.968% in 100 µs. Details were in Table 4.2.

First I look at intensity error. Keeping all other aspects of the simulation constant, one of the beams in the sequence had its intensity scanned. The fidelity achieved as a function of the intensity is shown in Figure 4.37. The intensity axis is shown as a multiplier of the optimal intensity, so that \( x = 1 \) represents the optimal sequence for all the lines. We see that shelving is highly insensitive to the 850 intensities – except for having the 850\(\pi\) too weak, the intensities can be orders of magnitude different with very little effect. The 393 intensity is (as expected) much more sensitive; but even so, it can be a factor of three overpowered (or 40% underpowered) and still exceed 99.9% fidelity.

Next, I consider errors in the pulse times. Figure 4.38 shows the shelving fidelity as a function of the fraction of the total time dedicated to a particular pulse. For instance, at \( x = 0.6 \) the red 393 curve shows the result when the seventeen 393 pulses together filled 60% of the total shelving time – the other 40% was divided among 850\(\sigma^+\) and 850\(\pi\) in the same ratio as in the optimal sequence (1.13 : 1, shown as a diamond marker). As in the previous graph, the shelving is resilient to changing the 850 pulses – as long as neither pulse makes up less than \( \sim 20\% \) of the total 850 allowance, the fidelity is very

Figure 4.33: Single pulse shelving simulation, from clock states, showing optimised shelving fidelity.
Figure 4.34: Shelving errors from each qubit state, for the simulations of Figure 4.33.

Figure 4.35: Optimal intensities for the simulations of Figure 4.33.
Figure 4.36: The best fidelities available for shelving from stretch states, for the three major methods discussed in this section, as a function of total shelving time. For multipulse, the maximum over the number \( n \) of repeats has been taken; for 850-at-angle, the maximum over all angles has been taken.

Table 4.3: Summary of the best optimised shelving simulations from Section 4.2.2. The very lowest error achieved with each method is listed, along with the total shelving time required. I also state the error that can be reached with just 10 \( \mu \)s shelving (the time that Steane allows for readout in [134]).
near its optimum. Again, the 393 pulse is much more sensitive, but not too much. As long as the 393 is on for between 62% and 99.6% of the sequence, the fidelity is at least 99.9%. The 393 pulses are each 5.5 µs long; a 0.1 µs timing error would increase the shelving error by only $10^{-6}$ absolute.

Figure 4.39 shows the effect of detuning the lasers from resonance (recall that the 393 is tuned to $S_{1/2} \rightarrow P_{3/2}^-$ and the 850 has components at $D_{3/2}^+ \rightarrow P_{3/2}^-$ and $D_{3/2}^+ \rightarrow P_{3/2}^-$. As may be expected, the 393 is most frequency-sensitive, but an error of $\gtrsim 2$ MHz is needed to significantly reduce the fidelity.

I calculated the effect of polarisation impurity in the laser beams, in Figure 4.40. I have assumed in every case that the impurity appears as $\sigma^-$ polarised light (I did not simulate, for instance, a mis-set waveplate), with an intensity that makes up the stated fraction of the relevant beam. The correctly polarised intensity is reduced to match, so that at a polarisation impurity of 1 the relevant beam is entirely $\sigma^-$ polarised. For the 850$\sigma^+$ beam, I assume both frequency components are affected to the same extent. This time the 850$\sigma^+$ is the most sensitive beam, and 850$\pi$ the least. Notice that even in the worst of these cases, a pure $\sigma^-$ 393 beam, the fidelity is still above 94%.

Figure 4.37: Multipulse shelving simulation with $n = 16$, from stretch states, varying the intensities from the optimum.
Figure 4.38: Multipulse shelving simulation, from stretch states, varying the pulse times from the optimum.

Figure 4.39: Multipulse shelving simulation, from stretch states, varying the laser frequencies.
Finally, the simulations were repeated for the best single shelving pulse (the peak of Figure 4.19). Figures 4.41-4.43 show a similar robustness to the multipulse method; with the exceptions that this time the fidelity is significantly harmed by having too much 850 power, and the single-pulse method is less sensitive to 850σ+ polarisation impurity.
Figure 4.41: Single pulse shelving simulation, from stretch states, varying the intensities from the optimum.

Figure 4.42: Single pulse shelving simulation, from stretch states, varying the laser frequencies.
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Figure 4.43: Single pulse shelving simulation, from stretch states, varying the polarisation impurities of the beams.
4.3 Experiments

4.3.1 850 nm Parallel to Magnetic Field

In an early experiment, the sequence (393, 850, 393, 850, 393) was implemented, on an ion prepared in $S_{1/2}^{1+}$. The 393 nm pulse time was 100 µs; the 850 nm pulse time was scanned. This time, the magnetic field had been aligned along the 850 nm beam direction, so the 850 nm $\pi$ component was very weak. The results, and a simulation of them, are shown in Figure 4.44. The simulation fits the data only if $\sim 2\%$ of the 850 nm beam is set to be $\sigma^-$ polarised; also the simulation assumes 1% initialisation error (prepared in $S_{1/2}^{3+}$). This initialisation error also includes fluorescence-detection errors. The best seven data points ($t_{850} \geq 300$ µs) have an average of 97.7(2)% shelving. Notice that, as the polarisation impurity of the 850 nm beam increases, the shelving becomes much faster for only a small decrease in shelving. But it is only a small decrease compared to the large overall shelving error. [Speed-up???]

![Figure 4.44: Experiment (black points) and simulation of shelving sequence (393, 850, 393, 850, 393). $I_{393} = 0.0097 I_0$, $I_{850} = 2680 I_0$. Simulation assumes 1% preparation impurity. Error bars on the experimental data points are statistical only.](image)
4.3. EXPERIMENTS

4.3.2 850 nm at Small Angle to Magnetic Field

In an attempt to improve the state preparation, we realigned the magnetic field along the 397 nm $\sigma$ beam (improving the purity of $\sigma^+$ light at the ion). Since the 850 nm beam was now at a small angle to the magnetic field, we discovered that it excited $\pi$ transitions at the ion strongly enough to effectively reclaim from $D_{3/2}^{4+5}$ – even after we added a second polarising-beam-splitter (PBS) to the 850 nm beam to improve its polarisation purity.

4.3.2.1 Various Results

The major aim of the experiments was to achieve the best possible fidelity, rather than to test rate equations theory. So we made many trials individually, with various parameters altered, rather than a series of experiments varying only one parameter at a time. The only feasible way to present such results is as a table, and so Table 4.4 shows a selection of results from our final set of experiments. In the next few sections I will select particular rows from the table and explain their significance.

Explanation of fields:

Row: An index number for reference.

Date: The date is in DDMMYY format.

File: Usually the data file is “CA43.xxx” where xxx is this number.

Fidelity, $\epsilon_{|0\rangle}$ and $1 - \epsilon_{|1\rangle}$: These are the fidelities and error probabilities as deduced by detecting fluorescence. Photon counting may give an erroneous reading even if the shelving were perfect, and no attempt is made here to subtract this contribution to the infidelity; typically the contribution is 0.1% infidelity.

$S_{1/2}^{4,+4}$ Preparation: As described below, the fidelity of population preparation depends on the frequency of the 397 nm $\sigma$ beam. This column shows whether the carrier frequency of this beam was tuned to $S_{1/2}^{4} \rightarrow P_{1/2}^{4}$ or $S_{1/2}^{3} \rightarrow P_{1/2}^{4}$ (the sideband excites out of the other hyperfine level of $S_{1/2}$ in both cases). For $3 \rightarrow 4$, the usual optical pumping pulse can be followed by a pulse with this same beam, with the EOM switched off, which should improve the preparation as discussed below.

t$_{393}$ and t$_{850}$: For multipulse sequences, these are the times per pulse. For single-pulse experiments, the time of the combined 393/850 pulse is given as t$_{393}$. 
$I_{393}$ and $I_{850}$: On 290507, a microscope slide pickoff (that reflected some light for spot-size and beam-power measurement) was removed from the $\sigma$ beams’ paths, to improve polarisation purity. From this point on, the listed intensities are less reliable because the beam powers were measured by different sensors.

Sequence: If the entry is a number, that number is $n$ representing the shelving pulse sequence $((393\text{ nm}, 850\text{ nm})^n, 393\text{ nm})$; “Single” refers to a single pulse during which both the 393 nm and 850 nm lasers were switched on.

854 nm Shutter: When the shutter was not used (“N”), the 854 was switched off only using its AOM; leakage through the AOM could contribute to $\epsilon_{|1\rangle}$ by desheling the ion. When the shutter was used (“Y”), the laser was blocked completely during the shelving and fluorescence detection phases.

### 4.3.2.2 Population-Preparation Improvement

For the early experiment of Figure 4.44, the 397 nm laser had its carrier tuned to $S^+_1\rightarrow P^+_1$, the sideband to $S^+_1\rightarrow P^+_1$. This allowed $S^+_1$ to be prepared simply by turning the EOM off. But we discovered that the population preparation was improved by exchanging the frequencies of carrier and sideband. The carrier is the more intense component, so the new tuning increased excitation from $S^+_1$ and so reduced its population. Also, the impact of any polarisation impurity (exciting out of the desired state $P^+_1$) is reduced. This configuration also allowed us to turn the EOM off briefly at the end of state preparation, to pump any remaining population from $S^+_1$ to $S^+_1$.

We performed an experiment that measured the rate at which the 397 nm $\sigma$ beam pumped out of $S^+_1$. Together with simulations, I deduce that the nominally $\sigma+$ beam contains $0.9(2)\%$ $\sigma-$ impurity (assuming all the depumping is due to this beam; in fact there is also a large contribution from the 397 nm Doppler beam leaking through its AOM, but the particular source of the impurity is irrelevant for these purposes). This improved from an earlier figure of 1.86(11)% before the pickoff was removed. If the carrier were tuned to $S^+_1\rightarrow P^+_1$, 0.9% polarisation impurity in the beam would prepare $S^+_1$ just 95.0% of the time ($S^+_1$ at 96.1%). Retuning the carrier to $S^+_1\rightarrow P^+_1$ immediately improves these figures to 98.7% and 99.85% respectively. Switching the EOM off for 100 $\mu$s prepares $S^+_1$ with probability 99.9979% (but the purity of $S^+_1$ barely changes; indeed, the “EOM off” pulse pumps out of $S^+_1$ if it is left on for more
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<td>97%</td>
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Table 4.4: Selected results obtained by shelving experiments using a circularly polarised 850 nm beam at 2.3(1)° to the magnetic field. Columns are explained in the main text. Table continues on the following two pages.
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<td>4 $\rightarrow$ 4</td>
<td>0.025</td>
<td>130</td>
<td>100</td>
<td>100</td>
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<td>Y</td>
<td>a</td>
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<td>011</td>
<td>98.6(2)%</td>
<td>0.28(8)%</td>
<td>97.4(2)%</td>
<td>4 $\rightarrow$ 4</td>
<td>0.025</td>
<td>130</td>
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<td>130</td>
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<td>019</td>
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<td></td>
<td>3 $\rightarrow$ 4 (some with EOM off)</td>
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<td>130</td>
<td>100</td>
<td>100</td>
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<td>3 $\rightarrow$ 4</td>
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<td>130</td>
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<td>3 $\rightarrow$ 4</td>
<td>0.025</td>
<td>130</td>
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<td>99.53(5)%</td>
<td>0.39(6)%</td>
<td>99.44(7)%</td>
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Continuation of Table 4.4.

*850 Changed to Rpara channel (to allow more precise timing [97]).

*Waveplate adjusted to improve 850 nm polarisation.
### 4.3. EXPERIMENTS

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<tr>
<th>Row</th>
<th>Date</th>
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<th>Preparation</th>
<th>$I_{393}$</th>
<th>$I_{850}$</th>
<th>$t_{393}$</th>
<th>$t_{850}$</th>
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<td>98.1(3)%</td>
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<td>120</td>
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</tbody>
</table>

Continuation of Table 4.4

*Extra 850 PBS cube inserted; Pickoff removed.

*397 nm Probe beam blocked. Leakage of mixed $\sigma\pm$ light through this AOM could have contributed to optical pumping infidelities.

*Waveplates adjusted to improve 397 nm $\sigma$ polarisation.
than \( \sim 300 \mu s \). Although this “EOM off” pulse is of little use in qubit preparation, it greatly reduces the contribution of \( S_{1/2} \) manifold preparation errors to the readout infidelity we measure.

### 4.3.2.3 Some Trends

The most noticeable trend in Table 4.4 is that the greatest fidelity improvement came from improving the population preparation (changing from \( 4 \rightarrow 4 \) to \( 3 \rightarrow 4 \)), rather than the readout itself. Between rows 31 and 34 \( \epsilon_{\{1\}} \) improved from \( 1.65(12)\% \) to \( 0.42(6)\% \), just by improving the state preparation; each improvement increased the fidelity. Pairs 22-23 and 30-31 are consistent with the 854 nm shutter reducing \( \epsilon_{\{1\}} \) by (a marginally significant) \( \sim 0.1\% \) (rows 35 and 37 show an opposite, much larger effect; although there was an hour’s gap between these two experiments and so some other parameter could have drifted in between them). It is better to have long, low intensity pulses than short bright ones: compare rows 38-40 with 41-44. The pulse times for rows 37-42 had been increased until \( \epsilon_{\{1\}} \) stopped improving, to ensure that they were long enough to effectively shelve the ion. The pairs 27-28 and 35-36 suggest that the single pulse method is more accurate than multi-pulse, although the simulations of Section 4.2 imply that this could reverse if the sequences were properly optimised. Note that the 850 nm beam is on for longer in total for the 400 \( \mu s \) single pulse than in the three 100 \( \mu s \) pulses of the multi-pulse sequence. What it does show is that there are no adverse coherent effects (such as EIT) between the 393 nm and 850 nm beams when they are on together (at least at the 0.1\% level), supporting the use of rate equations as a model.

High fidelities are seen in rows 22-26 (pulsed method, average fidelity for that day 99.63\%); rows 32-34 (average 99.67\%); 41-42 (99.7\%) and 43-45 (99.71\%). The first of these sets used multipulse sequences, the others were single 393+850 pulses. The last of these sets is discussed in detail in Section 4.3.2.5

### 4.3.2.4 Effect of \( \lambda/4 \) Waveplate Rotation

On 290507, the \( \lambda/4 \) waveplates in each of the \( \sigma \) beams was adjusted to improve their polarisation purity. As part of this process \( \epsilon_{\{1\}} \) was recorded for a variety of waveplate angles, for each beam in turn.

The 397 nm \( \sigma \) adjustment was made between rows 33 and 34 of Table 4.4. Initially the waveplate was at 28°; the best position was found to be 27° in an experiment with
4.3. EXPERIMENTS

Figure 4.45: \((1 - \epsilon_{[1]})\) as a function of waveplate angle for the three \(\sigma\) beams. In all cases: the preparation method was “3 \(\rightarrow\) 4; EOM off”, the 854 nm shutter was in use, \(I_{393} = 0.0052 I_0\), \(I_{850} = 100 I_0\) and there was a single 400 \(\mu s\) combined 393 nm and 850 nm shelving pulse (i.e. parameters are as rows 33 and 34 of Table 4.4). Data points at the same waveplate angle have been displaced horizontally for clarity. The angles are accurate to \(\pm \sim 1.5^\circ\). For 393 and 850, simulations are shown as a curve assuming perfect tilt. The simulations have been scaled so that the upper levels match the experiment.

preparation method “4 \(\rightarrow\) 4”. The state preparation was extremely sensitive in this case: at 27\(^\circ\) the probability of seeing the ion as shelved was 97.0(2)\%, while 28\(^\circ\) and 26\(^\circ\) achieved only 96.2(3)\% each. However, we see in Figure 4.45 that tuning the 397 nm to 3 \(\rightarrow\) 4, and using an EOM off pulse, greatly reduces the sensitivity to polarisation impurity.

The 393 nm and 850 nm adjustments were made just after the experiment of row 34. The 393 nm waveplate was originally at 70\(^\circ\), and 80\(^\circ\) was found to be a slight improvement – the waveplate was left in that position. The shelving seems insensitive to the 393 nm polarisation purity (or else the purity of the beam is poor even at the best waveplate angle). However, an earlier experiment showed that \(\epsilon_{[1]}\) rose by up to
10% (in that case, to 14%) when the 393 nm beam was completely $\sigma$– polarised.

For the 850 nm beam, we tried tilting the waveplate around an axis perpendicular to the beam direction (in this case, a vertical axis). Such tilting is a well-known technique to optimise the retardation of a waveplate. Specifically, a waveplate designed to give a specific retardation (in this case $\frac{1}{4}$ of a wavelength) can be tilted about its fast (slow) optical axis to increase (decrease) the relative retardation [140, Section 8.7.1]. As seen in Figure 4.45, a small anticlockwise tilt (estimated to be $5^\circ$, although the rotation was completely uncalibrated) gave an improvement of $0.25(9)\% \, (= 99.54(6)\% - 99.29(7)\%)$.

The waveplate rotation angle was set to $314^\circ$, which was its original setting.

The 393 and 850 experiments were simulated, with the laser parameters set as described in the caption. The simulations significantly underestimate the shelving error when the waveplate rotation is far off its optimum, particularly for the 850, for reasons we do not understand. It might be a symptom of inaccurate power measurements, or perhaps of the waveplates not being at the best tilt angle.

### 4.3.2.5 The Best Results

The highest experimentally-achieved fidelity was $99.77(4)\%$ (row 43). This result is statistically significantly different from rows 44 and 45 ($99.68(3)\%$ and $99.70(3)\%$), so we may be justified in claiming the higher figure by itself (Figure 4.46). The experiments of 43 and 44 were separated by $\sim 15$ minutes, and we know that the 850 nm power or polarisation purity fluctuate over this sort of timescale – the laser parameters could have been different for the two runs, leading to the different fidelities. If we do combine the three data sets, we obtain readout errors:

$$
\epsilon_{|0\rangle} = 0.18(2)\%; \quad \epsilon_{|1\rangle} = 0.41(3)\%; \quad F = 99.706(18)\%. \quad (4.10)
$$

This approaches the estimated target of $99.9\%$ for an operational quantum computer [134], although at $400 \mu s$ (plus fluorescence time) it is significantly slower than Steane assumes in that reference ($10 \mu s$). For each of these rows, the data were collected in 40 sets of 1000 sequences (500 for row 43), 20 sets for each qubit state. Figure 4.46 shows the errors calculated from each set individually, and it can be seen that they agree with each other within their uncertainties. The average errors for each row are also displayed.

