

Towards Large Scale Quantum Simulations with Trapped Ions: Programmable XY model, Precise Light Sensing, and Extreme High Vacuum

by

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Author's Declaration

I hereby declare that I am the sole author of this thesis. This is a true copy of the thesis, including any required final revisions, as accepted by my examiners.

I understand that my thesis may be made electronically available to the public.

Abstract

We are currently witnessing a revolution in quantum technologies. Today’s controllable quantum devices have reached a complexity that makes it practically intractable to fully simulate their dynamics using current classical supercomputers. Decades of fundamental research and development have led us to this point. In the coming years, billions of dollars in investments from governments and private entities are expected worldwide. Although general-purpose fault-tolerant quantum computers are expected to impact computing profoundly, today’s quantum devices are best suited for their analog quantum operation, where a well-controlled quantum simulator mimics the dynamics of the other quantum system being studied. This affords an advantage over classical simulators at the cost of a restricted set of physical phenomena that can be studied. Today’s quantum devices are already providing insights into large-scale entanglement, the underlying physics of high-temperature superconductivity, disordered quantum systems, and much more. Enhancing the capabilities of today’s analog quantum simulators requires adding more classes of interactions, reducing errors due to calibration and noise, and increasing the system size to allow larger-scale simulations.

The work described in this thesis directly addresses these core points for a system of trapped ions, which are ideal quantum simulators of the coupled dynamics of a large number of magnetic spins. First, the theory and experiment pertaining to the simulation of the anisotropic XY model on trapped ions has been presented. The theoretical proposal does not require added technical improvements over what has existed in the field for over a decade. The experimental validation is performed on a system with two $^{171}\text{Yb}^+$ ions. This directly enhances the repertoire of trapped ions simulators and opens avenues to the exploration of high-temperature superconductivity, superfluidity, and spin liquids. The second result is the demonstration of the highest resolution readout of optical intensity and polarization using a single $^{171}\text{Yb}^+$ ion as the field probe. The technique utilized the intensity- and polarization-dependent optical pumping of the ions as a signature to detect light parameters. This will be useful for the characterization of the optical addressing fields in trapped ion quantum simulators and hence for the calibration of large-scale quantum devices. Finally, the design and construction of a large-scale ion trapping apparatus for quantum simulation are described. The ion trap allows for the trapping of more than 50 $^{171}\text{Yb}^+$ ions, and the vacuum chamber used to house the trap with pressure below 1.5×10^{-12} mbar (measurement limited by pressure gauge saturation) likely sets a record for the lowest pressure achieved on a room-temperature trapped ions system. This increases the useful simulation time of large-scale trapped-ion devices and paves the way for further enhancement of the scale of the simulations performed. Together, these results are

another step in advancing the capabilities of today's quantum devices to explore physical phenomena far beyond the capability of classical supercomputers.

Acknowledgments

I had planned to write this section in the usual manner, but that would not do justice to my experience at the QITI (Quantum Information with Trapped Ions) lab. Joining the lab at its inception has been an exhilarating experience and I want to start by first acknowledging the builders: the first generation of the QITI lab.

The Builders

Sometimes I can't help but wonder, how the last few years have passed
A lot could've discouraged us, but we've been able to last
I'll call ourselves the builders! Rajibul, Sainath, Gilbert, and I
And in the grand scheme of things, we've really had a blast!

We walked into an empty room, with a heart full of glee
And trust me when things didn't work, sometimes I wanted to flee
But like a well oiled machine, we kept playing our part
And when we shifted the lab, we also took things apart

Rajibul is fun to work with! And he's not just great at science
He understands people well, knows it gets hard at times
In the times of difficulty, he has the demeanor of a monk
Even if sometimes it seems like, the plan is going to flunk!