The optical qubit/fluorescence detection phase of the readout used a collection time of $2$ ms, a bright-state photon count rate of $7600 \text{s}^{-1}$ and a detection threshold of $3.5$
4.3. EXPERIMENTS

Figure 4.46: Readout errors from rows 43, 44 and 45 of Table 4.4, both overall (filled symbols, to the right of the vertical gridline) and for each data subset (small dots, to the left). The statistical uncertainties (assuming binomial distribution) are also shown as errorbars.

photons – sequences that resulted in more counts than this were designated as “bright”. Figure 4.47 shows the photon histograms from the experiments of row 45.

We measured the fluorescence detection using 393 nm, 866 nm and 397 nm beams together, shelving the ion with high probability from both qubit states. The error probability was 0.04(2)% when measuring an unshelved ion and 0.16(3)% for a shelved one, giving a total of 99.903(17)% fidelity. Removing these numbers from the results above (all three combined), we obtain the error rate for just the shelving and state-preparation phases:

$$
\epsilon_{|0\rangle} = 0.14(3)\%; \quad \epsilon_{|1\rangle} = 0.26(4)\%; \quad \mathcal{F} = 99.80(2)\%. \quad (4.11)
$$

From Section 4.2.2.3 we can read directly off Figures 4.26-4.28 to see that the theoretical optimal shelving, for a single 400 µs pulse with the 850 nm beam at 2.3° to the magnetic field, is much higher fidelity than the experiment:

$$
\epsilon_{|0\rangle} = 0.056\%; \quad \epsilon_{|1\rangle} = 0.021\%; \quad \mathcal{F} = 99.962\%. \quad (4.12)
$$
Figure 4.47: Photon count histograms from row 45, using $2 \times 10^4$ sequences for each of $S_{1/2}^3$ and $S_{1/2}^{4,+4}$. The black vertical dashed line indicates the optimum threshold. The coloured curves show the ideal Poisson distributions, with just one free parameter (the mean number of counts $\lambda$). The departure from the theoretical Poisson distributions is due to a combination of shelving errors, power or frequency fluctuations of the fluorescence lasers, and non-Poissonian dark-count processes in the PMT (including cosmic rays [82]).

The intensities are $I_{393} = 0.00320 I_0$ and $I_{850} = 182 I_0$.

I set the simulation to use the intensities measured in the experiment ($I_{393} = 0.011 I_0$ and $I_{850} = 120 I_0$), and also simulated the 393 nm beam being at $2.79^\circ$ to the magnetic field, again as measured. Of these, the 393 nm intensity has by far the greatest effect. We obtain:

$$
\epsilon_{|0\rangle} = 0.205\%; \quad \epsilon_{|1\rangle} = 0.014\%; \quad \mathcal{F} = 99.891\%.
$$

There is still significant discrepancy with the experiment. One solution would be to add a 16% $\sigma-$ polarisation impurity to the 393 nm beam, that produces a reasonable match to the experiment ($\epsilon_{|0\rangle} = 0.19\%, \epsilon_{|1\rangle} = 0.21\%, \mathcal{F} = 99.80\%$), but this seems like an unrealistically large impurity.
4.4 Future Directions

We can replicate the experimental results just by changing $I_{393}$ to $0.0076I_0$ (30\% below the measured value, possible if the beam was misaligned, but still twice the theoretical optimum), and adding 0.13\% $\sigma$ impurity to the 850 nm beam. Both imperfections are very reasonable, and they are upper limits because I have assumed perfect state preparation.

4.4 Future Directions

To further improve the experimental fidelity of readout, we would need to overcome the current uncertainty about the experimental conditions (laser polarisations, intensities etc.). We can take inspiration from Biercuk et al. [141], who demonstrate the optimisation of a dynamic-decoupling sequence using experimental results (generated on demand in real time) as the quantity to be optimised. A similar approach could be used to optimise the readout fidelity, replacing the rate equations simulations.

We would need to improve the laser polarisation impurities, especially the 397 nm $\sigma$ beam. Polarisers are available (Glan-Taylor or Glan-Thompson polarisers [142]) with claimed extinction ratios of 100 000 : 1 (compared to polarising beamsplitter cubes such as we currently use, with claimed extinction ratios of 1000 : 1). Our polarisation purity may in fact be limited by birefringence in the viewports of our vacuum system, but we might be able to counteract this using carefully-set $\lambda/2$ and $\lambda/4$ plates in each beam, after the polariser. Or we might not be able to – the birefringence could change over time; or if it varies spatially over the window, different parts of the beam would experience different polarisation changes (on average, the polarisation state of the beam would become mixed).

We would also need to stabilise the laser intensities. Re-routing and thermally insulating the 850 nm fibre would help, but it may also be necessary to use noise-eaters (the power of a beam is monitored, and this feeds back to the AOM driver to keep the power constant). Improving the AOM extinctions (such as by detuning and reducing the power of the driver at the same time as operating the driver’s TTL switch) would also help.

The final requirement is a carefully thought-out optimisation procedure that can cope with noise in the function to be optimised. Biercuk et al. [141] successfully used the Nelder-Mead method, an optimisation algorithm that does not calculate the gradient
of the function it is optimising and is hence quite robust.

Such efforts may not be justified given that the operation of a quantum computer is thought to be much less sensitive to the readout fidelity than to the gate fidelity.

### 4.5 Comparison with the Literature

In 2007 Hume, Rosenband and Wineland \[85\] experimentally achieved a readout fidelity of 99.94\%, from an aluminium ion. This is almost as high as the best optimised simulations I performed in Section 4.2.2 which assumed ideal conditions and perfect fluorescence-detection. But the methods I have developed here are still valuable for their simplicity and robustness. In Section 4.2.3 we saw that the multipulse shelving method was highly resistant to changes in the 850 pulse lengths and intensities, and relatively resistant to errors in the 393 too. The procedure can be greatly simplified, to a single pulse with just two monochromatic laser beams, while the fidelity is barely affected. The processes do not depend on coherent beams or narrow linewidths (although the laser linewidths should not be significantly larger than the natural linewidths). And the shelving is fast, taking just a few microseconds to reduce the the average error below $10^{-3}$.

In contrast, methods that depend on coherent processes, such as that of Hume et al., require complex and precise pulse sequences (and in their case, a second ion). The particular method of Hume et al. is also very slow, taking 2 ms per cycle with each cycle having only 85\% fidelity (an average of 6.5 cycles were needed to achieve their high fidelity).

Optical qubits can be detected with very high fidelity. In $^{40}$Ca$^+$, our group has distinguished S$_{1/2}$ from D$_{5/2}$ with a fidelity of 99.9913(11)\% from $^{40}$Ca$^+$, taking $\sim 1$ ms. The 99.9\% level is reached after 200 $\mu$s, and if we use an adaptive method (that only collects data for as long as it takes to reach the desired fidelity) it is even faster \[82\]. The fidelity is limited by the photon collection efficiency and the D$_{5/2}$ lifetime. In Ba$^+$, that lifetime is so long that Kurz et al. could, "completely rule out the possibility of incorrect state determination", by using a very long (100 ms) detection period \[143\].

Other experimental readout fidelities, from hyperfine ground-level qubits, that have been reported are significantly lower than achieved in this work. One method, used in $^{171}$Yb$^+$ (Olmschenk et al. \[57\]) and $^{111}$Cd$^+$ (Acton et al. \[136\], both groups at the
4.5. **COMPARISON WITH THE LITERATURE**

University of Michigan), directly applies fluorescence-detection to the qubit. Both ions have large hyperfine splittings (12.6 GHz and 14.5 GHz in their respective $S_{1/2}$ levels), and so off-resonant excitation of the “dark” qubit state is low; and in Cd$^+$ there are no low-lying D-states and so a closed cycling transition can be used. There are low-lying D-states in Yb$^+$ but $^{171}$Yb$^+$ has nuclear spin $I = \frac{1}{2}$, so Olmschenk *et al.* can repump cleanly back to the “bright” qubit state by exploiting the fact that $F_i = 0 \rightarrow F_j = 0$ transitions are forbidden [57]. $^{111}$Cd$^+$ also has $I = \frac{1}{2}$, and that selection rule (together with large hyperfine splittings of $\approx 2$ GHz in $P_{1/2}$) is vital in both ions to allow a cycling transition from clock-state qubits. Olmschenk *et al.* report readout with 97.9(2)% fidelity in 1 ms [57]. Acton *et al.* report $>99.4$% in 15 ms, and also derive theoretical results for other ions [136]. Both methods would improve if higher photon collection efficiencies were possible.

For ions with metastable shelves, rapid adiabatic passage is a method for directly driving the qubit→shelf transition, with improved robustness compared to a basic $\pi$-pulse. It works by “chirping” the shelving pulse – scanning the laser frequency over the resonance while the amplitude is smoothly raised and lowered (e.g. a Gaussian envelope) [144]. Wunderlich *et al.* used this method on $S_{1/2} \rightarrow D_{5/2}$ in $^{40}$Ca$^+$, and achieved 99(1)% shelving transfer in 150 $\mu$s. However they have not yet attempted state-selective shelving from $^{43}$Ca$^+$. A similar method is being developed with $^{137}$Ba$^+$; so far only 60% transfer has been achieved, but the laser is still being stabilised [145]. Benhelm notes that a $\pi$-pulse shelving method can be made more accurate by using several pulses, each tuned to transfer the desired qubit state to a different state in $D_{5/2}$ achieving better than 99% fidelity overall [128, 72].

The methods of this chapter – both the readout process itself and the optimisation simulations – should work for other common ion species, provided that they have low-lying D-states and a hyperfine ground-state qubit. $^{87}$Sr$^+$, $^{137}$Ba$^+$ and $^{199}$Hg$^+$ might all be investigated; $^{137}$Ba$^+$ is especially interesting because of its large $S_{1/2}$ hyperfine splitting (8.0 GHz [145]), favourable branching ratios (Br$_{(r_{3/2} \rightarrow r_{5/2})} = 22$%; Br$_{(r_{3/2} \rightarrow r_{3/2})} = 3$% [143]) and long $D_{5/2}$ lifetime ($\approx 33$ s [146, 147]).
Chapter 5

40-43

Our group is working towards an entangling quantum phase gate between a $^{40}\text{Ca}^+$ ion and a $^{43}\text{Ca}^+$ ion. The motivations behind this experiment are as follows:

- An alternative to the standard “measure-the-syndrome-and-classically-correct” paradigm of quantum error correction involves performing classical AND gates directly on the ions. We have designed methods to convert a 40-43 phase gate into such an AND gate. Demonstrating the phase gate would lead naturally to an attempt on the AND gate, and then to error-correction experiments.

- It might turn out to be preferable to use $^{40}\text{Ca}^+$ rather than $^{43}\text{Ca}^+$ for certain quantum operations; but $^{43}\text{Ca}^+$ clock-state qubits will almost certainly be the best way to store quantum information as a memory. Being able to transfer quantum information between ions of the different isotopes would be necessary in such a case.

- With the previous 40-40 gate [75], the states $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$ were indistinguishable. $^{40}\text{Ca}^+$ and $^{43}\text{Ca}^+$ can be read out independently and so complete state tomography becomes possible [148].

To give detailed descriptions of the theory behind such a gate is beyond the scope of this thesis [149, 150, 151, 74]. Instead I shall take a practical perspective, and describe early experiments towards this goal. Despite significant experimental effort to realise this gate, our attempts were unsuccessful. Diagnostic experiments to investigate the reasons for this are described in this chapter. The eventual result was to show that our present trap has significant failings regarding this project, and this has motivated us to
design and build a new apparatus for future experiments.

5.1 Introduction

Our “wobble” gate uses the method of Leibfried et al. [73], which is based on ideas from Milburn, Schneider and James [152] and Wang, Sørensen and Mølmer [70, 153]. A more detailed discussion can be found in [74], in the context of a two-\(^{40}\text{Ca}^+\) ion gate; I shall describe it qualitatively here.

5.1.1 Light-Motion Interaction

The coherent couplings between light and ion-motion can be divided into two types, although this represents a convenient distinction of notation and imagery rather than different physical processes (they are both derived from the same Hamiltonian [74, Section 3.2]).

5.1.1.1 Resolved Sideband Interactions and Cooling

The first variety is the quantised simple harmonic oscillator. Each vibrational normal mode (with angular frequency \(\omega_z\)) splits each existing state into a ladder of energy levels separated by \(\hbar\omega_z\). An atomic transition of frequency \(\omega_0\) gains sidebands, of frequency \(\omega_0 + m\omega_z\) for integer \(m\). If \(m > 0\) (\(m < 0\)) it is a blue (red) sideband and the transition connects \(|\downarrow, n\rangle\) with \(|\uparrow, n + m\rangle\). An example is given in Figure 5.1 that illustrates the technique of resolved Raman sideband cooling.

The lowest temperature to which an ion can be cooled is ultimately limited by the ion’s atomic properties [154]. The Doppler limit \(T_D\) is the minimum that can be reached by simple Doppler cooling, approximating the ion as a two-level system. The recoil limit \(T_R\) is a lower bound for any laser-cooling method, corresponding to the random recoil “kick” the ion experiences during the spontaneous relaxation phase. For \(^{40}\text{Ca}^+\) cooled on the 397 nm transition, and assuming an isotropic trapping potential of 500 kHz (to work out the mean motional excitation):

\[
T_D = \frac{\hbar}{2\tau k_B} = 0.54 \text{ mK} \approx 7 \text{ quanta} \quad (5.1)
\]

\[
T_R = \frac{\hbar^2}{m\lambda^2 k_B} = 3.0 \mu\text{K} \approx 0.04 \text{ quanta} \quad (5.2)
\]
5.1. INTRODUCTION

Figure 5.1: [Top] Illustration of 1st red and 1st blue sidebands (s.b.) of an internal state transition $|\downarrow\rangle \rightarrow |\uparrow\rangle$. When a $\pi$-pulse is performed from the lower to the upper state, the 1st red (blue) sideband removes (adds) one motional quantum $\hbar \omega_z$. [Bottom] Illustration of pulsed Raman sideband cooling. The ion starts in $S_{1/2, -1/2}$. Step 1: a red sideband Raman $\pi$-pulse is applied to remove one quantum of vibrational energy from the ion. Step 2: a near-resonant (80 MHz red-detuned), $\sigma^-$ polarised 397 nm beam is applied to repump the ion from $S_{1/2, +1/2}$ to $S_{1/2, -1/2}$. Because the recoil energy is typically much less than $\hbar \omega_z$, the repump step does not often change the motional state, and on average the ion loses almost one vibrational quantum per cycle. There is no red sideband out of the motional ground state $|S_{1/2, -1/2}, 0\rangle$ so, in the ideal case, the ion has a high probability of ending up there after several cycles.
where \( m \) is the mass of an ion, \( \tau \) is the lifetime of \( P_{1/2} \) and \( \lambda = 397 \text{ nm} \). Our Doppler cooling actually achieves much higher temperatures than the limit suggests, because we typically are not tuned precisely to the (optimal) half-fluorescence point, and use intensities much greater than the saturation intensity, broadening the transition.

5.1.1.2 Optical Dipole Force

The second picture describes the optical dipole force. Suppose that an ionic state is shifted by \( \delta E \) due to the light shift from an optical field (with a particular frequency and polarisation). Then if the strength of the field varies with position, an ion in that state will feel a force proportional and parallel to the amplitude gradient of the field (towards the stronger (weaker) field if \( \delta E < 0 \) (\( \delta E > 0 \))). An example of such a spatially-varying light field is the standing wave set up by two intersecting non-parallel laser beams of the same frequency (see also Figure 5.2).

We use two beams derived from the same laser (397 master/slave) to ensure the beams are mutually coherent. In fact, we set up a *travelling* standing wave by setting the beams to slightly different frequencies (using the AOMs). The two beams have a difference wavevector that lies along the trap axis, so the standing wave travels in that direction and only affects the axial motional mode(s) of the ion(s). For now consider just one ion with mass \( m \) (assumed to start in the ground state of motion), and suppose the Raman beams have a difference frequency that is close to the axial frequency \( \omega_z \) (detuned from it by \( \delta_z \)). The travelling standing wave will sweep over the ion such that the ion feels a force oscillating at frequency \( \omega_z + \delta_z \). The damping of the axial mode is negligible and so we can treat the mode as a classical undamped simple harmonic oscillator subject to a periodic, slightly off-resonant driving force. The ion oscillates at \( \omega_z \) with amplitude modulation at \( \delta_z \), so it returns to rest at time \( t = t_r = \frac{2\pi}{\delta_z} \). We call this a “wobble” pulse, because of the ion’s motion.

The quantum description [74, 155] is that the ion is in a coherent state \( |\alpha\rangle \), the state that best resembles classical harmonic oscillators. Coherent states are eigenstates of the annihilation operator \( \hat{a} \):

\[
\hat{a} |\alpha\rangle = \alpha |\alpha\rangle ,
\]

(5.3)

where \( \alpha \) takes complex values \( \alpha = |\alpha| e^{i\phi} \). The mean number of quanta in a coherent
5.1. INTRODUCTION

The state is
\[ \langle \alpha | \hat{N} | \alpha \rangle = \langle \alpha | \hat{a}^\dagger \hat{a} | \alpha \rangle = |\alpha|^2. \] (5.4)

The position and momentum (here using the operators in the Heisenberg picture) have expectation values
\[ \langle \alpha | \hat{z}(t) | \alpha \rangle = \langle \alpha | \sqrt{\frac{\hbar}{2m\omega_z}} (\hat{a}^\dagger e^{i\omega_z t} + \hat{a} e^{-i\omega_z t}) | \alpha \rangle = 2|\alpha|z_0 \cos(\omega_z t - \phi) \] (5.5)
\[ \langle \alpha | \hat{p}(t) | \alpha \rangle = \langle \alpha | i\sqrt{\frac{m\hbar}{2\omega_z}} (\hat{a}^\dagger e^{i\omega_z t} - \hat{a} e^{-i\omega_z t}) | \alpha \rangle = -2|\alpha|z_0 \omega_z \sin(\omega_z t - \phi) \] (5.6)

where
\[ z_0 = \sqrt{\frac{\hbar}{2m\omega_z}}, \] (5.7)

which shows how the coherent state resembles the classical harmonic oscillator.

As the ion is driven by the travelling standing wave wobble pulse, \( \alpha(t) \) travels round a circle in the complex plane (equivalently, round a circle in z-p phase space, in a frame rotating at \( \omega_z \)). It starts at zero (the ground state), returning to zero at time \( t_r = \frac{2\pi}{\delta_z} \).

The ion’s overall wavefunction gains a phase \( \Phi \) proportional to the area of this circle: after a single complete cycle we have
\[ \Phi(t_r) = -\frac{\pi}{2} \left( \frac{F_m}{\delta_z} \right)^2. \] (5.8)

The amplitude of the dipole force is \( F_m = \eta \Omega = \delta_k z_0 \Omega \) where \( \eta \) is the Lamb-Dicke parameter, \( \delta_k \) is the difference between the wavevectors of the two beams, and \( \Omega \) is the Rabi frequency.

By itself this phase is uninteresting, because global phases are irrelevant in quantum mechanics. But we could start with the ion in a superposition of states, such that each state feels a different light shift and thus a different value of \( F_m \). Each component of the superposition picks up a different phase shift, and so the travelling standing wave acts as a single-qubit phase gate. Of course, simpler phase gates are available that are faster and have higher fidelities – such as applying a single laser beam to provide a constant differential light shift between the qubit states. But the above process generalises easily to a two-qubit controlled-phase gate.

5.1.1.3 Same-Species Gate

Two \(^{40}\text{Ca}^+\) ions are trapped in the same potential, so there are now two axial modes of the ions moving collectively: centre-of-mass motion (CoM) with frequency \( \omega_z \) and
stretch motion (Str) at $\omega_z\sqrt{3}$. Each of these modes behaves as described above. The light field is set up so that $S_{1/2, +1/2}$ and $S_{1/2, -1/2}$ experience opposite light shifts. The ion spacing is carefully set so that it is an integer number of wavelengths of the standing wave (Figure 5.2). So at any time, the ions feel forces of equal magnitude – in the same direction if both ions are in the same internal state, in opposite directions if they are in different internal states. The Raman beams’ difference frequency is chosen to be close to the Str frequency ($\omega_z\sqrt{3} + \delta_z$) – being far off resonant from the CoM mode means that only the Str is significantly excited. And the Str mode is only excited when the ions feel oppositely directed forces, when they are in different states. Only in that case will the travelling standing wave be able to drive the Str oscillation, and thus give the ions (collectively) a phase shift $\Phi$ as given by (5.8). Careful choice of $\delta_z$ provides $\Phi = \frac{\pi}{2}$, and so we achieve the controlled phase gate

$$ \hat{G}_{40-40} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & i & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. $$

(5.9)

In previous work our group implemented this gate with fidelity 83% [75].

Figure 5.2: Illustration of two ions in a travelling standing wave, spaced a whole number of wavelengths apart. In this case they are assumed to be in the same internal state, and so experience equal forces $F$ in the same direction. White arrows indicate the beam directions.
There are several subtleties to implementing the gate; such as ensuring that the static light shifts induced by each Raman beam are equal for both qubit states (to reduce single-qubit phase shifts). To cancel out other single-ion phase shifts (such as magnetic field drift, or the static two-photon light shift), we do a spin-echo sequence on both ions. The wobble pulse is divided into halves, placed symmetrically on either side of the spin-echo $\pi$-pulse (similar to Figure 5.6). The $\pi$-pulse reverses the direction with which the qubits precess with respect to single-ion light shifts, unwinding the accumulated unwanted phase. But the collective effect of the wobble pulse depends on the relative spin-state of the ions (both the same or both different), and so the wobble phase is summed over both pulses and the two-qubit gate works. See Dr. Home’s thesis for very full details [74].

### 5.1.1.4 Mixed-Species Gate

The two-qubit gate $\hat{G}$ can be applied to a mixed crystal of $^{40}\text{Ca}^+$ and $^{43}\text{Ca}^+$. In this case the ions have different atomic structure – in particular, very different qubit frequencies of $\sim 5 \text{ MHz}$ and $\sim 3 \text{ GHz}$ respectively. Nevertheless, the gate should still work because the oscillating force is applied close to the trap frequency $1.702\omega_1^2$ and is independent of the qubit frequencies. The ions will respond differently to the light field; the forces are different in magnitude for each ion, and for each of the four possible two-qubit states. It also becomes impossible to cancel out the single qubit phase shifts: assuming typical beam parameters, if the $^{40}\text{Ca}^+$ light shifts are balanced then the $^{43}\text{Ca}^+$ qubit states are differentially shifted by $\sim 30 \text{ kHz}$ [149]. But by separating two gate pulses with single-qubit carrier $\pi$-pulses, we can ensure that the gate reduces to $\hat{G}_{40-40}$.

### 5.1.2 Mixed-Isotope Readout

To show that our gate leaves the ions entangled, we must be able to read-out from both ions at the end of each sequence. The large isotope shift between the ions, and the hyperfine structure of $^{43}\text{Ca}^+$, allow us to stimulate and detect fluorescence from each ion separately. $^{40}\text{Ca}^+$ fluoresces $\sim 5$ times more strongly than $^{43}\text{Ca}^+$ under the experimental conditions, and so uses a shorter counting period; $^{40}\text{Ca}^+$ fluorescence is

\footnote{The Str frequency for two $^{40}\text{Ca}^+$ ions is $\omega_s \sqrt{3} \approx 1.732\omega_z$, where $\omega_z$ is the centre-of-mass frequency; the small mass difference between $^{40}\text{Ca}^+$ and $^{43}\text{Ca}^+$ changes the vibrational modes slightly. For the 40-43 crystal, the Str frequency $\omega_{s,40-43} = 1.702\omega_z$ and the CoM frequency $\omega_{c,40-43} = 0.981\omega_z$ [149].}
done first to minimise error due to decay of the D_{5/2} shelf.

The ions are shelved using a single pulse containing both 393 nm \( \sigma^+ \) and 850 nm \( \sigma^- \). 1.938 GHz sidebands are imposed on the 393 nm beam using an EOM so that when the carrier frequency is resonant with \(^{40}\text{Ca}^+\), the upper sideband excites the \( \text{S}_{1/2} \rightarrow \text{P}_{3/2} \) transition in \(^{43}\text{Ca}^+\). This allows it to shelve from both ions simultaneously. The 850 nm beam is tuned and polarised for EIT readout of \(^{40}\text{Ca}^+\) (see Figure 4.1), and the pulse time is set for highest fidelity from that ion (up to \( \sim 90\% \)). Then the \(^{43}\text{Ca}^+\) readout fidelity reaches \( \sim 90\% \) without further adjustment. It seems likely that further optimisation would allow higher fidelities. Figure 5.3 shows a test with simultaneous Rabi oscillations of \(^{43}\text{Ca}^+\) and \(^{40}\text{Ca}^+\).

At the end of each sequence, the ions are deshelled by the 854 nm beam tuned in-between the isotopes’ resonances.

![Figure 5.3: Independent carrier oscillations of \(^{43}\text{Ca}^+\) (using microwaves) and \(^{40}\text{Ca}^+\) (using Raman laser beams) with Rabi frequencies 5.4 kHz and 95 kHz respectively, testing the simultaneous readout. The horizontal time axis is shared by both plots, but note the \( \times 10 \) scaling factor for \(^{43}\text{Ca}^+\).](image-url)
5.1.3 Pulse Sequence

Figures 5.4-5.6 show an experimental pulse sequence for testing the 40-43 wobble gate. The sequence has several phases.

1. Cooling 2. Experiment 3. Readout

1. Cooling

(a) Doppler cooling. To reduce the final temperature achieved by Doppler cooling, the $^{40}\text{Ca}^+$ 397Doppler beam is reduced in power narrowing the effective linewidth. It is returned to normal at the end of this 1.5 ms pulse (using the “Set DAC (fixed)” instruction).
(b) **Continuous Raman cooling.** We cannot perform pulsed Raman cooling immediately after Doppler cooling, because the Doppler temperature is not low enough. The ions could have a high motional excitation that could not be efficiently cooled by the pulsed method. So we use 5 ms of continuous Raman sideband cooling. The 397σ beam itself repumps out of $S_{1/2, +1/2}$ (Figure 5.1); it is $\approx 90$ MHz red-detuned, so the rate is small enough that the Raman transitions can occur. By applying the beams continuously, this method can efficiently cool from a wide range of initial motional states.

(c) **Pulsed Raman cooling.** Continuous cooling reduces the Com and Str
excitations to $\bar{n} \lesssim 3$, and it is feasible to perform pulsed Raman cooling. We repeatedly apply the following sequence $\sim 20$ times:

i. CoM red sideband $\sim \pi$-pulse (18–38 $\mu$s)

ii. 397$\sigma$ repump

iii. Str red sideband $\sim \pi$-pulse (35–50 $\mu$s)

iv. 397$\sigma$ repump

The sideband pulses are driven by $R_{||}$ and $R_{63}$ (see Figure 2.5). The frequencies are measured in advance by a scan similar to Figure 5.12 below; the Marconi synthesizers (3 and 4, Figure 2.7) are set to these frequencies and the X and Y switches are used to select the relevant frequency for each pulse.
The $\pi$-pulse times are then measured on each sideband, and the sequence set appropriately. Since the Rabi frequency falls as $\bar{n}$ falls, we add cooling pulses to the sequence in groups of five, measure the $\pi$-time after each change and use the result as the pulse time of the next group. We get best results by interleaving CoM and Str pulses. Figure 5.5 shows the pulsed cooling sequence from Figure 5.3 in more detail. During these experiments we achieved temperatures down to $\bar{n} \sim 0.1$ (although $\bar{n} \sim 0.3$ was more common).

Note that both Raman cooling methods act only on the $^{40}\text{Ca}^+$ ion; the $^{43}\text{Ca}^+$ is a mostly inert spectator. More information about this “sympathetic” cooling can be found in [93].

2. **Experiment.** In this phase we perform the actual experiment, which could be a measurement of motional coherence or heating rate, or a test of the wobble pulse as shown in Figure 5.6. The wobble pulse is split into two parts, applied either side of a spin-echo $\pi$-pulse on each ion, to cancel out single-ion phase shifts. The variable-length microwave pulse allows the $^{43}\text{Ca}^+$ state to be chosen, and then the gate attempts to transfer the state to the $^{40}\text{Ca}^+$ so that Ramsey interference fringes are observed as the microwave pulse length is scanned. Also shown are the “Set DAC” instructions that allow us to scan the phase of the final $\frac{\pi}{2}$-pulses, for tomography of the entangled state [74].

3. **Readout.** As described in Section 5.1.2.

## 5.2 Crystal issues and Ion Ejection

### 5.2.1 Crystallisation

Crystallising a 40-43 pair has always been difficult, and it subjectively seemed much worse during the time of these experiments. On good days, the ions would be in a linear axial crystal but would swap positions with frequency of order once per 3 minutes. We normally try to keep the ions in the same position during an experiment, so that they feel the same laser intensities (it is often easy to tell what position they are in, because they give different count rates even with the PMT). Sometimes it will subjectively be very hard to crystallise the ions – they will exist in a cloud, or in a “pseudo-crystal” such as the cigar shape described below. “Pseudo-crystals” appear well localised on the
camera, as opposed to clouds that are often almost invisibly diffuse. They also have much higher count rates than clouds – sometimes as much as an axial crystal if the 397 nm Doppler beam is a little red-detuned.

**Left-Hand and Right-Hand Crystals** These are the desired axial crystals, named for the position of the $^{40}\text{Ca}^+$ ion as seen on the camera images.

**Cigars** “Cigars” is the name we have given to various pseudo-crystals that lie axially like a proper crystal, but in which the ions are in motion so that the camera shows a single elliptical blob. Cigars come in various lengths, and they might be qualitatively different: we watched short (≈ 5 pixels on camera) cigars turn into longer ones (≈ 6 pixels), with the latter having 30% higher fluorescence, and the change between the two configurations taking 7 s one time and ~ 0.5 s another. Sometimes long cigars look peanut-shaped.

**Line of Sight Pseudo-Crystal** The ions appear to be aligned radially in the trap, one behind the other in the line-of-sight of the imaging system. They look like a single blob on the camera, slightly larger than a single ion appears, at the location expected for a single ion. If the fluorescence laser is switched between exciting $^{40}\text{Ca}^+$ and $^{43}\text{Ca}^+$, the blob is visible for both isotopes and it does not move significantly (i.e. it is not the case that one of the ions is hot and in a large orbit that is not visible). We cannot tell whether, if this pseudo-crystal was viewed from the side, it would look like a proper crystal or like a cigar.

Figure 5.7 shows some of these situations.

### 5.2.2 Ion Ejection

In the week starting 25th August 2008, we had great trouble loading the trap. Ions would vanish for very little reason. It was very hard to add a single $^{40}\text{Ca}^+$ to a $^{43}\text{Ca}^+$; we often got two $^{40}\text{Ca}^+$ ions (which very rarely happens normally). Then, for a few days, $^{40}\text{Ca}^+$ ions would often vanish from the trap while leaving the $^{43}\text{Ca}^+$. There would often be no noticeable problem with any lasers, and we could not satisfactorily pin the problems on variability of the RF trap drive amplitude (which we monitored).

It was during this period that I made the electrode noise measurements of Section 5.3. Over the next few days, the problem gradually went away, until by 9th September
Approximate trap centre

Figure 5.7: Some images of crystals and pseudo-crystals, for 40-43. Endcap voltages 240 V and 238 V; RF amplitude $140 \, \text{V}_{\text{pk-pk}}$ ($\approx 700 \, \text{mV}_{\text{pk-pk}}$ on monitor); axial frequency $\omega_z \approx 2\pi \times 475 \, \text{kHz}$; radial frequency $\omega_r \sim 2\pi \times 700 \, \text{kHz}$.

2008 we were doing single-$^{40}\text{Ca}^+$ Raman pulsed sideband cooling (heating rate a few hundred quanta/s).

### 5.3 Electrode Noise and RF Harmonics

#### 5.3.1 RF Correlation

If a trapped ion is not located precisely at the null point of the radio-frequency (RF) electric field, it will experience an oscillating force at that frequency. The resultant motion is called micromotion, and we avoid it by using DC electric fields to adjust the position of the ion onto the null point. We detect micromotion by photon arrival-time correlation. The ion is made to fluoresce with the Doppler cooling beams, with the
397 nm beam detuned near the half-fluorescence point. The computer records the time-of-arrival of photons detected by the PMT, and counts them in bins based on the phase of the trap RF at the arrival time. When micromotion forces the ion towards (away from) the oncoming beam, it will be Doppler-shifted closer to (further from) resonance and the count rate will increase (decrease). The computer plots a graph of counts vs. RF phase, and the shape of the graph allows us to tune the voltage on the DC compensation electrodes to minimise the micromotion. As well as the usual horizontal 397 nm Doppler beam, we have a vertical beam so that we can detect micromotion along both radial axes (we expect negligible micromotion along the axial direction).

During this series of experiments, RF correlation scans showed a high frequency, small amplitude oscillation (Figure 5.8, bottom). This is seen in horizontal and vertical directions, even when optimally compensated, with single $^{40}\text{Ca}^+$ and with 40-43, and for both Left- and Right-Hand crystals and Line-of-Sight. Fitting sine functions to various correlation scans shows that this is an oscillation at five times the RF frequency (i.e. 32 MHz). It must be phase-coherent with the RF to show up in the scans.

### 5.3.2 RF Harmonics

We have looked at the trap RF, and the DC electrodes, using oscilloscopes and a spectrum analyser to look for harmonics of the RF. The RF does have harmonics, but the fifth harmonic is not especially strong (19 dB below the fundamental, Figure 5.9) as the correlation results might suggest. The DC electrodes also seem to pick up the RF and harmonics – with the harmonics relatively stronger. For instance, using a spectrum analyser connected (via a 500 Hz high-pass filter) to the cable between the high-voltage DC supply and the feedthrough, the fundamental and third harmonic both reach $-10$ dBm (Figure 5.10).

### 5.3.3 Electrode Noise

In 2003 Jonathan Home [156] used a spectrum analyser to measure noise near the trap axial frequency (500 kHz) picked up by the trap’s DC electrodes from the trap RF. I repeated this measurement on 29th August 2008, and found that noise levels had not increased.

The spectrum analyser’s 50 Ω input was connected to the BR/BL cable – this is a coaxial cable whose central conductor is attached to the BR trap DC electrode, and the
Figure 5.8: RF Correlation scans for a single $^{40}\text{Ca}^+$ ion. There is $\approx 3\%$ uncertainty in the horizontal axis scale. Trap RF period is 157 ns. [Top] Normal scan (horizontal Doppler beam) showing oscillation at the RF frequency $f_{\text{RF}}$. The ion’s vertical position is not optimal. [Bottom] Scans with horizontal and vertical beams, showing anomalous $5 \times f_{\text{RF}}$ oscillation. No visible oscillation at $f_{\text{RF}}$ because the ion is well compensated.
shield to the BL electrode. The BR electrode is usually used as the microwave antenna (the microwave amplifier was disconnected for this test). For each value of the trap RF amplitude, the spectrum analyser was set to a variety of resolution bandwidths (10 Hz to 10 kHz) and the power at 500 kHz was measured. This procedure was repeated for several settings of the trap RF, and also with the analyser’s 50 Ω input terminated – this latter measurement shows the analyser’s noise floor, which was subtracted from all the other measurements.

I made two measurements with the RF switched off. They were almost indistinguishable from the noise floor, so they are not included with the rest of the results in Table 5.1 and Figure 5.11. The power per unit bandwidth was found by fitting straight lines to a log-log plot of the data: let $P$ be the power measurement and $b$ be the bandwidth, then the fit

$$\log_{10}(P) = m \log_{10}(b) + c$$  \hspace{1cm} (5.10)

implies

$$P = 10^c b^m$$  \hspace{1cm} (5.11)
Figure 5.10: Trap RF and harmonics as picked up by the Near Endcap and measured with a spectrum analyser. RF amplitude was $145\,\text{V}_{\text{pk-pk}}$. Four sweeps were made with the analyser, for different frequency ranges (the different coloured lines). A $-20\,\text{dB}$ attenuator was used for the two ranges highest in frequency – their traces have been adjusted for this. The measurements were made for RF on and off. The RF frequency (6.364 MHz) and its harmonics are marked as solid black vertical lines.

where $10^c$ is the power per unit bandwidth. $m$ was equal to 1 within the uncertainty of the fit for all the data except for $160\,\text{V}_{\text{pk-pk}}$ ($m = 1.08(3)$) and the noise floor ($m = 1.015(11)$).