What do I say about Sainath and Gilbert, making progress every passing day
When you're surrounded by folks like them, It's easier to keep fear at bay
For anything involving optics or code, Gilbert could always take the load
And Sainath can do everything, he doesn't even have to be told

Ohh! And as much as I'd like to claim, that the builders were just us
Rajibul always made sure, talent always kept flowing
Within a year of our start, we were joined by Roland and Manas
Roland settled in the UK, where his little one is growing.

If I'm gonna talk about builders, Lewis deserves a special mention
When it comes to building stuff, no detail escapes his attention
With Anthony, Monica and Yu-Ting, the 'four rod' has a new set of wings
There is no doubt in my mind, you will all do really amazing things

Sakshee, Shilpa and Fabien, old and new additions to the blade trap arsenal
There will be several challenges ahead, but you are onto something phenomenal,
Now listing everyone who contributed, is far beyond my poetic ability
To all the people I've missed, that's simply my lyrical incapability

The best decision I've made, was to join the lab at its start
For all that you all gave me, thank you from the bottom of my heart
My experience at the QITI lab, I will forever cherish
Whatever I learned from you all, it will certainly never perish

I meant it when I said that this was the best career decision. I want to now thank Rajibul for giving me this opportunity. He is a fantastic scientist with a great eye for detail and a very good communicator. I have learned a lot about effective communication and presentation from observing him. He has ensured that the lab culture is positive and pleasant while ensuring productivity. And it has been thoroughly enjoyable writing papers with him, going over each line and figure until we were completely satisfied. And not just the writing, but also the occasional banter, was fun. The best part is that we have planned a lot of stuff to write, so wherever I go, I will at least be able to enjoy it longer.

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Dedication

This is dedicated to my family.

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Chapter 1

Introduction

Heavier-than-air flying machines are impossible.

– Lord Kelvin, Engineer, Mathematician, and Physicist, 1895

There is no likelihood man can ever tap the power of the atom. The glib supposition of utilizing atomic energy when our coal has run out is a completely unscientific Utopian dream, a childish bug-a-boo.

– Robert Millikan, Physicist, 1928

We never experiment with just one electron, or atom or small molecule. In thought experiments, we assume that we do; this invariably entails ridiculous consequences.

– Erwin Schrödinger, Physicist, 1952

Any sufficiently advanced technology is indistinguishable from magic.

– Arthur C. Clarke, Science Fiction Writer, 1962

On 17 December 1903 at Kitty Hawk, North Carolina, Wilber and Orville flew the Wright flyer, a flying machine powered on a mere twelve horsepower gasoline engine. They proved to the world that heavier-than-air machines could fly. The view that humans could not harness nuclear energy for useful purposes was held not only by one Nobel laureate, Robert Millikan, but even by Earnest Rutherford [1]. Yet, it is possible that you are reading this thesis on a device that was charged on or plugged into a grid powered with nuclear power. And Schrödinger, who did not consider quantum jumps to be real, almost certainly did not expect [2, 3] that part of the 1989 Nobel Prize in physics would be awarded to Wolfgang Paul for the invention of the Paul trap [4], a device that would soon be used to trap single atomic ions and also observe quantum jumps [5, 6].

I am starting my introduction with quotes from scientific stalwarts that have not stood the test of time, but my intention is not to mock, not even the slightest bit. The progress of science and technology has been so mind-boggling that it is not possible for anyone to predict the future. Arthur C. Clarke put it rather aptly that “*Any sufficiently advanced technology is indistinguishable from magic*”. Today, quantum technologies seem to be the beginning of another such upheaval.

The first quantum revolution was fueled by the newfound understanding of quantum mechanics and gave us technologies such as modern electronics, the laser, the atomic clock, and MRI scanners. This led to computers, the global positioning system, biomedical imaging equipment, and other technologies that have transformed the global economy on an unprecedented scale. The first quantum revolution harnessed the power of quantum mechanics to a great extent, but the manipulation of individual quantum objects was beyond reach. Today we are witnessing the second quantum revolution, where single quantum objects like atoms, electrons, molecules, photons, etc. are routinely manipulated in the lab. This opens up new avenues for metrology and sensing [7, 8, 9], computation [10, 11], and understanding physics and chemistry [12, 13, 14] that can drastically surpass the scale of current technologies. In the words of Prof. Ivan Deutsch [15], “The second quantum revolution is accelerating—and with eyes wide open to the opportunities and real challenges, the revolution will deliver”.