Jonathan performed measurements up to $180\,\text{V}_{\text{pk-pk}}$, whereas the maximum RF amplitude I could obtain was $\approx 166\,\text{V}_{\text{pk-pk}}$. This could possibly be a sign of degradation of the Colpitts oscillator that drives the RF. But since there is perhaps less noise now than in 2003, it seems that the oscillator is not to blame for our current problems.
5.4 Raman Motional Spectra

5.4.1 Observation of Radial Mode in Axial Motion-Coupling Raman Scans

During previous experiments, a “mystery-mode” was sometimes observed in Raman sideband frequency scans, when a mixed crystal or two $^{40}\text{Ca}^+$ ions were being used. We observed this mode during the current experiments, both in a mixed crystal and with a single $^{40}\text{Ca}^+$. An example scan is shown in Figure 5.12. We have good evidence that this is the radial oscillation mode – it varies with the trap’s RF voltage, and matches radial secular frequencies found by tickling (see Section 2.2.1).

We do not understand how we manage to excite the radial mode with Raman beams that should be very well aligned with the trap axis ($\sim \pm 3^\circ$). It has of order half the Rabi frequency of the axial modes (e.g. a single $^{40}\text{Ca}^+$ with $\omega_r = 2\pi \times 580\ \text{kHz}$ and $\omega_z = 2\pi \times 470\ \text{kHz}$: radial sideband $\pi$-pulse time $t_{\pi,r} = 35\ \mu\text{s}$ and axial sideband $\pi$-pulse time $t_{\pi,z} = 14\ \mu\text{s}$ with continuous Raman sideband cooling only; $t_{\pi,z} = 24\ \mu\text{s}$ when $\bar{n}_z \approx 0.16$).

5.4.2 Heating Rates

The temperature of a vibrational mode can be measured from Raman sideband scans such as Figure 5.12. Let $R$ be the height of the red sideband peak divided by the height of the blue sideband peak (the heights are measured above the shelving baseline in that

<table>
<thead>
<tr>
<th>RF Voltage in $V_{pk-pk}$</th>
<th>Power per unit bandwidth = $10^{16}$ / aW Hz$^{-1}$</th>
<th>This Work</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1.1</td>
<td>Jonathan Home [156]</td>
</tr>
<tr>
<td>60</td>
<td>1.9(7)</td>
<td></td>
</tr>
<tr>
<td>90</td>
<td>4.7</td>
<td></td>
</tr>
<tr>
<td>110</td>
<td>5.1(7)</td>
<td></td>
</tr>
<tr>
<td>160</td>
<td>7.7(1.3)</td>
<td></td>
</tr>
<tr>
<td>180</td>
<td>21</td>
<td></td>
</tr>
</tbody>
</table>

Table 5.1: Noise power as picked up by the trap’s DC electrodes. The spectrum analyser’s noise floor (2.01(14) aW/Hz for this work; 3.97 aW/Hz for [156]) has been subtracted.
Figure 5.11: Noise power as picked up by the trap’s “BR” DC compensation electrode. The spectrum analyser’s noise floor (2.01(14) aW/Hz for this work; 3.97 aW/Hz for [156]) has been subtracted. Similar recordings were made from the endcap electrodes.

part of the scan). Then the mean occupation of that mode is $\bar{n}$ quanta where

$$
\bar{n} = \frac{R}{1 - R}.
$$

(5.12)

By doing one scan with the measurement immediately after sub-Doppler cooling, and another scan with a delay between the cooling and the measurement, we can measure the rate at which the ion heats up. Such heating can be caused by noise on the electrodes, photon scattering, collisions with gas molecules etc.

During the last three months of 2005, the heating rate of a single $^{40}\text{Ca}^+$ ion was measured more than thirty times [74]. The heating rate was usually less than 10 quanta per second (qps). Sometimes, for reasons unexplained, it would rise to 10s of qps, the highest measured rate being $\approx 200$ qps.

We measured the heating rate of a 40-43 crystal on 24th July 2008. The Str (CoM) mode heating rate was found to be $\approx 180$ qps ($\approx 570$ qps). A similar, measurement on 20th August found $\sim 150$ qps ($\sim 200$ qps). We qualitatively expect the Str mode to be less susceptible to heating than the CoM, because the ions are so close together that
Figure 5.12: Raman sideband scan of a single $^{40}$Ca$^+$ ion, showing axial and radial sidebands. The ion was first cooled with forty sideband cooling pulses, and then prepared in the unshelved qubit state. A Raman probe pulse of $t_{\pi,z} = 28 \mu$s was then applied, followed by readout. 200 sequences were performed for each frequency setting of the Raman probe. The carrier (no motional component) is at 0 kHz and highly overdriven. The dashed vertical lines show the location of the axial sidebands at $\pm 470$ kHz (measured using the blue sideband; the red sideband is not visible because the ion is cold, mean axial vibrational excitation $\bar{n}_z < 0.3$). The solid vertical lines show the positions of the radial sidebands, measured by tickling to be 604 kHz. The sidebands are approximately equal heights, showing that the radial mode is hotter than $\bar{n}_r \gtrsim 3$. 
small changes in the electric field affect them equally

For a single $^{40}\text{Ca}^+$ ion, three measurements found the ion heating rate to be $\approx 200$ qps, $\approx 20$ qps and $\approx 80$ qps on 9th and 11th September. The heating rate thus seems to be greater than in 2005.

5.4.3 Motional Coherence

It is possible to measure the coherence time of the vibrational states using a Ramsey sequence. The ion is cooled, prepared in an equal superposition of qubit states, and has a blue sideband $\pi$-pulse applied. After a variable delay time, the sideband pulse is applied again. Then we apply a carrier $\frac{\pi}{2}$-pulse whose phase is scanned, and finally the state is read out. The result is Ramsey fringes whose amplitude (as a function of the delay time) reveal the decoherence rate. See [74] for details.

For a single $^{40}\text{Ca}^+$, our measurement of the coherence time was $\approx 6$ ms for axial frequency 470 kHz (The figure in [74] was 76(30) ms – more than ten times better). We also did this for a mixed crystal (coherent manipulations were only applied to $^{40}\text{Ca}^+$, with $^{43}\text{Ca}^+$ being a spectator). Then the Str (CoM) mode had coherence times of 0.186(7) ms (160(60) ms). This contrasts sharply with the heating rate measurements, where the CoM was found to heat more strongly than the Str mode. We would also expect the CoM to decohere faster. We do not know what could cause the CoM coherence to be so much longer in this measurement (based on delays of up to 10 ms), nor why our single $^{40}\text{Ca}^+$ measurement is much worse than previously.

One source of decoherence of the Str mode is given by Roos et al. [157]. They show that the ions’ radial motion – specifically the antiphase “rocking” modes – couples to the axial motion in a mathematically similar way to Kerr nonlinearities in optics. The amplitude of the rocking motion affects the ions’ mean separation, and hence the Coulomb force between them. Each additional quantum in a rocking mode changes the Str frequency, and Roos et al. detected this in experiments. Specifically: let the radial trap frequency be $\omega_x = \omega_y$; let the angular frequencies of the CoM, Str and rocking modes be $\omega_z, \omega_s = \omega_z\sqrt{3}$ and $\omega_k = \sqrt{\omega_x^2 - \omega_z^2}$ respectively; let $n_{k,x}$ and $n_{k,y}$ be the numbers of phonons in the two perpendicular rocking modes; let $\alpha$ be the fine structure constant, $m$ be the ionic mass and $c$ the speed of light; then the “cross-Kerr coupling
5.4. RAMAN MOTIONAL SPECTRA

constant” $\chi$ is

$$\chi = -\omega_s \left(1 + \frac{\omega_s^2}{8\omega_k^2 - 2\omega_z^2} \right) \frac{\omega_z}{\omega_k} \left(\frac{2\hbar\omega_z}{\alpha^2 mc^2}\right)^{\frac{1}{2}}$$

(5.13)

and the shift in the Str frequency is

$$\delta \omega_s = (n_{k,x} + n_{k,y} + 1) \chi.$$  

(5.14)

Their experiments found the shift to be significantly lower than this theory predicts. For our experiments, taking $\omega_z = 2\pi \times 460$ kHz and $\omega_x = 2\pi \times 750$ kHz, we get $\chi = -11 \text{ Hz} \times 2\pi$. To give a coherence time of $\approx 0.2$ ms would require the rocking modes to have a total of $\sim 200$ quanta, while we expect Doppler-cooling to leave the ions at 0.5–2 mK implying 6–25 quanta in these modes.

5.4.4 Schrödinger Cats

Let us return to the single-qubit geometric phase gate described in Section 5.1.1.2. Previously we only considered the case where the coherent state returned to $|\alpha = 0\rangle$ at the end of the wobble pulse that creates the travelling standing wave. But suppose the wobble pulse duration $t$ did not equal the return time $t_r = \frac{2\pi}{\delta z}$. Then the two parts of the wavefunction (that were originally the qubit states $|\uparrow\rangle$ and $|\downarrow\rangle$) will have very different values of $|\alpha\rangle$. Such a state – being superpositions of two states that are “far apart” in some parameter – is often called a Schrödinger Cat state. The overlap integral between the parts will be small if they have large motional excitations. Therefore, if the wobble pulse is placed in the gap of a Ramsey experiment, the fringe contrast will be low except for $t \approx t_r$.

We performed Schrödinger Cat experiments to try to diagnose possible problems with our wobble pulses when we could not make the two-qubit gate work. A Ramsey spin-echo sequence (scanning the phase of the final $\frac{\pi}{2}$-pulse) had a detuned wobble pulse of length $t$ in its first gap. For a single $^{40}\text{Ca}^+$, plotting Ramsey fringe contrast $A$ against $t$ gives Figures 5.13 and 5.14. Both sets of data are fitted with the function [73]:

$$A = ne^{-\gamma t}e^{-2|\alpha_A|^2\left(\sin\left(\frac{4q_A}{2}\right)\right)}$$

(5.15)

where: $n$ is a normalisation constant (that includes imperfect readout etc.); $\gamma$ is a phenomenological decay constant; $|\alpha_A| = \sqrt{n + 1/2} |\Delta \alpha|$ indicates how far apart the superposed states become in phase space; $\delta_{\text{eff}}$ is approximately the detuning of the
travelling standing wave from the motional frequency (it is not exact because large motions cause the ions to leave the Lamb-Dicke regime \[158\]); \( t_{\text{eff}} = \frac{2\pi}{\delta_{\text{eff}}} \). Table 5.2 and the figures that follow, show the data and the fits.

| Figure | Ion(s)     | Set \( \delta/2\pi \) | \( \gamma / \text{s}^{-1} \) | \( |\alpha_A| \) | \( \delta_{\text{eff}}/2\pi \) | \( t_{\text{eff}} \) |
|--------|------------|------------------------|---------------------|------------|------------------------|----------------|
| 5.13   | \( ^{40}\text{Ca}^+ \) | 10                     | 1800(300)            | 1.72(2)    | 11.680(10)             | 85.6           |
| 5.14   | \( ^{40}\text{Ca}^+ \) | 15                     | 2900(400)            | 1.257(16)  | 16.28(6)               | 61.4           |
| 5.15   | \( ^{40}\text{Ca}^+ & ^{43}\text{Ca}^+ \) | 10                     | 9700(300)            | 0.668(7)   | 9.94(15)               | 100            |
| 5.16   | \( ^{40}\text{Ca}^+ & ^{43}\text{Ca}^+ \) | 10                     | 22200(500)           | 1.26(4)    | 11.50(14)              | 87             |
| 5.17   | \( ^{40}\text{Ca}^+ & ^{43}\text{Ca}^+ \) | 34                     | 7400(600)            | 0.93(4)    | 12.28(10)              | 81             |

Table 5.2: Parameters from recent Schrödinger cat experiments. The first two rows use single \( ^{40}\text{Ca}^+ \) ions; the last three rows used \( ^{40}\text{Ca}^+ - ^{43}\text{Ca}^+ \) two-ion crystals.

The single \( ^{40}\text{Ca}^+ \) experiments are of a similar quality to those in \[74\]. For instance, in two experiments with \( \delta = 2\pi \times 10 \text{kHz} \) he finds \( \gamma = 3500 \text{s}^{-1} \) and \( \gamma = 2000 \text{s}^{-1} \), and \( \alpha_A = 1.49 \) and \( \alpha_A = 1.44 \); which are all of the same order as the first two rows of Table 5.2.
However, it is immediately apparent that the 40-43 experiments are extremely poor. The return of coherence, seen so clearly in the single ion results, is of much lower amplitude, presumably because of the very high decoherence rate of the Str mode compared to a single ion. Also note that for the final row (Figure 5.17), where $\delta = 2\pi \times 34$ kHz from the Str mode, the second peak is expected at $\sim 30\, \mu s$. Instead it seems delayed until $\sim 80\, \mu s$.

## 5.5 Conclusion

The Str coherence time of $\sim 200\, \mu s$ is too short to allow high-fidelity motional operations with the 40-43 crystal, and is probably responsible for the failure of our attempts at the gate. A serious practical problem is decrystallisation of 40-43 pairs. This impedes all work with the ions, including experiments to find the source of the motional decoherence. Our current opinion is that some unknown electrical problem causes decrystallisation, and possibly the decoherence too. We have tried grounding the electrode power supplies to various different positions, or leaving them floating, in attempts to eliminate ground loops. We were unable to produce a consistent improvement. Also, physically
For some time, the group has aimed to replace the current trap with a new one (as described in Section 7.1). This would be of the same basic design but a factor of 2.4 smaller (ion to RF electrode distance), allowing tighter confinement of the ions. In particular, we expect to be able to reach higher axial frequencies (allowing easier ground-state cooling, without the need for continuous Raman cooling) and have a tighter radial potential to reduce decrystallisation. We have decided to invest our efforts on this new apparatus rather than attempt to solve the problems in the current system.
Figure 5.16: Schrödinger cat experiment with a 40-43 pair. $\delta = 2\pi \times 10 \text{kHz}$ from Str.

Figure 5.17: Schrödinger cat experiment with a 40-43 pair. $\delta = 2\pi \times 34 \text{kHz}$ from Str.
Chapter 6

Dynamic Decoupling

The use of spin-echoes [159] to improve the coherence of a quantum state is well known [58, 62]. A set of qubits, each in a superposition state, will accumulate phase offset errors if they precess at slightly different frequencies. This decoherence (or, more precisely, dephasing), is clearly a problem if the qubits are part of some quantum memory. Inserting a $\pi$-pulse in the middle of the storage time can “unwind” the excess phase acquired due to this frequency difference, and restore the quantum information at the end of that time. However, if the frequency offsets vary with time, the acquired phases will no longer be equal-and-opposite in the two halves of the storage delay, and there will be uncorrected errors in the stored information.

In this chapter I derive a pulse sequence that can correct for such time-varying frequency errors. In the literature this is called “dynamic decoupling”, to distinguish it from the situation that often obtains in NMR experiments where only a static frequency error needs to be compensated for. The phrase “bang-bang decoupling” is often used in this context [160], emphasizing that a (ideal) $\pi$-pulse causes a step change to the system (as opposed to some form of continuous adjustment to the Hamiltonian).

With $n$ specifically timed $\pi$-pulses, I prove that we can cancel out all the dephasing that would be caused by the magnetic field varying as an $(n - 1)$th order polynomial function of time. It turns out that this pulse sequence has been independently derived before, for a different dephasing model, and has been extensively studied especially in the solid-state qubit community. Recently it has also been applied to an ensemble of trapped-ion qubits in a Penning trap [141]. I review the relevant literature.

Finally I describe the experiments I performed to implement the sequence on a single $^{43}\text{Ca}^+$ ion, demonstrating that 20 $\pi$-pulses can increase the coherence time of a
magnetic-field sensitive qubit $\sim 75$-fold (compared to an experiment with no protection).

6.1 Theory

A convenient way to measure the phase acquired by a qubit is to use a Ramsey experiment [161]. The basic Ramsey experiment, illustrated in Figure 6.1, starts with a qubit initialised in an eigenstate (say, $|0\rangle$). A coherent pulse with area $\pi/2$ puts the qubit in the equal superposition $|R\rangle = (|0\rangle - i|1\rangle)/\sqrt{2}$ (I assume that all the $\pi/2$-pulses are about the $x$ axis). The qubit freely precesses for time $\tau$, the precession being approximately tracked by the oscillator that drives the pulses. If the oscillator is very close to the same frequency as the qubit splitting ($\delta \ll \frac{1}{\tau}$, where $\delta$ is the frequency detuning between qubit and oscillator), the second $\pi/2$-pulse will transfer the qubit to state $|1\rangle$. However, if $\delta$ is moderate, that second pulse will still leave the qubit in a superposition of $|0\rangle$ and $|1\rangle$. In a real experiment the phase $\phi$ of the second $\pi/2$-pulse is varied, yielding fringes that reveal the phase difference accumulated during $\tau$. The probability of measuring the state $|0\rangle$ is $(\sin(\tau \delta + \phi/2))^2$.

![Figure 6.1: The basic Ramsey sequence.](image)

Measuring a single qubit only yields $|0\rangle$ or $|1\rangle$, so we must average over many repeats of the sequence with the same $\phi$ to measure the probability and obtain a single data point of the fringe. If $\delta$ changes significantly during the averaging, we will obtain fringes with reduced contrast. Adding a $\pi$-pulse at time $\tau/2$ (Figure 6.2) causes any phase difference acquired during the first half of the sequence, to be cancelled out by an equal and opposite phase difference in the second half. This needs $\delta$ to remain constant over the timescale of $\tau$, but it can now vary between successive sequences (provided $\delta$ is much less than the Rabi frequency).

By inspection, one notices that if $\tau$ is divided by two $\pi$-pulses into intervals in the ratio 1:2:1 (Figure 6.3), the qubit becomes immune to a frequency error that varies linearly with time. The graphical interpretation is, of course, just an expression of an
Figure 6.2: A single spin-echo sequence.

integral:

\[
\phi_{err} = \int_{0}^{\frac{1}{4}} \delta(t) \, dt - \int_{\frac{1}{4}}^{\frac{3}{4}} \delta(t) \, dt + \int_{\frac{3}{4}}^{1} \delta(t) \, dt
\]  \hspace{1cm} (6.1)

where \( t = \frac{\text{time}}{\tau} \). We can prove that \( \phi_{err} = 0 \) if the frequency error is an arbitrary straight line \( \delta(t) = a + bt \):

\[
\phi_{err} = \int_{0}^{\frac{1}{4}} \delta(t) \, dt - \int_{\frac{1}{4}}^{\frac{3}{4}} \delta(t) \, dt + \int_{\frac{3}{4}}^{1} \delta(t) \, dt
\]

\[
= \left[ at + \frac{b}{2} t^2 \right]_{0}^{\frac{1}{4}} - \left[ at + \frac{b}{2} t^2 \right]_{\frac{1}{4}}^{\frac{3}{4}} + \left[ at + \frac{b}{2} t^2 \right]_{\frac{3}{4}}^{1}
\]

\[
= a \left( \frac{1}{4} - \frac{3}{4} + \frac{1}{4} + 1 - \frac{3}{4} \right) + \frac{b}{2} \left( \frac{1}{16} - \frac{9}{16} + \frac{1}{16} + 1 - \frac{9}{16} \right)
\]

\[
= 0 .
\]  \hspace{1cm} (6.2)

Figure 6.3: [Top] Two spin-echo \( \pi \)-pulses can compensate for a linearly varying frequency error. [Bottom] The phase accumulated is shown graphically.

To generalise spin-echos, I started with a guess that a sequence with \( n \pi \)-pulses could compensate for \( \delta(t) \) being an \((n-1)\)th order polynomial \( \delta(t) = p_0 + p_1 t + p_2 t^2 + \cdots + \)
Perfect, instantaneous $\pi$-pulses occur at times $\alpha_1 \tau$, $\alpha_2 \tau$, ..., $\alpha_n \tau$, where $0 < \alpha_1 < \alpha_2 < ... < \alpha_n < 1$. We must then solve

$$0 = \phi_{\text{err}}$$

$$= \int_0^{\alpha_1} \delta(t) \, dt - \int_{\alpha_1}^{\alpha_2} \delta(t) \, dt + \cdots + (-1)^n \int_{\alpha_{n-1}}^{1} \delta(t) \, dt$$

$$= \left[ p_0 t + \frac{p_1}{2} t^2 + \cdots + \frac{p_{n-1}}{n} t^n \right]_{0}^{\alpha_1} - \left[ p_0 t + \frac{p_1}{2} t^2 + \cdots + \frac{p_{n-1}}{n} t^n \right]_{\alpha_1}^{\alpha_2} + \cdots$$

$$+ (-1)^n \left[ p_0 t + \frac{p_1}{2} t^2 + \cdots + \frac{p_{n-1}}{n} t^n \right]_{\alpha_{n-1}}^{1} = p_0 \left( \alpha_1 - \alpha_2 + \alpha_1 + \alpha_3 - \alpha_2 + \cdots + (-1)^n (1 - \alpha_n) \right) +$$

$$\frac{p_1}{2} \left( \alpha_1^2 - \alpha_2^2 + \alpha_1^2 + \alpha_3^2 - \alpha_2^2 + \cdots + (-1)^n (1 - \alpha_n^2) \right) + \cdots$$

$$\frac{p_{n-1}}{n} \left( \alpha_1^n - \alpha_2^n + \alpha_1^n + \alpha_3^n - \alpha_2^n + \cdots + (-1)^n (1 - \alpha_n^n) \right)$$

$$= \sum_{j=0}^{n} \frac{p_j}{j+1} \left( (-1)^n - 2 \sum_{i=1}^{n} (-1)^i \alpha_i^j \right)$$

Equation (6.3) must be independently true for each $p_j$, because they can take any (real) value. So we obtain a set of simultaneous equations for the times $\alpha_i$.

$$(-1)^n - 2 \sum_{i=1}^{n} (-1)^i \alpha_i^j = 0 \quad \forall j = 1, 2, \ldots, n. \quad (6.4)$$

The solution is by no means obvious, but for individual cases of $n$ (up to 8) Mathematica can solve the equations exactly in terms of polynomial roots. For $n \leq 5$ the solutions are particularly simple (Table 6.1).

<table>
<thead>
<tr>
<th>$n$</th>
<th>$\alpha_1$</th>
<th>$\alpha_2$</th>
<th>$\alpha_3$</th>
<th>$\alpha_4$</th>
<th>$\alpha_5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$\frac{1}{2}$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>$\frac{1}{4}$</td>
<td>$\frac{3}{4}$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>$\frac{1}{4} (2 - \sqrt{2})$</td>
<td>$\frac{1}{2}$</td>
<td>$\frac{1}{4} (2 + \sqrt{2})$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>$\frac{1}{8} (3 - \sqrt{5})$</td>
<td>$\frac{1}{8} (5 - \sqrt{5})$</td>
<td>$\frac{1}{8} (3 + \sqrt{5})$</td>
<td>$\frac{1}{8} (5 + \sqrt{5})$</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>$\frac{1}{4} (2 - \sqrt{3})$</td>
<td>$\frac{1}{4}$</td>
<td>$\frac{1}{2}$</td>
<td>$\frac{3}{4}$</td>
<td>$\frac{1}{4} (2 + \sqrt{3})$</td>
</tr>
</tbody>
</table>

Table 6.1: The timing of the $\pi$-pulses for $n$-pulse Uhrig spin-echo sequences, for $n$ up to 5. The $\frac{1}{2}$ pulses are at $t = 0$ and $t = 1$. These numbers are plotted in Figure 6.4.

In Figure 6.4 I plot the times of the $\pi$-pulses, for $n$ up to 8. I also discovered that plotting the $\alpha_i$ against $\frac{i}{n+1}$ seems to lay all the points on the same curve – highlighted in Figure 6.5. This curve is rotationally symmetric about $(\frac{1}{2}, \frac{1}{2})$, and seems to tend to
6.2 Proof that the UDD Sequence Solves the Equations

Figure 6.4: For sequences with \( n = 1 \) to 8 \( \pi \)-pulses, the time \( \alpha_i \) of each pulse is plotted. This figure complements Table 6.1.

\((0,0)\) and \((1,1)\). One simple function that fits the requirements is

\[
\alpha_i = \left( \sin \left( \frac{\pi \cdot i}{2 \cdot n + 1} \right) \right)^2,
\]

and indeed that function precisely reproduces the \( \alpha_i \) found from Equation 6.4 and is the curve plotted in Figure 6.5. The formula’s usage is illustrated by Figure 6.6. The formula (6.5) was numerically shown to solve the simultaneous equations (6.4). It can also be proved analytically \[162\] Section 2.3 (and this work, section 6.2).

6.2 Proof that the UDD Sequence (6.5) Solves Equations (6.4)

6.2.1 A Lemma

We will need to show that

\[
\sum_{r=0}^{n} \binom{2n}{2r} = 2^{2n-1}
\]

where \( \binom{n}{k} = \binom{n}{k} \) is a binomial coefficient.
Figure 6.5: $\alpha_i$ plotted against $\frac{i}{n+1}$ seems to lay all the points on the same curve. Equation (6.5) is shown as a dotted curve.

Figure 6.6: A 4-pulse UDD spin-echo sequence whose timings are taken from Equation (6.5).

It is well known that

$$(1 + x)^m = \sum_{k=0}^{m} \binom{m}{k} x^k. \quad (6.7)$$
Replacing $m$ with $2n$, and splitting odd and even terms we get

$$(1 + x)^{2n} = \sum_{k=0}^{2n} \binom{2n}{k} x^k$$

$$= \sum_{r=0}^{n} \binom{2n}{2r} x^{2r} + \sum_{r=0}^{n-1} \binom{2n}{2r+1} x^{2r+1} \tag{6.8}$$

Consider setting $x$ to $-1$. Then

$$(1 + (-1))^{2n} = \sum_{r=0}^{n} \binom{2n}{2r} (-1)^{2r} + \sum_{r=0}^{n-1} \binom{2n}{2r+1} (-1)^{2r+1}. \tag{6.9}$$

$$0 = \sum_{r=0}^{n} \binom{2n}{2r} - \sum_{r=0}^{n-1} \binom{2n}{2r+1} \tag{6.10}$$

so

$$\sum_{r=0}^{n} \binom{2n}{2r} = \sum_{r=0}^{n-1} \binom{2n}{2r+1}. \tag{6.11}$$

Now consider setting $x$ to $1$. Then

$$2^{2n} = \sum_{r=0}^{n} \binom{2n}{2r} + \sum_{r=0}^{n-1} \binom{2n}{2r+1}. \tag{6.12}$$

But we have already shown that the two sums are equal, so

$$\sum_{r=0}^{n} \binom{2n}{2r} = \sum_{r=0}^{n-1} \binom{2n}{2r+1} = \frac{1}{2} 2^{2n} \tag{6.13}$$

$$= 2^{2n-1} \tag{6.14}$$

QED.

### 6.2.2 Useful Results

$$(\sin(z))^{2n} = 2^{-2n} \left( \frac{2n}{n} \right) + 2^{1-2n} \sum_{k=0}^{n-1} (-1)^{n-k} \binom{2n}{k} \cos(2(n-k)z) \quad n \in \mathbb{N}^+ \tag{6.15}$$

$$\sum_{k=0}^{n} (-1)^{k} \cos(ak) = \frac{\cos \left( \frac{a}{2} (a + n(a + \pi)) \right) \cos \left( \frac{n}{2} (a + \pi) \right)}{\cos \left( \frac{n}{2} \right)} \tag{6.16}$$

$$\sum_{k=0}^{n} (-1)^{k} \sin(ak) = \frac{\cos \left( \frac{a}{2} (a + n(a + \pi)) \right) \sin \left( \frac{n}{2} (a + \pi) \right)}{\cos \left( \frac{n}{2} \right)} \tag{6.17}$$

These forms are from Wolfram Functions [163, 164, 165]. They can be derived using the complex exponential forms of sine and cosine.

$$\cos(A + B) = \cos(A) \cos(B) - \sin(A) \sin(B) \tag{6.18}$$

is the standard cosine Double Angle Formula.
6.2.3 The Proof

We wish to prove that
\[
(-1)^n - 2 \sum_{i=1}^{n} (-1)^i \alpha_i = 0 \quad \forall j = 1, 2, \ldots, n \tag{6.20}
\]
is solved by
\[
\alpha_i = \left( \sin \left( \frac{\pi}{2} \frac{i}{n+1} \right) \right)^2, \tag{6.21}
\]
which I shall do by proving the convenient rearrangement
\[
\mathcal{U} = \sum_{l=0}^{n-1} (-1)^l \left( \sin \left( \frac{\pi I + 1}{2 n + 1} \right) \right)^{2j} = -\frac{1}{2} (-1)^n \quad \forall j = 1, 2, \ldots, n \tag{6.22}
\]
I present a direct, but longwinded, proof. A less direct but much shorter proof can be found in Ref [162].

We start by expanding the power of sine in (6.22), using (6.16).
\[
\mathcal{U} = \sum_{l=0}^{n-1} (-1)^l \left( \sin \left( \frac{\pi I + 1}{2 n + 1} \right) \right)^{2j} = -\frac{1}{2} (-1)^n \quad \forall j = 1, 2, \ldots, n \tag{6.23}
\]
Exchange the order of summation, and rearrange.
\[
= (-1)^j \frac{2}{4^j} \sum_{m=0}^{j-1} (-1)^m \left( \frac{2j}{m} \right) \sum_{l=0}^{n-1} (-1)^l \cos \left( \pi(j - m) \frac{l + 1}{n + 1} \right) + (-1)^j \left( \frac{2j}{j} \right) \sum_{l=0}^{n-1} (-1)^l \right) \tag{6.24}
\]
\[
= (-1)^j \frac{2}{4^j} \sum_{m=0}^{j-1} (-1)^m \left( \frac{2j}{m} \right) \sum_{l=0}^{n-1} (-1)^l \cos \left( \pi(j - m) \frac{l + 1}{n + 1} \right) + (-1)^j \left( \frac{2j}{j} \right) \left\{ \begin{array}{ll} 0 & n \text{ even} \\ 1 & n \text{ odd} \end{array} \right. \tag{6.25}
\]
Use the cosine Double Angle Formula, to expand.
\[
= (-1)^j \frac{2}{4^j} \sum_{m=0}^{j-1} (-1)^m \left( \frac{2j}{m} \right) \sum_{l=0}^{n-1} (-1)^l \cdot \cos \left( \pi \frac{j - m}{n + 1} \right) \cos \left( \pi \frac{l - m}{n + 1} \right) - \sin \left( \pi \frac{j - m}{n + 1} \right) \sin \left( \pi \frac{l - m}{n + 1} \right) + (-1)^j \left( \frac{2j}{j} \right) \left\{ \begin{array}{ll} 0 & n \text{ even} \\ 1 & n \text{ odd} \end{array} \right. \tag{6.26}
\]
6.2. PROOF THAT THE UDD SEQUENCE SOLVES THE EQUATIONS

Use the summation formulae (6.17) and (6.18).

\[
= \frac{(-1)^j}{4^j} \left( 2 \sum_{m=0}^{j-1} (-1)^m \binom{2j}{m} \right)
\cdot \left( \cos \left( \frac{\pi}{n+1} \right) \cos \left( \frac{\pi}{2} \left( \frac{j-m}{n+1} + 1 \right) \right) \right)
\begin{aligned}
&- \sin \left( \frac{\pi}{n+1} \right) \sin \left( \frac{\pi}{2} \left( \frac{j-m}{n+1} + 1 \right) \right) \cos \left( \frac{\pi}{2} \pi \left( \frac{j-m}{n+1} + 1 \right) \right) \\
&+ \frac{(-1)^j}{4^j} \left( \frac{2j}{j} \right) \left\{ \begin{array}{ll} 0 & n \text{ even} \\ 1 & n \text{ odd} \end{array} \right. \\
&\cos \left( \frac{\pi}{2} \left( \frac{j-m}{n+1} + 1 \right) \right) \\
&+ \sin \left( \frac{\pi}{2} \left( \frac{j-m}{n+1} + 1 \right) \right) \\
&+ \frac{(-1)^j}{4^j} \left( \frac{2j}{j} \right) \left\{ \begin{array}{ll} 0 & n \text{ even} \\ 1 & n \text{ odd} \end{array} \right.
\end{aligned}
\]

(6.27)

Use the cosine Double Angle Formula again, but this time contracting.

\[
= \frac{(-1)^j}{4^j} \left( 2 \sum_{m=0}^{j-1} (-1)^m \binom{2j}{m} \right)
\cdot \cos \left( \frac{\pi n - 1}{2} \left( \frac{j-m}{n+1} + 1 \right) \right) \cos \left( \frac{\pi}{2} \pi \left( \frac{j-m}{n+1} + 1 \right) \right)
\begin{aligned}
&- \sin \left( \frac{\pi n - 1}{2} \left( \frac{j-m}{n+1} + 1 \right) \right) \sin \left( \frac{\pi}{2} \pi \left( \frac{j-m}{n+1} + 1 \right) \right) \cos \left( \frac{\pi}{2} \pi \left( \frac{j-m}{n+1} + 1 \right) \right) \\
&+ \frac{(-1)^j}{4^j} \left( \frac{2j}{j} \right) \left\{ \begin{array}{ll} 0 & n \text{ even} \\ 1 & n \text{ odd} \end{array} \right. \\
&\cos \left( \frac{\pi}{2} \pi \left( \frac{j-m}{n+1} + 1 \right) \right) \\
&+ \sin \left( \frac{\pi}{2} \pi \left( \frac{j-m}{n+1} + 1 \right) \right) \\
&+ \frac{(-1)^j}{4^j} \left( \frac{2j}{j} \right) \left\{ \begin{array}{ll} 0 & n \text{ even} \\ 1 & n \text{ odd} \end{array} \right.
\end{aligned}
\]

(6.28)

And one final use of a Double Angle Formula (in expansion).

\[
= \frac{(-1)^j}{4^j} \left( 2 \sum_{m=0}^{j-1} (-1)^m \binom{2j}{m} \right)
\cdot \cos \left( \frac{\pi}{2} \pi \left( \frac{j-m}{n+1} + 1 \right) \right)
\begin{aligned}
&- \sin \left( \frac{\pi}{2} \pi \left( \frac{j-m}{n+1} + 1 \right) \right) \\
&+ \frac{(-1)^j}{4^j} \left( \frac{2j}{j} \right) \left\{ \begin{array}{ll} 0 & n \text{ even} \\ 1 & n \text{ odd} \end{array} \right.
\end{aligned}
\]

(6.30)
Now, if \( j - m + n - 1 \) is odd, then \( \sin \left( \frac{\pi}{2} (j - m + n - 1) \right) = 0 \). But if \( j - m + n - 1 \) is even, then \( \cos \left( \frac{\pi}{2} (j - m + n - 1) \right) = 0 \) and the whole term vanishes. So

\[
\mathcal{U} = \frac{(-1)^j}{4^j} \left( 2 \sum_{m=0}^{j-1} (-1)^m \binom{2j}{m} \left( \cos \left( \frac{\pi}{2} (j - m + n - 1) \right) \right)^2 \right)
\]

(6.31)

Notice that when \( m = j \),

\[
\cos \left( \frac{\pi}{2} (j - m + n - 1) \right) = \begin{cases} 
0 & n \text{ even} \\
1 & n \text{ odd} 
\end{cases}
\]

(6.32)

So we can absorb the final term into the main summation, because \( \binom{n}{r} = \binom{n}{n-r} \).

\[
\mathcal{U} = \frac{(-1)^j}{4^j} \sum_{m=0}^{2j} (-1)^m \binom{2j}{m} \left( \cos \left( \frac{\pi}{2} (j - m + n - 1) \right) \right)^2
\]

(6.33)

\[
= \frac{(-1)^j}{4^j} \sum_{m=0}^{2j} (-1)^m \binom{2j}{m} \begin{cases} 
0 & j - m + n \text{ even} \\
1 & j - m + n \text{ odd} 
\end{cases}
\]

(6.34)

\[
= \frac{(-1)^j (-1)^{j+n}}{4^j} \sum_{m=0}^{2j} \binom{2j}{m} \begin{cases} 
0 & j - m + n \text{ even} \\
1 & j - m + n \text{ odd} 
\end{cases}
\]

(6.35)

\[
= \frac{(-1)^n}{4^j} \sum_{k=0}^{j} \binom{2j}{2k} j + n \text{ odd}
\]

(6.36)

\[
= \frac{(-1)^n}{4^j} \sum_{k=0}^{j-1} \binom{2j}{2k+1} j + n \text{ even}
\]

(6.37)

Use (6.15)

\[
\mathcal{U} = -\frac{1}{2} \left( -1 \right)^n
\]

(6.38)

QED.