The two revolutions were founded on the basis of deep fundamental research in the twentieth century. In 1900 Max Planck introduced the concept of quantized energy levels when he postulated that energy of radiation can only have certain discrete values and the minimal increment is proportional to the frequency of the radiation. Although the idea of quantized energy levels was merely introduced as a clever mathematical trick to quantitatively explain the phenomenon of blackbody radiation, this set the stage for the development of quantum mechanics. Einstein’s work on the photoelectric effect in 1905 further supported Planck’s hypothesis and put forth the notion of the corpuscular nature

of light, with photons being the constituent particles of light.

In 1913 the idea of quantization was applied by Niels Bohr to explain the structure of atoms. The Bohr model of the atom was based on the premise that the electrons orbit the nucleus only at quantized energy levels. Bohr’s model of the atom was further expanded by De Broglie’s matter-wave hypothesis: matter has wave properties. He proposed that matter in motion had an associated wavelength and explained that the quantization of atomic energies was because an electron could only encircle the nucleus in orbits that were integral multiples of the wavelength. And finally by mid-1926, building on these developments, Schrödinger’s wave mechanics gave us the equation that describes a quantum-mechanical wave: the Schrödinger equation.

The Schrödinger equation is one of the most impactful equations in modern physics and has been solved and tested in small systems in great detail [16, 17]. Over the next few decades, the approximate solutions of the Schrödinger equation formed the basis for our understanding of much of chemistry [18], why atoms have the size they do [19, 20, 21], why some materials are transparent while others absorb light [22], why some materials are semiconductors [23], etc. The first quantum revolution was the result of scientific knowledge created from approximate solutions of the Schrödinger equation applied to relevant problems. There has been a great deal of progress in computational and approximation techniques over the past several decades; however, applying this equation to large-scale problems of importance suffers from a fundamental limitation: If X amounts of resources (such as computer memory) are needed to study a system with a single particle, the amount of resources required to study N particles is X^N . This exponential scaling of the computational resources is what makes quantum systems so hard to simulate on classical computers.

This exponential scaling prompted Feynman to suggest [24] in 1981 that “... if you want to make a simulation of nature, you better make it quantum mechanical” at a lecture at the first conference on the physics of computation. This was picked up quickly by researchers, and the blending of the two fields of quantum physics and information science began. In fact, in 1980 Yuri Manin [10, 25] and Paul Benioff [26] had already started working on the lines of using quantum resources for computation. In 1982 [27] Paul Benioff explained how the general computational model of the Turing machine [28] was in a sense incomplete and proposed the concept of the quantum Turing machine. David Deutsch, in 1985 took these ideas further and formalized the idea of a universal quantum computer [29]. The next decade was marked with several quantum algorithms, the most notable among them being Peter Shor’s prime factorization algorithm [30] and Lov Grover’s search algorithm [31]. A mathematical proof that quantum computers could factor large prime numbers meant that, at least in principle, it was possible to build devices that could break existing

encryption protocols [32]. This sparked great academic and commercial interest in the field and in 2000 DiVincenzo, in a seminal paper [33], set the formal requirements for a general-purpose quantum computer. Over the next two decades, several proof-of-principle quantum computers with a small number of qubits were constructed on systems of trapped ions and superconducting circuits [34, 35, 36, 37].

Today we are in the age of noisy intermediate scale quantum (NISQ) devices. The term NISQ was coined by John Preskill [38] to describe devices with 50-100 qubits that are not error corrected. It is quite awe-inspiring that these devices operate at a scale where no classical machine can simulate their dynamics in complete detail. This sentiment is shared by governments around the world; the United States recently passed the National Quantum Initiative (NQI) act, Canada declared its national quantum strategy, UK has its National Quantum Information Programme (UKNQTP), the EU has the Quantum Technologies Flagship and China has their own quantum mission. The private sector too has joined the race with a wide range of investments at all levels, from giant multinational companies like Google, IBM, and Microsoft to startups like Rigetti, Quantinuum, IonQ, etc. The last few years have been replete with researchers claiming quantum supremacy [39], i.e., quantum computers had a distinct advantage over classical ones for the specific task that was performed [40, 41, 42, 43, 44, 45].

With this amazing progress and even more amazing buzzwords, it might seem to an outsider that quantum computers can solve all our problems and that the world is about to be a very different place very soon. I would be wary of painting such a picture. For example, the best-known classical algorithms for solving NP-complete problems¹ have an exponential scaling. The most quantum computers can do to help solve these problems is to use the Grover’s search algorithm [31] and get square root improvement. Obviously, the scaling is still exponential. Quantum computers face much the same challenges that classical computers face in tackling these problems [46]. So, if a logistics company is trying to solve the traveling salesman problem [47] (to find the most efficient route to deliver their packages and potentially save billions of dollars in fuel cost) quantum computers may not be as helpful as we once thought. As Scott Aronson puts it “Quantum magic by itself is not going to do the job”²

¹A quick refresher on complexity classes from a non-computer scientist
P: Solvable by classical computers in polynomial time
NP: The solutions can be verified in polynomial time
NP-Complete: Also in NP, if you can solve one (in polynomial time), you can solve all

²We have no proof that no classical or quantum algorithm for solving NP-complete problems exists. But if there is one, it would have to exploit the structure of the problem in a way that has never been done before. And many people have tried!

Then what is the second quantum revolution all about? The class of problems which can be solved on a quantum computer in polynomial time (BQP) has many useful problems, and an exponential speedup is expected in machine learning [48, 49, 50], matrix inversion [51], recommender systems [52], semidefinite programming [53, 54] and simulating the physics of atoms and molecules [55, 56]. The implications of this are profound for the natural sciences, material science, medicine, and drug discovery. However, NISQ devices will not break cryptography, produce drugs to cure cancer, or help generate cleaner energy to solve the global climate crisis. The bottleneck is the number and quality of the qubits. For example, breaking n -bit RSA, the most commonly used encryption algorithm, requires $\mathcal{O}(n)$ logical(error corrected) qubits, and the realistic estimate of the number of physical qubits required to break 2048 bit RSA is between³ 10^6 and 10^7 . Using a general-purpose quantum computer for practically useful tasks seems to be out of reach for the time being.

Where NISQ devices truly shine is in their analog mode of operation, and by analog, I mean one device being the analog of the other. In the classical and quantum computation literature, any model with discrete inputs that evolves in discrete times is digital, and everything else is analog [15]. The universal quantum computer that we have discussed so far is a digital device. The concept of analog models has also existed in classical computation; for example, Shannon proposed a general purpose analog computer (GPAC) comprising of a set of basic components: adders, multipliers, integrators, and amplifiers based on mechanical and electrical elements. Today, NISQ devices are being used in the analog mode as quantum optimizers [57], hybrid quantum classical models such as variational quantum eigensolvers (VQEs) [58, 59], and simulators of many-body quantum physics [14, 60]. For the exploration of many-body physics today’s NISQ devices are already offering a practical quantum advantage [61]. These analog quantum simulators are special-purpose quantum computers that directly realize the interactions in the quantum system under study. Their major advantage is that the systems can easily scale to large sizes and are limited only by errors in the calibration of the parameters and decoherence. There are a variety of experimental platforms that are well-suited for quantum simulation, including but not limited to trapped ions [62, 63], neutral atoms [64, 65, 66], superconducting circuits [67, 68], and photons [69]. These devices are already allowing researchers to gain significant insight into disordered quantum systems [70], large-scale entanglement [71], high temperature superconductivity [72, 73] long range spin dynamics [74, 75] and much more.