### 6.2.4 Optimality

I have not formally proved that the UDD pulse sequence is optimal – i.e. I have not proved that to cancel out an \( (n-1) \)th order polynomial \textit{requires} \( n \) pulses; only that \( n \) are sufficient. However, the following argument suggests that \( n \) pulses are necessary in general.

The polynomial is described by \( n \) real numbers \( p_j \) that must be independently cancelled by the sequence. So all \( n \) of the equations (6.24) are needed. To solve \( n \) simultane-
ous equations generally requires one to solve for \( n \) variables. Here, these are the times of the \( n \) pulses; so \( n \) pulses are required.

It seems likely that the UDD sequence is the only solution to the equations, and hence is optimal for cancelling magnetic field drifts in the polynomial model.

6.3 The Literature

6.3.1 Theory

The pulse sequence defined by (6.5), and illustrated in Figure 6.6 had been previously discovered by G"otz S. Uhrig [166]. He derived it in the context of a qubit that interacts with a bath of bosons via the Hamiltonian

\[
H = \sum_i \omega_i b_i^{\dagger} b_i + \frac{1}{2} \sigma_z \sum_i \lambda_i \left( b_i^{\dagger} + b_i \right) + E
\]  

(6.39)

where \( \lambda_i \) and \( \omega_i \) are properties of the bath that define its spectral density; \( b_i^{(\dagger)} \) are (creation) annihilation operators for quanta in the bath; \( E \) is an energy offset; and \( \sigma_z \) is a Pauli spin operator acting on the qubit (assumed to be a spin-half particle). The sequence was found to provide optimal protection from decoherence in that model, and numerical simulations showed that it outperformed the standard CPMG sequence (6.40, below). The detailed derivation [162] treats a sequence of \( \pi \)-pulses as a filter in the frequency domain. Uhrig demands that the first \( n \) derivatives of the filter function vanish in the low frequency limit, which leads to Equations (6.4). The general technique of using a sequence of pulses to protect a qubit (which originated in the field of Nuclear Magnetic Resonance) is called Dynamical Decoupling (DD); the sequence of Equation (6.5) has become known as Uhrig DD (UDD).

Since this first appearance in the literature, UDD has been shown to have other remarkable properties. Lee, Witzel and Das Sarma [167] showed that UDD is the optimal decoupling process for \textit{any} dephasing Hamiltonian, provided that \( \tau \) is short compared to the timescale of the noise. They claim that, with each added pulse, UDD cancels out successive powers of \( \tau \) in the decoherence of the spin-echo signal. However, their chosen formalism (expanding the time evolution operator as a double sum of products of Hamiltonians) leads to a set of simultaneous nonlinear equations that grows exponentially with \( n \) – as opposed to the linearly growing set in [162] and this work. They are therefore able to algebraically prove the claim only for \( n \leq 9 \), with numerical “proof”
for \( n \leq 14 \). Similarly, Dhar et al. \[168\] had earlier derived UDD sequences for \( n \leq 4 \) but did not find the general formula (although their 5-pulse sequence disagrees with UDD).

Other authors \[169, 141, 170\] continue with the treatment of UDD as a filter. Cywiński in particular \[169\] lists the filter functions of a variety of DD pulse sequences, and shows numerically and algebraically that UDD is by far the best in the limit \( \omega \tau \ll n \). Biercuk et al. \[170\] derive the filter function for UDD where the \( \pi \)-pulses have non-zero length (rather than being idealised \( \delta \)-functions).

However, for longer times \( \tau \) or higher noise frequencies, UDD is not the best \[169\]. In particular it is overtaken by the simpler Carr-Purcell-Meiboom-Gill (CPMG) sequence, in which the \( \pi \)-pulse times are given by

\[
\alpha_i = \frac{\frac{1}{2} + i - 1}{n}
\]

for \( i = 1, \ldots, n \). See also Figure 6.7. CPMG has been used for many years in NMR experiments \[171\], although not usually in the context of a quantum memory. The Meiboom-Gill contribution to CPMG is that each \( \pi \)-pulse has a phase shift of \( \frac{\pi}{2} \) (or \( -\frac{\pi}{2} \), although it should be the same for each pulse) relative to the \( \frac{\pi}{2} \)-pulses. The sequence can be described as \( 90^\circ_x, 180^\circ_y, 180^\circ_y, \ldots, 90^\circ_x \) where the subscript indicates the axis of rotation in the Bloch sphere. This does not improve the noise-filtering properties of the sequence, but it prevents imperfections in the \( \pi \)-pulses from accumulating. This may be useful to improve the contrast in our experiments (without biasing the measurement of the coherence time). But it probably won’t help in practical usage of the sequence – in a quantum computer we want to be able to dynamically decouple any initial qubit state, not just \( (|0\rangle - i|1\rangle)/\sqrt{2} \) that is prepared here, and in the general situation the Meiboom-Gill phase shift gives no benefit on average.

6.3.2 Experiment

Biercuk et al. have provided the only experimental implementation of UDD so far \[141, 170, 172\]. They used a 4.5 T superconducting-magnet Penning trap and an ensemble of \( \sim 1000 \) \(^{9}\)Be\(^+\) ions, with qubit states in \( S_{1/2} \) (\(|m_I = 3/2, m_J = 1/2\rangle\) and \(|m_I = 3/2, m_J = -1/2\rangle\)). The qubit splitting is \( \approx 124 \) GHz with field sensitivity \( \approx 28 \) MHz/mT, and they achieve \( \pi \) times of \( \approx 185 \) µs.

In Ref \[170\] they show (in simulation and experiment) that UDD is much more robust than CPMG against detuned or wrong-length pulses. They also experimented
with injecting magnetic field noise with various power spectra. When they injected noise whose power spectrum is proportional to frequency ($S(\omega) \propto \omega$), UDD maintained high phase coherence for much longer than CPMG. However, they also tried noise with power inversely proportional to frequency ($S(\omega) \propto \omega^{-1}$) – although UDD still won at short times, the coherence fell sharply while CPMG was still maintaining some coherence. With their ambient noise (power spectrum $S(\omega) \propto \omega^{-4}$) CPMG is almost as good as (or better than) UDD for most times, to within the experimental precision.

In a later paper, they show [141] that pulse sequences can be optimised for any given, specific noise spectrum that may exist in some experiment. Such a sequence can outperform both CPMG and UDD, even in the high-fidelity (low noise/short time) regime where UDD is more generally optimal. They are able to perform the optimisation experimentally, where at each step of the algorithm the proposed sequence is applied to the ions and the coherence measured.

In fact, their third paper [172] makes such optimisation much simpler. They use numerical modelling to minimise the integral of an $n$-pulse sequence’s filter function over some range of frequencies $[0, \omega_c]$, where $\omega_c$ is some high-frequency cut-off of the noise spectrum. Note that only the filter is involved in this optimisation – the noise is still unknown. The optimum sequence depends on $\tau' \equiv \omega_c \tau$, a spectrum-independent measure of the total sequence time. UDD is taken as the initial guess at $\tau' = 0$, and the sequence diverges away from it as $\tau'$ increases. Having calculated a large number of sequences, for a variety of values of $\tau'$, they start their experiment. As before, they do an optimisation procedure using the experimental results as the feedback. But this time, the sequences are selected only from the pre-calculated set, optimising in just
one dimension \((\tau')\). This is far easier than the \(n\)-dimensional task of optimising each pulse location individually. Once the sequence has been selected, it is simply scaled uniformly to match the desired qubit storage time. Surprisingly the procedure is shown (in simulation) to perform very nearly as well as full optimisation, outperforming the fixed sequences UDD and CPMG. Their experiment also shows it preserving coherence better than CPMG and UDD for synthesised noise. However, it is worse for their ambient magnetic field noise that does not have a sharp high-frequency cutoff.

### 6.4 Our Experiment

#### 6.4.1 AC Field Compensation

I have used our hyperfine \(^{43}\text{Ca}^+\) stretch-state qubit to verify that UDD (and CPMG) are highly effective at lengthening the coherence time of a single ion qubit. Our group has already measured the coherence time of a clock-state qubit to be \(T_2 = 1.2(2)\) s \([58]\); if a single spin-echo pulse were used, no decoherence was detectable (at the 1% level) in a 1 second Ramsey gap. It would thus be intolerably slow to use clock states in this experiment, combined with the fact that we can only prepare those states with probability \(\sim \frac{1}{7}\).

An initial worry was that the qubit frequency varies with time due to the 50 Hz mains. Ben Keitch \([97]\) found that the frequency varied by \(\approx 10\) kHz pk-pk over a whole AC cycle. We can drive the qubit at a Rabi frequency of up to 18 kHz; a 10 kHz detuning would thus significantly degrade the fidelity of a \(\pi\)-pulse. Increasing the power of the microwaves is the obvious solution, but more powerful amplifiers at GHz frequencies are expensive. We currently use a Minicircuits ZVE-8G that puts out nearly 29 dBm \(\approx 750\) mW (nominally 33 dBm \(\approx 1.8\) W at the 1 dB compression point) and costs more than \$1000. The ZVE-3W-83 costs \$200 more for an extra 1 dB – a factor of 1.26. Since the Rabi frequency is proportional to the amplitude of the oscillating magnetic field at the ion, which is proportional to the square root of the radiated microwave power, the Rabi frequency would rise by only 12%. A 20 W amplifier would increase the Rabi frequency by a factor of 5, at a cost of \(\approx £1500\).

Keitch attempted to use a Spicer SC-20 field-cancelling system \([97]\). This is a commercial system that measures the magnetic field with two sensors, each measuring the field along three perpendicular axes. It uses a feedback circuit to try to keep the field be-
tween the sensors constant by sending current through three large, perpendicular coils. The user can adjust the gain of the feedback loop and the relative weighting of each sensor separately for each axis. But although he tried a wide variety of settings, the unit was unable to reliably cancel out field fluctuations, including the 50 Hz mains.

The AC line field should be easy to cancel because it is regular and stable. One idea is to use a line-locked 50 Hz signal to frequency-modulate the microwave synthesizer (on an analogue channel). The microwaves would thus follow the ion’s frequency, and the base microwave frequency could still be set by communication with the computer via the RS-232 serial port. However, we must also be able to use analogue phase modulation so that we can alter the phase of the final $\frac{\pi}{2}$-pulse in Ramsey experiments, and our synthesizers do not allow frequency and phase modulation at the same time.

Instead, I installed a 20-turn coil to allow a deliberate 50 Hz field to be driven to oppose the AC line field. A 10(2) µF capacitor is connected in parallel with the coil, as a crude low-pass filter. The coil’s resistance is 0.135(5) Ω (from a four-terminal measurement) so the approximate cutoff frequency of the filter is $\frac{1}{2\pi R C} = 120(20)$ kHz. The coil is placed with its axis parallel to the fixed magnetic field (which is parallel with the $\sigma$-polarised beams), close to the window through which $R_{\parallel}$ enters the vacuum system (see Figure 2.5).

First I tried to drive the coil directly from the mains (with step-down transformers including a variable one), but this leads to the “correction” field being out of phase with the ambient field, and the phase is not adjustable. The eventual solution was to drive the coil with a signal generator (Stanford Research Systems DS345). We could, of course, use a phase-locked-loop to keep the signal synchronised with the mains, but instead I choose a simpler method.

The Stanford has a mode in which it emits a burst (an integer number of periods) of signal in response to some trigger, and then waits for the next trigger. While it waits, the output voltage is held constant at its value at the end of the burst. The trigger options include triggering from the mains. This gives us a 50 Hz signal that accurately follows the mains, provided that one can be sure that the Stanford finishes its cycle before the next trigger (otherwise it misses the next cycle completely). We must therefore set the signal frequency to just over 50 Hz: 50.2 Hz seems to work well with the following settings.
AMPL → as required, typically around 2 V for these experiments.
FREQ → 50.2 Hz
SWEEP/MODULATE → BURST
BRST CNT (Burst Count) → 1
SWEEP ON/OFF → ON
PHASE → as required, typically around 100° for these experiments.
TRIG SOURCE → LINE

The Stanford expects 50 Ω output impedance; I pass the signal through 44 Ω resistance in series with the 20-turn coil.

To tune up the system to do useful cancelling of the AC, it is convenient to use a Gaussmeter and an oscilloscope. In Figures 6.8 and 6.9 I show an example. The Gaussmeter probe is set near the trap, and fed into one 'scope channel; the Stanford output is fed into another (it doesn’t go to the coil); and the 'scope is set to display the difference between them. I then adjust the amplitude and phase offset of the Stanford to minimise the (peak-to-peak) amplitude of the difference signal. Figure 6.8 shows an example of success. The measured magnetic field is clearly not a pure sine wave, having a strong third harmonic (see Figure 6.9) that remains in the difference trace.

Since the Stanford is not driving the coil yet, the measured AC B-field doesn’t change and the procedure does not obtain the correct signal amplitude. To do this I set up the following timed sequence experiment (Figure 6.10). It contains two complete subsequences separated by a delay; each subsequence has its own population preparation, microwave probe pulse and readout. The microwave power is reduced to give a Rabi frequency of \( \approx 960 \) Hz. Both pulses are at the same frequency, and separated by a time \( t \) (strictly, \( t \) is the time from the end of the first pulse to the beginning of the second pulse). The microwave frequency was scanned; at each step in frequency the sequence was repeated 100 or 200 times, with the number of times the ion was shelved being recorded separately for each subsequence. The resonance frequencies for the microwave pulses are revealed as dips in their own shelving vs frequency plots; once both resonances were seen the scan was stopped and saved. The data were analysed by fitting a carrier shape (6.41) to each graph (Figure 6.11), and we are interested in the difference between the two frequencies. The fit is:

\[
1 - n_{\text{Shelved}} = b + a \frac{\Omega^2}{2 \left( \Omega^2 + \left( \omega - \omega_0 \right)^2 \right)} \left( 1 - \cos \left( \sqrt{\Omega^2 + \left( \omega - \omega_0 \right)^2} \right) \right) \quad (6.41)
\]
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Figure 6.8: An example of setting the phase of the Stanford to cancel out the AC magnetic field. Here, that angle is 114°, and was set by attempting to minimise the pk-pk amplitude of the difference signal (the Stanford amplitude was also adjusted). Note that the difference is calculated only in the 'scope, and is not a magnetic field measurement. Both 'scope channels were set to “AC coupled” to remove DC offsets.

where \( b \) is the vertical offset and \( a \) the vertical scaling, both for imperfect readout; \( \Omega \) is the Rabi frequency; \( \omega \) is the frequency of the incident microwaves and \( \omega_0 \) the resonant frequency.

To optimise the Stanford amplitude I set \( t \) to a value such as 26.20 s where the frequency difference is particularly large (see Figure 6.13). I repeated the frequency scan for various settings of the amplitude, until the frequency difference became \( \lesssim 1 \) kHz. This setting was then kept. A series of scans, with \( t \) varying over a full mains cycle of 20 ms, were then made to check that the compensation was good.

Figures 6.12 and 6.13 show the results of two such experiments. The first is lower resolution (2 ms time steps and 1 kHz frequency steps) than the second (1 ms time steps and 0.5 kHz frequency steps). In both cases we see the AC variation has been greatly reduced, from 20 kHz to 4 kHz in Figure 6.12 and from 19 kHz to 7 kHz in Figure 6.13. The poorer performance of the latter is because the AC field changes slowly over time...
Figure 6.9: [Top] A 0.1 s sample of the AC line field, as measured by the Gaussmeter. Arbitrary vertical units. [Bottom] Fourier Transform of the AC line field measured by Gaussmeter; from a 1 s sample.

(for instance, if mains-powered devices are switched on or off), and the scan was done seven days after setting the phase and amplitude. Notice also that, while the uncancelled data does not perfectly resemble the Gaussmeter-measured field in Figure 6.8, there is a third harmonic residual clearly visible in the field-cancelled data. The Stanford is also an arbitrary waveform generator, so it would probably be possible to cancel that and other harmonics if necessary.

A $\pi$-pulse with Rabi frequency $2\pi \times 18$ kHz, assumed to have perfect fidelity at zero detuning, has 95% fidelity at a detuning of 4 kHz; 82% at 8 kHz; and only 23% at 20 kHz. These are the respective approximate worst case fidelities of $\pi$-pulses with the coil well-tuned (Figure 6.12), with the coil imperfectly tuned (Figure 6.13) and with no coil in use. Without using the coil, some $\pi$-pulses would have extremely low fidelities and the experiment would be impossible.
6.4. OUR EXPERIMENT

Figure 6.10: The sequence of pulses used to measure how the ion’s microwave resonance frequency varies due to the magnetic field due to AC mains currents. The sequence is triggered to always start at the same point in the mains cycle.

6.4.2 Spin-Echo Sequences

To implement DD sequences (mostly Uhrig, but also CPMG for comparison), I inserted an appropriately-timed series of \( \pi \)-pulses in the gap of a Ramsey experiment. The qubit was initially prepared in \((|0\rangle - i|1\rangle)/\sqrt{2}\) by a \( \frac{\pi}{2} \)-pulse, left for a delay \( \tau \) (including the refocussing \( \pi \)-pulses, if any), and measured with a second \( \frac{\pi}{2} \)-pulse. The phase of the second pulse was scanned, using the analogue phase modulation control of the Agilent synths and a DAC channel. The fringes obtained were fit by a sine function, whose frequency was constrained to \( \pm 15\% \) of the average frequency obtained from an unconstrained fit. We are only interested in the amplitude of that sine, which is the contrast of the fringes and is plotted in the graphs.
Figure 6.11: A fitted microwave frequency scan that comprises a single datum of Figure 6.13. The gap time was 30.28 ms and the AC compensation coil was not in use, leading to a frequency shift of -2.4(2) kHz.