The other very important application of quantum devices, both NISQ and smaller scale, is quantum sensing. This involves using quantum-mechanical objects as sensors to measure electric and magnetic fields, pressure, acceleration, and temperature. What is considered

³However, the estimates are getting smaller because of algorithmic advances. Just a few years ago it was 10^9 .

as a weakness of quantum devices in other applications is precisely the strength here: the extreme sensitivity to external perturbations. In some sense, quantum sensing imposes fewer technical challenges in technology development than other quantum applications primarily because scaling to large system sizes is not required. In fact, even in the history of semiconductors, light sensors found commercial viability decades before computers [7].

Since the very beginning of the quantum race, trapped ions have been at the forefront. This is made possible by their key characteristics, which we shall go over.

1. Tunable interactions and all-to-all connectivity

In condensed matter physics, many-body spin-spin interaction Hamiltonians form the foundation for understanding the collective behavior of particles in solids, leading to phenomena like magnetism, quantum phase transitions, spin liquids, and topological matter. Trapped ions are very well suited to simulate many-body-interacting spin Hamiltonians of the form

$$H_{\text{eff}} = \sum_{i < j} J_{ij} \sigma_x^i \sigma_x^j + B_{\text{eff}}^x \sum_i \sigma_x^i + B_{\text{eff}}^z \sum_j \sigma_z^j, \quad (1.1)$$

where σ_x^i and σ_z^i are the Pauli spin-1/2 matrices representing the spin components of the i -th spin. J_{ij} is the matrix element determining the interaction strength between the Hamiltonians of the form defined in Eq. (1.1) can be considered to be the native interaction set of a trapped ions quantum simulator.

Each spin is encoded in the internal energy levels of a single ion. When more than one ions are trapped in an ion trap, the Coulomb repulsion pushes them away from each other and at typical distances between spins in an ion trap (1-10 μm) the inherent spin-spin interactions are negligible. The interactions are mediated by the exciting of their collective motion through laser-based spin-dependent forces. This allows for a great deal of tunability in their interactions, for example power-law type interactions $J_{ij} \approx 1/|i-j|^\alpha$ with $\alpha \in (0, 3)$, which are readily achievable. The externally mediated interactions also allow for the couplings to be switched on/off on demand.

Collective excitation of ions can also be used as a computational resource [76] and, for the purpose of quantum simulation, these have been used to simulate the Dicke model [77, 78, 79]

$$H = \omega_c a^\dagger a + \omega_z \sum_{j=1}^N \sigma_j^z + \frac{2\lambda}{\sqrt{N}} (a + a^\dagger) \sum_j \sigma_j^x, \quad (1.2)$$

on a system of upto 70 spins [80]. Here a , $a^\dagger$ are the bosonic annihilation and creation operators, σ_i^x and σ_i^z are the Pauli spin-1/2 matrices representing the spin components of the i -th spin respectively. The Dicke model is of broad interest as it exhibits rich physics including quantum phase transitions and non-ergodic behaviour [81].

2. Long Coherence Time

Trapped ions were used to establish the coherence record, with a coherence time of more than an hour [82] having been recorded. The reason for such high coherence is that spins can be encoded in long-lived metastable and the so-called “clock states” in the ground hyperfine manifold of the ions and these long-lived states offer a high degree of isolation from the environment [63, 83]. Due to the high coherence of the qubit, implementations of single-ion and two-ion operations are mainly limited by the experimental imperfections like environmental noise, laser and control errors, ion heating, etc. However, even with these imperfections, trapped ion systems have some of the highest coherence time/gate time ratios for quantum computers and a long simulation time for quantum simulators. Only recently one and two qubit gates have been performed [84] with a fidelity of 99.99916(7)% and 99.97(1)% respectively.

3. High State Preparation and Measurement Fidelity

The spin encoding scheme in the internal energy levels of the ions also allows for excitation to auxiliary excited states through strong optical transitions. The excitation drives population dynamics between the qubit levels through optical pumping, and the selection rules of the excitation allow for state-dependent fluorescence readout. This results in high State Preparation and Measurement Fidelity (SPAM). The optical pumping initializes the state of the ions with a purity of $> 99.9\%$ [85] within a few microseconds, and it is possible to achieve much higher purity by increasing the pumping time. With trapped ions, SPAM fidelities of $> 99.9\%$ have been shown consistently [86, 87, 63].

4. Free from Fabrication Imperfections

Among the biggest sources of defects in the manufacturing of modern electronics is the semiconductor industry are fabrication imperfections. As quantum devices become more advanced and scale to larger number of qubits, they will also be susceptible to fabrication imperfections. The trapped ion qubits are not fabricated, and hence each ion’s internal structure is the same, and this is guaranteed by nature. The clock states also offer the advantage of making the ions less susceptible to environment-induced changes in the internal structure.

This is an exciting time for researchers in the field. Continued progress will require deep collaboration between physicists, chemists, mathematicians, and engineers. From the point of view of enhancing the capabilities of the NISQ devices, the following research directions seem to have the most potential for impact.

1. **Increase the system size to larger number of qubits**
2. **Increasing the native interaction set of a device**
3. **Allowing better calibration of devices to reduce calibration errors**
4. **Reducing decoherence to increase the usable time of the devices**

The work described in this thesis broadly serves towards building useful quantum technologies both for quantum simulations and quantum sensing and directly addresses the above four research directions. The experiments presented were performed on $^{171}\text{Yb}^+$ ions. Now I will give a brief outline of the work.

In **Chapter 2**, I provide a brief introduction to the field of quantum simulation of trapped ions. The goal is to keep the thesis self-contained and to set the background and notation for the rest of the chapters. Additionally, conventional experimental methods in an ion trap quantum information processing laboratory are introduced, while simultaneously the experimental setup employed in our laboratory is discussed.

In **Chapter 3**, I will describe how we demonstrated, both theoretically and experimentally, that XY-type couplings leading to an effective Hamiltonian of the form

$$H_{\text{eff}} = \sum_{i < j} J_{ij}^x \sigma_x^i \sigma_x^j + \sum_{i < j} J_{ij}^y \sigma_y^i \sigma_y^j, \quad (1.3)$$

are part of the native interactions available on a system of trapped ions (with individual control over J_{ij}^x and J_{ij}^y). The main insight of this work is that spin-dependent forces, which have been the backbone of entangling operations on trapped ions [63], can also be applied in parallel on the same motional modes of trapped ions and the theory presented discusses when this is possible. The proof-of-principle experimental demonstration was performed on two $^{171}\text{Yb}^+$ ions.

This directly enhances the available interactions in trapped-ion NISQ devices and would lead to the exploration of several interesting phenomena, such as exploring the ground-state order of frustrated XY-type models, understanding high-temperature superconductivity, and exploring exotic quantum phases such as spin liquids.

In **Chapter 4**, I will describe the theory and experiments leading to the highest resolution sensing of optical intensity and polarization, to date, using a single trapped $^{171}\text{Yb}^+$ ion as a field probe. The technique utilizes the intensity and polarization-dependent optical pumping of $^{171}\text{Yb}^+$ ions as a signature to extract the light parameters and the resolution is only limited by the fundamental limit imposed by the absorption cross section of a resonant light detector.

The technique applies directly to the characterization and calibration of optical addressing fields in large-scale ion- and atom-based quantum computers. The technique will also be useful for characterizing light sources in optical lithography systems.