Each sequence still has to be synchronised with the 50 Hz mains. Despite the AC compensation coil, the mains frequency shift is still far too high to be corrected by the DD sequences. But by triggering each sequence with the mains, the accumulated phase shift from the mains is almost identical for each repeat of the sequence, therefore it does not cause loss of fringe contrast. Instead, the fringe has a phase offset. Random noise, or oscillations that aren’t at a multiple of 50 Hz, do of course lead to loss of contrast and need to be decoupled by the π-pulses.

Crude fits to the data are also shown on the graphs – modelling the data as a constant followed by a shifted half-Gaussian:

$$a_1 e^{-a_2 \left( \max(0, \tau - a_3) \right)^2}$$  \hspace{1cm} (6.42)

This is a phenomenological fit, with no physical basis, and is only intended to guide the viewer’s eye and estimate a coherence time.

The first series of experiments (23rd January 2009) are shown in Figure 6.15. They were performed without the use of the AC compensation coil, and so the π-pulses might
have very low fidelity at certain times in the AC mains cycle.

The second set of experiments (6th March 2009) used the AC compensation coil, which allowed me to use long sequences with confidence that the $\pi$-pulses would remain at high fidelity. Sometimes, when a scan gave a poorer contrast than expected for the delay time, I would check the microwave resonant frequency and find it had shifted, requiring the DD scan to be repeated. I also started using the Meiboom-Gill phase shift for the $\pi$-pulses, because preliminary experiments implied a small improvement (but see Figure 6.17).

The third set of experiments (12th and 13th March 2009) used the compensation coil, and to maintain a constant, high fidelity for the $\pi$-pulses I checked and set the microwave frequency before every scan. This set included the data of Figure 6.16 which used CPMG and UDD sequences with the same number of $\pi$-pulses.

The fourth set of experiments (16th and 17th April 2009) included five-pulse sequences performed with and without the Meiboom-Gill phase shift. This is essentially equivalent to testing the Uhrig sequence for both $|R\rangle = (|0\rangle - i|1\rangle)/\sqrt{2}$ and
Figure 6.13: Comparison of the shift in the qubit frequency due to the 50Hz mains, with and without the compensation coil. The Stanford’s phase and amplitude were last adjusted 7 days previously. The time from the start of the sequence (the start of the 397 Master pulse, which was just a marker because that laser was turned off) to the start of the first microwave pulse was 2.3485(5) ms. This data taken on the same day as the 6-pulse data of Figure 6.16.

\[ |+\rangle = (|0\rangle + |1\rangle)/\sqrt{2}. \] Results are shown in Figure 6.17.

Finally Figure 6.18 collects all the UDD results together (that use the AC compensation coil and Meiboom-Gill phase shifting – that is, from the second, third and fourth sets of experiments), to compare the effect of number of pulses. The fits are then used to estimate a coherence time – which is taken as the time at which the contrast falls to half its initial value. That is,

\[
\text{coherence time} = a_3 + \sqrt{-\frac{\ln(\frac{1}{2})}{a_2}} \tag{6.43}
\]

using the parameters from (6.42).
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6.4.2.1 Conclusions

All the experiments show that dynamic decoupling is extremely effective at prolonging the phase coherence of the qubit. In a basic Ramsey experiment with no $\pi$-pulses, the contrast stays above half its initial value for $\approx 0.45 \text{ ms}$. With just a single $\pi$-pulse, the standard spin-echo sequence increases this to $\approx 2 \text{ ms}$. Six pulses keep coherence for $\approx 12 \text{ ms}$, and twenty pulses, $\approx 28 \text{ ms}$. Notice also that the contrast does not decay exponentially; instead it seems to fall linearly with time, or even have a plateau of high contrast at short delays and then a sharp drop. This tells us that the noise in our trap is highly correlated over these timescales; Cywiński [169, Section III] says that signal $\propto e^{-\tau / T_2}$ only occurs when the noise autocorrelation time is much smaller than $T_2$. One more thing to notice from Figure 6.18 is that the results are reliably similar from day to day.

Figure 6.14: A 20-pulse Uhrig sequence. This one has 40 ms between the two $\frac{\pi}{2}$-pulses.
The amplitude of the magnetic field noise can be estimated, even though we have been unable to calculate it precisely from detailed simulations and fits to the data.

Consider, for instance, the $n = 0$ Ramsey experiments. The coherence vanished for $\tau \gtrsim 0.8$ ms, so in 0.8 ms the spurious accumulated phase was $\sim \pi$ and the angular frequency error was $\delta \approx \pi/\tau \approx 4$ kHz. This corresponds to a magnetic field of $\approx 1.5$ mG.

The sequence was repeated identically 200 times for each point of the Ramsey fringe, taking 4 s for each point, and it is the change in magnetic field over this timescale that gives measurable dephasing. So we see that the magnetic field fluctuation at the 4 s timescale is $\approx 1.5$ mG.

The average fidelity of each $\pi$-pulse is approximately 98% for $n = 3$ to 20 pulses, which is what we may expect given the residual field variations of Figures 6.12 and 6.13.

Figure 6.16 shows that the CPMG sequence is just as good, if not better, at maintaining fringe contrast as UDD. This matches the findings of Cywiński [169] in the long time or high noise regime.

---

1 An example of such a calculation is from [169], but it requires measurements with large $n$ and small $\tau$ that we are currently unable to perform.
6.4. OUR EXPERIMENT

Unfortunately I have not been able to test the sequences’ effectiveness in the short time regime. This is partly because the large variability in the fringe contrasts I measured would obscure any subtle variability due to real effects; and partly because our finite \( \pi \) time imposes a minimum \( \tau \) that can be tested for a given number of pulses. To speed up the experiments, it would be desirable to emulate Biercuk et al. [141, 170] and not do a phase scan at all. They scanned only the delay time, and simply recorded the probability of shelving after the final \( \frac{\pi}{2} \)-pulse. Unfortunately that may not be practical for us; our fringes also have different phase offsets for different Ramsey delays. This is probably due to the residual AC mains field, which is constant for every experimental run and hence does not reduce the fringe contrast, but could give the qubit a phase shift that varies with the delay time. The Biercuk method would confuse this for loss of phase contrast.

Figure 6.17 shows data with and without the Meiboom-Gill phase shift. Preliminary experiments suggested that the Meiboom-Gill phase shift improves the initial contrast, although it was not expected to affect the decoherence time. In fact, it seems to make
Figure 6.17: Comparing five-pulse UDD sequences with and without the Meiboom-Gill phase shift on the $\pi$-pulses. AC compensation coil in use.

little difference to either figure. In CPMG sequences, the phase shift works partially because there are equal gaps between $\pi$-pulses; this is not true for UDD, which may explain this result.
Figure 6.18: Comparing UDD sequences with from 0 to 20 $\pi$-pulses [top] or 0 to 6 $\pi$-pulses [bottom]. The different symbols denote the number of $\pi$-pulses used for that sequence; different colours for the same symbol indicate data from different days. Hollow symbols are anomalous data points excluded from the fits. AC compensation coil in use.
Figure 6.19: The coherence time, as measured by (6.43), is plotted against the number of UDD $\pi$-pulses. A straight line provides a reasonable fit to the data, especially if the point at 20 pulses is excluded from the fit.
Chapter 7

Conclusion

This thesis described work concerned with detection and protection of quantum bits, focusing on trapped ions and $^{43}\text{Ca}^+$ in particular.

The first stage was to develop a full rate equations model of the states and transitions of a $^{43}\text{Ca}^+$ ion. It includes the 4S, 4P and 3D levels and automatically calculates hyperfine structure. While such simulations do not include coherent effects such as dark resonances, and thus disagree with experimental data in some circumstances, they are accurate enough to predict and explain the results of experiments with far off-resonant laser beams. This is relevant for readout and sympathetic cooling.

The speed of rate-equations simulations allows them to be used to optimise an electron-shelving readout method in $^{43}\text{Ca}^+$. The procedure uses pulses of tuned, $\sigma^+$ polarised 393 nm light to transfer ions from $S_{1/2}^4$ to $D_{5/2}$, while causing as few transfers as possible from $S_{3/2}^3$. Approximately 10% of the time, the ion is transferred to $D_{3/2}$ instead; the procedure repumps back to $S_{1/2}^4$ with pulses of 850 nm light, carefully tuned and polarised to minimise unwanted transfer to $S_{1/2}^3$. The predicted maximum fidelity of the process was 99.968% at a time of 100 $\mu$s. Restricting the time to 10 $\mu$s allows 99.958% fidelity.

The shelving method could be simplified while retaining high fidelity by using a single pulse in which all three laser beams ($393\sigma^+, 850\sigma^+, 850\pi$) are switched on. This achieves up to 99.965% fidelity, but is significantly slower than the multipulse method. Even simpler, a single circularly-polarised 850 nm beam at a small angle ($\sim 2^\circ$) to the magnetic field direction achieves up to 99.963% fidelity in 300 $\mu$s. The shelving was shown to be robust against errors of pulse timing, laser intensity and beam polarisation.

Experimentally, a readout fidelity of up to 99.77(4)% was performed, including all
error sources. We remove the measured error due to fluorescence detection (0.097(17)\%) to obtain the fidelity for shelving alone: $F = 99.87(2)\%$ in 400\ $\mu$s. Despite the method’s predicted robustness, this is an error five times larger than the theoretical optimum – possibly due to setting the 393 intensity twice as high as is ideal, and having 0.13\% $\sigma$-impurity in the 850 beam.

Experiments were performed with a mixed pair of ions, $^{40}\text{Ca}^+$ and $^{43}\text{Ca}^+$. In contrast with the pure $^{40}\text{Ca}^+$ case, we discovered high heating and motional decoherence rates, as well as frequent decrystallisation and other problems. This prevented us from reaching our aim – an entangling phase gate between the two isotopes. As I describe below, we will soon make several major improvements to the apparatus. We decided it would not be efficient to spend any more time tracking down the problems, since the trap would soon be replaced anyway.

Dephasing of qubits is a major source of errors in quantum information processing. A spin-echo pulse sequence was derived that can eliminate phase errors when the dephasing is caused by a frequency drift that is an arbitrary polynomial in time. If its highest-order term is $t^{n-1}$, then $n$ $\pi$-pulses are required and should be spaced at times

$$\tau \sin^2\left(\frac{\pi}{2\frac{n}{n+1}}\right), \tau \sin^2\left(\frac{\pi}{2\frac{n}{n+1}}\right), \ldots, \tau \sin^2\left(\frac{\pi}{2\frac{n}{n+1}}\right)$$

where the qubit’s original state is recovered at $t = \tau$. The derived sequence is the same as the one that had previously been derived by Uhrig, by treating the sequence as a filter function; I have reviewed the relevant literature on this dynamical decoupling method.

The sequence was implemented on a single trapped $^{43}\text{Ca}^+$ ion. But first, to improve the $\pi$-pulse fidelity, a coil was installed to cancel out the (50 Hz component of the) magnetic field of the mains. The sequence was then tested. Using 0, 1, 3, 5, 6, 10 and 20 $\pi$-pulses gave coherence times of, respectively, 0.4 ms, 1.9 ms, 5.7 ms, 9.8 ms, 12 ms, 18 ms and 30 ms. Twenty pulses gave a 75-fold enhancement, using the ambient noise environment of our experiment. The simpler CPMG pulse sequence was equally effective, which suggests that our ambient noise is outside the low-frequency regime where UDD would be optimal. We saw no significant change between performing $\pi$-pulses about the $x$ or $y$-axes.
7.1 Future Developments

We have begun constructing a new trap and vacuum chamber, with several benefits over the current apparatus. The trap will be a linear Paul trap like our current one, but $\approx 40\%$ of the size (ion-electrode distance = 0.5 mm). We hope to reach secular frequencies up to $\omega_r = 2\pi \times 3.6 \text{ MHz}$ and $\omega_z = 2\pi \times 2 \text{ MHz}$. The vacuum chamber will be based on an octagon rather than the current hexagon – this will allow laser access both parallel and perpendicular to the magnetic field, so that $\pi$-polarised light is available for optical pumping into clock states, or testing the faster shelving methods. The new trap’s higher secular frequency will make ground-state cooling significantly easier than it is currently, because the Doppler limit will then be $\bar{n}_z \approx 2$. We should be able to omit the slow continuous sideband cooling step in motional experiments. We will be able to use higher aspect ratios (much stronger radial than axial potential), without reducing axial frequency, compared with in our current trap, which should improve the crystallisation of 40-43 pairs. We will be able to make a better study of mixed crystals than described in this work, and aim to implement the mixed-species quantum logic gate and use it for a classical AND gate. Furthermore, we have recently purchased a pair of Toptica TA-SHG110 lasers producing 130 mW at 397 nm for use as a Raman laser with $^{43}\text{Ca}^+$. Higher Raman beam intensities allow the beams to be further detuned for a given Rabi frequency, reducing gate decoherence due to photon scattering.

The chamber and trap electrodes will be made out of 316 stainless steel, which is less magnetisable than standard stainless steel; we expect this to reduce the stray magnetic fields at the ion. Two coaxial feedthroughs will be included for more efficient transfer of microwave signals to the ion. The feedthroughs will be connected inside the chamber, allowing microwaves both in and out (passing the ion on the way): this gives us the flexibility to terminate the transmission line with a 50 $\Omega$ absorber, a reflective open/closed circuit or some other terminator, whichever turns out to give the highest Rabi frequency.

Even though multi-well microtraps will become increasingly important in the future for demonstrating the scalability of ion-trap quantum computing, a simple, low-heating-rate trap such as this will remain useful for many interesting experiments.
Appendix A

Hyperfine Structure of $^{43}\text{Ca}^+$

The following graphs show the hyperfine structure of the transitions of $^{43}\text{Ca}^+$. Each hyperfine component is drawn as a thick black solid vertical line. Its $x$-position indicates the frequency of the component, and the height shows the branching ratio of that component. The branching ratio from an upper state $j$ to a lower state $i$ is given by:

$$\text{Br}_{j\rightarrow i} = \frac{\Gamma_{j\rightarrow i}}{\sum_k \Gamma_{j\rightarrow k}} = \frac{\Gamma_{j\rightarrow i}}{\Gamma_j}$$  \hspace{1cm} (A.1)$$

where $\Gamma_{j\rightarrow i}$ is the spontaneous transition rate from $j$ to $i$, and $\Gamma_j$ is the total decay rate out of $j$ to any level. The branching ratio also indicates the strength of stimulated transitions between $i$ and $j$ (see Section 3.1.2.1).

Each hyperfine component is labeled as $F_j \rightarrow F_i$ (upper to lower). Also shown for 397 nm and 393 nm are the positions of the $^{40}\text{Ca}^+$ resonance, as a dotted line (the height of this line is not significant). Note that the 850 nm component $P_{3/2}^3 \rightarrow D_{3/2}^3$ is forbidden.
APPENDIX A. HYPERFINE STRUCTURE OF $^{43}$CA$^+$

Figure A.1:

$397$ nm $4P_{1/2} \rightarrow 4S_{1/2}$

Branching ratio

Frequency detuning in MHz relative to the centre of gravity

Figure A.2:

$866$ nm $4P_{1/2} \rightarrow 3D_{3/2}$

Branching ratio

Frequency detuning in MHz relative to the centre of gravity
Figure A.3:

Figure A.4:
Figure A.5:
Appendix B

The Transitions Suite: Users’ Guide

This is the users’ manual for the major functions in my Transitions suite of programs. The basic principles are described in Sections 3.1 and 3.2 so this appendix will be of use mostly to those who want to use the programs.

B.1 Setting Up

At the start of any MATLAB session where Transitions is to be used, the user must run “transitionsSetup.m”: tranStruct = transitionsSetup. The structure tranStruct contains information about the ion: Einstein A coefficients, a list of the states and their quantum numbers, \( M_{spont} \) etc. The nature of its fields is explained in the help comment (type help transitionsSetup). You may use several different structures at the same time, simply by saving the output of transitionsSetup to a different variable. This allows you to, for example, compare \(^{40}\text{Ca}^+\) and \(^{43}\text{Ca}^+\).

To change the ion or atom you are using, you must edit the function “transitionsGlobals.m”. This contains data such as the nuclear spin, Einstein A coefficients and which major levels you wish to use. Despite its name, none of the file’s contents is global in scope. Instead, the function returns a structure containing that data, in a form that can be input into transitionsSetup. For example, suppose you have set up “transitionsGlobals40.m” with data about \(^{40}\text{Ca}^+\). Type

\[
\text{tranStruct40} = \text{transitionsSetup(transitionsGlobals40)};
\]
to use it. If `transitionsSetup` is given no input, it uses “transitionsGlobals.m” by default. Currently, “transitionsGlobals.m” is set up for $^{43}\text{Ca}^+$. The command

```octave
tranStruct.levData = transitionsZeemanData(tranStruct, B)
```

will apply a magnetic field $B$ to the ion. $B$ is in Tesla: $1 \text{T} = 10^4 \text{G}$. You may use this command as often as you wish to change the field. Only the linear Zeeman shifts are calculated, and no attempt is made to mix the states.

### B.2 Adding and Using Lasers

Initially, no laser light exists in the model. Lasers are stored in matrices, with each row representing a laser. Suppose you already have a list of lasers, called `lasers` (if you don’t, simply define it as the empty matrix `[]` or `{}`), that you wish to add to. Use the command:

```octave
lasers = transitionsAddLaser(tranStruct, lasers, ...
{newName oldName intensity detuning});
```

where `newName` is a string that you wish to call the new laser; `intensity` is the initial intensity of the laser in saturation intensities; `detuning` is the frequency difference, in $s^{-1}$ (angular units), between the laser and the centre-of-gravity of the sublevels of the level addressed by the laser. `oldName` is a string specifying a template on which to base your laser. An `oldName` of ‘866+’ causes your new laser to be 866 nm with a polarisation of $\sigma+$. ‘397|’ or ‘850−’ define 397 nm $\pi$ polarised or 850 nm $\sigma−$ polarised lasers respectively. 854 nm and 393 nm are available as well. A laser of a particular wavelength is assumed to address one fine-structure line only, e.g. using ‘866+’ means that your laser will only affect the $4P_{1/2} \leftrightarrow 3D_{3/2}$ transition (but all the hyperfine components of it) no matter what its detuning. To define new template lasers (e.g. for using a different type of ion), edit “transitionsGlobals.m”.