In **Chapter 5**, I will describe the design and construction of a large-scale ion trapping apparatus, the blade trap system. The trap is engineered for the trapping of more than 50 ions in a linear chain, and the design and fabrication of the trap electrodes are discussed in detail. The vacuum system is an extreme high vacuum (XHV) chamber, with background pressure $P < 1.5 \times 10^{-12}$ mbar, likely the lowest recorded pressure in a room temperature ion trapping apparatus. The setup is fully constructed and was recently moved from the clean assembly area (in another building) to our laboratory.

In **Chapter 6**, I conclude the thesis with a brief summary and outlook for future work.

Chapter 2

Quantum Simulation with Trapped Ions

The purpose of this chapter is to set the background and the notation necessary for the rest of the chapters of the thesis and to give the reader an introduction to standard experimental procedures in an ion-trap based quantum information processing laboratory. We will go over the physics of how ions are trapped in an ion trap using radio frequency (RF) and direct current (DC) voltages and the form of the trapping potential created by an ion trap. We will discuss the classical and quantum dynamics of cold trapped ions and how laser-based forces on a system of ions lead to an effective spin-spin interaction. After discussing the relevant theoretical framework, we shall go over the standards operations in a trapped-ion quantum information processing laboratory with a specific focus on $^{171}\text{Yb}^+$ and the experimental apparatus in our laboratory.

2.1 Physics of Ion traps

Fig. 2.1 shows a schematic cartoon of the type of trap used in our lab¹. This trap achieves trapping using a combination of DC and RF voltages applied to the trap electrodes. Such traps are often referred to as 2D Paul traps after Wolfgang Paul² who first explored the

¹For a detailed description of our trap, its electrode fabrication, and derivations/simulations of the potentials and equations of motion you can refer to my masters thesis [88] where the construction of this device has been documented.

²Wolfgang Paul and Hans Dehmelt received half of the 1989 nobel prize “for the development of the ion trap technique”. The other half was awarded to Norman F. Ramsey “...for the invention of the separated

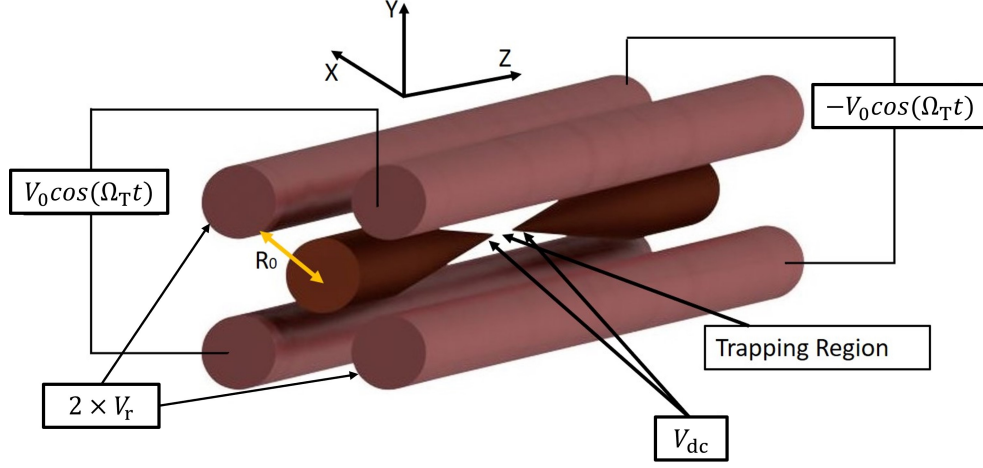


Figure 2.1: Ion Trap Schematic

Cartoon schematic of a four rod Paul trap. The radiofrequency voltage with amplitude $\pm V_0$ and frequency Ω_T is applied on diagonally opposite pairs of rod electrodes and DC voltages are applied on both the rods and the needles.

idea of using radiofrequency voltages to trap charged particles.