The `newName` given to a laser when it was created allows you to change its detuning or intensity at any time. Use

```octave
lasers = transitionsChangeDetuning(lasers, name, detuning);
```

to change the detuning of the laser called `name`, stored in the matrix `lasers`, to `detuning` $s^{-1}$ (use `detuning*2e6*pi` to specify detuning in MHz).

```octave
lasers = transitionsChangeIntensity(lasers, name, intensity);
```
works similarly for intensity in $I_0$.

Although $M^{spont}$ is generated by `transitionsSetup` and stored in `tranStruct`, you must keep track of $M^{stim}$ yourself. The matrix of stimulated transitions due to the set of lasers `lasers` is calculated by

```matlab
stimMatrix = transitionsGenStim(tranStruct, lasers);
```

It is a good idea to keep at least two different laser lists and $M^{stim}$s: one for lasers that you keep fixed, and one for lasers being scanned. This will make your simulation faster.

## B.3 Solving

This code finds the steady state sublevel populations:

```matlab
transMatrix = spontMatrix + stimMatrix1 + stimMatrix2 + ...;
solution = transitionsSteadySolve(transMatrix);
```

The vector `solution` contains the population of each sublevel. You do not need to worry about adding the normalisation constraint manually: `transitionsSteadySolve` does it for you.

There is no special function for handling time-dependent modelling, but we only need MATLAB’s own matrix exponential function `expm`. Given a `time` in seconds, and an initial vector of populations `initial` the code

```matlab
pulseMatrix = expm(transMatrix*time);
final = pulseMatrix * initial;
```

returns `final`, the population vector that results from evolving `initial` for `time` seconds.

Sometimes we want to keep `transMatrix` constant and calculate how the populations change over time. In this case we can gain a significant speed-up by splitting the matrix exponential into two parts (algorithm by Simon Webster). First run

```matlab
[v,d]=eig(transMatrix);
```

once to calculate the eigenvectors `v` and eigenvalues `d`. Then, inside the loop that scans the `time`, we can use

```matlab
pulseMatrix = real(v*diag(exp(diag(d*time)))/v);
```

The speed gain is a factor of $\sim 2$. 

B.4 Utility Functions

The indices corresponding to each level are listed in Table B.1.

<table>
<thead>
<tr>
<th>Level</th>
<th>Starts at Row</th>
<th>Ends at Row</th>
</tr>
</thead>
<tbody>
<tr>
<td>4S$_{1/2}$</td>
<td>1</td>
<td>16</td>
</tr>
<tr>
<td>3D$_{3/2}$</td>
<td>17</td>
<td>48</td>
</tr>
<tr>
<td>3D$_{5/2}$</td>
<td>49</td>
<td>96</td>
</tr>
<tr>
<td>4P$_{1/2}$</td>
<td>97</td>
<td>112</td>
</tr>
<tr>
<td>4P$_{3/2}$</td>
<td>113</td>
<td>144</td>
</tr>
</tbody>
</table>

Table B.1: Indices of the $^{43}$Ca$^+$ levels in the matrices and vectors produced by the
_Transitions_ functions

The routine _transitionsLevFind_ can be used to find the indices of a particular set of states. For instance,

```plaintext
transitionsLevFind(tranStruct, 4, [1,0], 1/2, 3, 0)
```

tells you that the 4S$_{1/2}$ and 4P$_{1/2}$ substates can be found at indices 4 and 100 (NOT necessarily respectively). The order of arguments (after the data structure) is $n$, $L$, $J$, $F$, $M_F$. Any of the arguments can be scalar, vector or matrix. One or more of the rightmost arguments may be omitted to allow that quantum number to take any value. E.g.

```plaintext
transitionsLevFind(tranStruct, [3,4], [0,1,2], 3/2)
```

finds the indices of all states with $n = 3$ or 4, $L = 0$, 1 or 2 and $J = 3/2$. It can also understand spectroscopic notation:

```plaintext
transitionsLevFind(tranStruct, '4P_{1/2}(4,4)')
```

The underscore “_” or the braces “{“ can be omitted. But if hyperfine components are specified they must be in parentheses “()”. The function _transitionsSpecNote_ (by Andrew Steane) converts between spectroscopic notation and [$n$, $L$, $J$, $F$, $M_F$] lists, in either direction.
This example MATLAB script file creates (a low-resolution version of) Figure 3.1. It demonstrates many of the commands described in this appendix.

% Based on coolingWithSidebands2009_04_29.m

% Automatically define tranStruct if not already done.
if (exist('tranStruct','var') ~= 1)
    tranStruct = transitionsSetup
end

% Set up magnetic field.
tranStruct.levData = transitionsZeemanData(tranStruct, 1.5e-4);
% Define a short-named copy of levData, for later reference.
lD = tranStruct.levData;
% Define the laser intensities in saturation intensities.
totalIntensity866 = 170;
totalIntensity397 = 14;

% Find the indices of the levels.
indS4 = transitionsLevFind(tranStruct, 4,0,1/2,4,0);
indS3 = transitionsLevFind(tranStruct, 4,0,1/2,3,0);
indP4 = transitionsLevFind(tranStruct, 4,1,1/2,4,0);
% Just for a change, demonstrate spectroscopic notation.
indP3 = transitionsLevFind(tranStruct, '4P1/2(3,0)');

% Detuning of 397 is the energy shift of the P_1/2 level, minus
% that of the S_1/2 level. The first column shows the frequency
% addressed by the carrier; the second column is the sideband.
% All 12 possible choices are included here.
detunings397 = ...
[1D(indP4,7)-1D(indS3,7) 1D(indP4,7)-1D(indS4,7); ...
1D(indP4,7)-1D(indS3,7) 1D(indP3,7)-1D(indS4,7); ...
1D(indP3,7)-1D(indS3,7) 1D(indP4,7)-1D(indS4,7); ...
1D(indP3,7)-1D(indS3,7) 1D(indP3,7)-1D(indS4,7); ...
1D(indP4,7)-1D(indS4,7) 1D(indP4,7)-1D(indS3,7); ...
1D(indP3,7)-1D(indS4,7) 1D(indP4,7)-1D(indS3,7); ...]
\[ 1D(\text{indP4,7}) - 1D(\text{indS4,7}) \quad 1D(\text{indP3,7}) - 1D(\text{indS3,7}); \ldots \]
\[ 1D(\text{indP3,7}) - 1D(\text{indS4,7}) \quad 1D(\text{indP4,7}) - 1D(\text{indS4,7}); \ldots \]
\[ 1D(\text{indP3,7}) - 1D(\text{indS3,7}) \quad 1D(\text{indP3,7}) - 1D(\text{indS3,7}); \ldots \]
\[ 1D(\text{indP4,7}) - 1D(\text{indS3,7}) \quad 1D(\text{indP3,7}) - 1D(\text{indS3,7}); \ldots \]
\[ 1D(\text{indP3,7}) - 1D(\text{indS4,7}) \quad 1D(\text{indP3,7}) - 1D(\text{indS4,7}); \ldots \]
\[ 1D(\text{indP4,7}) - 1D(\text{indS4,7}) \quad 1D(\text{indP3,7}) - 1D(\text{indS4,7})] \]

% Frequency values to plot in MHz. Change the number between the
% colons to change the resolution. I used 5 for my plot in the
% thesis.
freqs = -1500:50:2000;
% Predefine the array that will hold the results, for efficiency.
results = zeros(length(freqs),12);

% Loop over all choices of 397 carrier and sideband frequency.
for itD = 1:12
    detuning397c = detunings397(itD,1);
    detuning397s = detunings397(itD,2);
    % Carrier: has 74% of the total 397 intensity.
lasersFixed = [];
    lasersFixed = transitionsAddLaser(tranStruct, lasersFixed, ...
        {'397c+','397+', totalIntensity397*0.74/2, detuning397c});
    lasersFixed = transitionsAddLaser(tranStruct, lasersFixed, ...
        {'397c-','397-', totalIntensity397*0.74/2, detuning397c});
    % Sideband: has 13% of the total 397 intensity.
lasersFixed = transitionsAddLaser(tranStruct, lasersFixed, ...
        {'397s+','397+', totalIntensity397*0.13/2, detuning397s});
    lasersFixed = transitionsAddLaser(tranStruct, lasersFixed, ...
        {'397s-','397-', totalIntensity397*0.13/2, detuning397s});

    % Calculate the stimulated transitions matrix for the fixed 397nm
    % laser.
    stimMatrixFixed = transitionsGenStim(tranStruct, lasersFixed);
    % The spontaneous decay matrix is also constant, so we can add
    % these two fixed matrices together now to reduce the amount of
    % work the program does at each data point.
    transMatrixFixed = (stimMatrixFixed + tranStruct.spontMatrix);
lasersScanned = [];
% 866 beam. Its detuning is initially set to 0, because we'll
% scan it soon.
lasersScanned = transitionsAddLaser(tranStruct, lasersScanned, ...
    {'866+', '866+', totalIntensity866/2, 0});
lasersScanned = transitionsAddLaser(tranStruct, lasersScanned, ...
    {'866-', '866-', totalIntensity866/2, 0});

for itF = 1:length(freqs)
    % Change detuning.
    freq = freqs(itF);
    lasersScanned = transitionsChangeDetuning(lasersScanned, ...
        '866+', (freq)*2*pi*1e6);
    lasersScanned = transitionsChangeDetuning(lasersScanned, ...
        '866-', (freq)*2*pi*1e6);
    stimMatrixScan = transitionsGenStim(tranStruct, lasersScanned);
    transMatrix = transMatrixFixed + stimMatrixScan;
    % Actually find the steady-state populations here.
    solutionVector = transitionsSteadySolve(transMatrix);
    % Add together the populations of all of the P_{1/2} states, and
    % save as a result.
    results(itF, itD) = sum(solutionVector(97:112));
end
end

%%

% Plot a graph of the results
figure1 = figure('Color',[1 1 1], 'Visible','on');
figure(figure1);
axes1 = axes('Parent',figure1);

% Choose some pretty colours.
coloursSat = 1;
coloursVal = 0.75;

colours = [0 coloursSat coloursVal; 1/4 coloursSat coloursVal; ... 
1/2 coloursSat coloursVal; 3/4 coloursSat coloursVal];

plot(axes1, freqs', results(:,1), '-', 'Color', hsv2rgb(colours(1,:)));
hold('on')
plot(axes1, freqs', results(:,2), '-', 'Color', hsv2rgb(colours(2,:)));
plot(axes1, freqs', results(:,3), '-', 'Color', hsv2rgb(colours(3,:)));
plot(axes1, freqs', results(:,4), '-', 'Color', hsv2rgb(colours(4,:)));
plot(axes1, freqs', results(:,5), ':', 'Color', hsv2rgb(colours(1,:)));
plot(axes1, freqs', results(:,6), ':', 'Color', hsv2rgb(colours(2,:)));
plot(axes1, freqs', results(:,7), ':', 'Color', hsv2rgb(colours(3,:)));
plot(axes1, freqs', results(:,8), ':', 'Color', hsv2rgb(colours(4,:)));

% Add a horizontal line indicating the experimental result, 4.7%
plot(axes1, [freqs(1) freqs(end)], [0.047 0.047], '--k');

set(axes1, 'XGrid','on', 'YGrid','on', ... 
'XMinorTick','on', 'YMinorTick','on')
xlabel(axes1, '866 Frequency Relative to Centre of Gravity / MHz');
ylabel(axes1, 'Population of P_{1/2}');

% Define the legend that explains the colour code of the lines.
% Sorry it looks such a mess; each line of the legend had to be
% chopped in half to fit LaTeX's line-length limit.
legend(...
['Carrier on S_{1/2}^{4}\rightarrow P_{1/2}^{4};'... 
'Sideband on S_{1/2}^{4}\rightarrow P_{1/2}^{4}', ... 
'Carrier on S_{1/2}^{4}\rightarrow P_{1/2}^{3};'... 
'Sideband on S_{1/2}^{4}\rightarrow P_{1/2}^{3}', ... 
'Carrier on S_{1/2}^{3}\rightarrow P_{1/2}^{4};'... 
'Sideband on S_{1/2}^{3}\rightarrow P_{1/2}^{4}', ... 
'Carrier on S_{1/2}^{3}\rightarrow P_{1/2}^{3};'... 
'Sideband on S_{1/2}^{3}\rightarrow P_{1/2}^{3}', ... 
'Carrier on S_{1/2}^{3}\rightarrow P_{1/2}^{4};'... 
'Sideband on S_{1/2}^{3}\rightarrow P_{1/2}^{4}', ... 
'Carrier on S_{1/2}^{3}\rightarrow P_{1/2}^{3};'... 
'Sideband on S_{1/2}^{3}\rightarrow P_{1/2}^{3}', ... 
'Carrier on S_{1/2}^{3}\rightarrow P_{1/2}^{4};'... 
'Sideband on S_{1/2}^{3}\rightarrow P_{1/2}^{4}', ... 
'Carrier on S_{1/2}^{3}\rightarrow P_{1/2}^{3};'... 
'Sideband on S_{1/2}^{3}\rightarrow P_{1/2}^{3}', ... 
'Carrier on S_{1/2}^{3}\rightarrow P_{1/2}^{4};'... 
'Sideband on S_{1/2}^{3}\rightarrow P_{1/2}^{4}', ... 
'Carrier on S_{1/2}^{3}\rightarrow P_{1/2}^{3};']... 
'Sideband on S_{1/2}^{3}\rightarrow P_{1/2}^{3}', ... 
'Carrier on S_{1/2}^{3}\rightarrow P_{1/2}^{4};'... 
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'Carrier on S_{1/2}^{3}\rightarrow P_{1/2}^{3};'... 
'Sideband on S_{1/2}^{3}\rightarrow P_{1/2}^{3}', ... 
'Carrier on S_{1/2}^{3}\rightarrow P_{1/2}^{4};'... 
'Sideband on S_{1/2}^{3}\rightarrow P_{1/2}^{4}', ... 
'Carrier on S_{1/2}^{3}\rightarrow P_{1/2}^{3};'... 
'Sideband on S_{1/2}^{3}\rightarrow P_{1/2}^{3}', ... 
'Carrier on S_{1/2}^{3}\rightarrow P_{1/2}^{4};'... 
'Sideband on S_{1/2}^{3}\rightarrow P_{1/2}^{4}', ... 
'Carrier on S_{1/2}^{3}\rightarrow P_{1/2}^{3};'... 
'Sideband on S_{1/2}^{3}\rightarrow P_{1/2}^{3}', ... 
'Carrier on S_{1/2}^{3}\rightarrow P_{1/2}^{4};'... 
'Sideband on S_{1/2}^{3}\rightarrow P_{1/2}^{4}', ... 
'Carrier on S_{1/2}^{3}\rightarrow P_{1/2}^{3};'... 
'Sideband on S_{1/2}^{3}\rightarrow P_{1/2}^{3}', ... 
'Carrier on S_{1/2}^{3}\rightarrow P_{1/2}^{4};'... 
'Sideband on S_{1/2}^{3}\rightarrow P_{1/2}^{4}', ... 
'Carrier on S_{1/2}^{3}\rightarrow P_{1/2}^{3};'... 
'Sideband on S_{1/2}^{3}\rightarrow P_{1/2}^{3}', ... 
'Carrier on S_{1/2}^{3}\rightarrow P_{1/2}^{4};'... 
'Sideband on S_{1/2}^{3}\rightarrow P_{1/2}^{4}', ... 
'Carrier on S_{1/2}^{3}\rightarrow P_{1/2}^{3};'... 
'Sideband on S_{1/2}^{3}\rightarrow P_{1/2}^{3}', ... 
'Carrier on S_{1/2}^{3}\rightarrow P_{1/2}^{4};'... 
'Sideband on S_{1/2}^{3}\rightarrow P_{1/2}^{4}', ... 
'Carrier on S_{1/2}^{3}\rightarrow P_{1/2}^{3};'... 
'Sideband on S_{1/2}^{3}\rightarrow P_{1/2}^{3}', ... 
'Carrier on S_{1/2}^{3}\rightarrow P_{1/2}^{4};'... 
'Sideband on S_{1/2}^{3}\rightarrow P_{1/2}^{4}', ... 
'Carrier on S_{1/2}^{3}\rightarrow P_{1/2}^{3};'... 
'Sideband on S_{1/2}^{3}\rightarrow P_{1/2}^{3}', ... 
'Carrier on S_{1/2}^{3}\rightarrow P_{1/2}^{4};'... 
'Sideband on S_{1/2}^{3}\rightarrow P_{1/2}^{4}', ... 
'Carrier on S_{1/2}^{3}\rightarrow P_{1/2}^{3};'... 
'Sideband on S_{1/2}^{3}\rightarrow P_{1/2}^{3}', ... 
'Carrier on S_{1/2}^{3}\rightarrow P_{1/2}^{4};'... 
'Sideband on S_{1/2}^{3}\rightarrow P_{1/2}^{4}', ... 
'Carrier on S_{1/2}^{3}\rightarrow P_{1/2}^{3};'... 
'Sideband on S_{1/2}^{3}\rightarrow P_{1/2}^{3}', ... 
'Carrier on S_{1/2}^{3}\rightarrow P_{1/2}^{4};'... 
'Sideband on S_{1/2}^{3}\rightarrow P_{1/2}^{4}', ... 
'Carrier on S_{1/2}^{3}\rightarrow P_{1/2}^{3};'... 
'Sideband on S_{1/2}^{3}\rightarrow P_{1/2}^{3}', ... 
'Carrier on S_{1/2}^{3}\rightarrow P_{1/2}^{4};'... 
'Sideband on S_{1/2}^{3}\rightarrow P_{1/2}^{4}', ... 
'Carrier on S_{1/2}^{3}\rightarrow P_{1/2}^{3};'... 
'Sideband on S_{1/2}^{3}\rightarrow P_{1/2}^{3}', ... 
'Carrier on S_{1/2}^{3}\rightarrow P_{1/2}^{4};'... 
'Sideband on S_{1/2}^{3}\rightarrow P_{1/2}^{4}', ...
B.5. EXAMPLE

['Carrier on $S_{1/2}^{4}$\rightarrow $P_{1/2}^{4}$;'
' Sideband on $S_{1/2}^{3}$\rightarrow $P_{1/2}^{3}$], ... 

['Carrier on $S_{1/2}^{4}$\rightarrow $P_{1/2}^{3}$;'
' Sideband on $S_{1/2}^{3}$\rightarrow $P_{1/2}^{3}$], ... 

'Experimental P Population: 4.7%')
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