As shown in Fig. 2.1, an oscillating voltage is applied to one pair of diagonally opposite electrodes and an out-of-phase voltage is applied to the other diagonally opposite pair of electrodes. The oscillating voltages provide confinement in the radial (XY) direction, and the DC voltage applied to the needle electrodes creates confinement in the Z direction. Typically, we also apply a DC voltage $2 \times V_r$ to one pair of diagonally opposite electrodes to achieve anisotropic trapping strength along the two radial directions in the trap. The potential created at the trapping from the above voltages is

$$\phi = \kappa V_0 \cos(\Omega_T t) \left(\frac{x^2 - y^2}{R_0^2} \right) + V_r \left(1 + \frac{x^2 - y^2}{R_0^2} \right) + \frac{\kappa' V_{dc}}{z_0^2} \left(z^2 - \frac{1}{2}(x^2 + y^2) \right) \quad (2.1)$$

The first term is from the oscillating voltages applied to the rods, second from the DC voltages applied to the rods and the third from the DC voltages applied to the needles. Here, κ and κ' are constants that depend on the exact geometry of the trap, R_0 is the radial ion-rod distance as depicted in Fig. 2.1, z_0 is the distance (along the Z direction) from the trapping center to the needle tips. Note that ϕ is the electric potential while the

oscillatory fields method and its use in the hydrogen maser and other atomic clocks”.

mechanical potential felt by an ion with charge q is $q\phi$. The electric potential in the Z direction is static and corresponds to a harmonic confining potential and can be written as

$$q\phi_Z = \frac{1}{2}m\omega_z^2 z^2, \quad (2.2)$$

where m is the mass of the ion, and $\omega_z = \sqrt{2\kappa'qV_{dc}/z_0^2m}$.

The potential in the XY direction can be written as

$$\phi = (\kappa V_0 \cos(\Omega_T t) + V_r) \left(\frac{x^2 - y^2}{R_0^2} \right) - \kappa' V_{dc} \left(\frac{(x^2 + y^2)}{2z_0^2} \right) \quad (2.3)$$

It can be shown that the equations of motions for the potential above are described by the Mathieu equations

$$\begin{aligned} \frac{d^2 x}{d\zeta^2} + [a_x + 2q_x \cos(2\zeta)] x &= 0 \\ \frac{d^2 y}{d\zeta^2} + [a_y + 2q_y \cos(2\zeta)] y &= 0, \end{aligned} \quad (2.4)$$

where $\zeta := \Omega_T t/2$, $a_x = (4q/m\Omega_T^2)(2\kappa V_r/R_0^2 - \kappa' V_{dc}/z_0^2)$, $a_y = -(4q/m\Omega_T^2)(2\kappa V_r/R_0^2 + \kappa' V_{dc}/z_0^2)$, $q_x = -q_y = 4q\kappa V_0/(m\Omega_T^2 R_0^2)$.

These equations represent a forced harmonic oscillator, and solutions can be found using Floquet theory [89] and, in general, there are either stable or unstable solutions possible. Stable solutions are those where the position stays finite for all time. A good way to visualize the operating parameters for the ion traps that lead to successful trapping is to find regions in the (a_i, q_i) plane that lead to stable or unstable solutions. It can be shown that the boundaries of the stable regions are enclosed with contour lines that mark solutions with periodicity π and 2π . Fig. 2.2 shows a stability diagram of Mathieu's equations with the first stable region marked (see Chapter 9 in Ref. [89] for detailed derivations of these stability regions).

When stable solutions exist in both radial directions, the solution to the Mathieu equations up to the first order in $q_{x/y}$ is given as [90]

$$\begin{aligned} x(t) &= C_x \cos(\omega_x t + \phi_x) \left[1 + \frac{q_x}{2} \cos(\Omega_T t) \right] \\ y(t) &= C_y \cos(\omega_y t + \phi_y) \left[1 + \frac{q_y}{2} \cos(\Omega_T t) \right], \end{aligned} \quad (2.5)$$

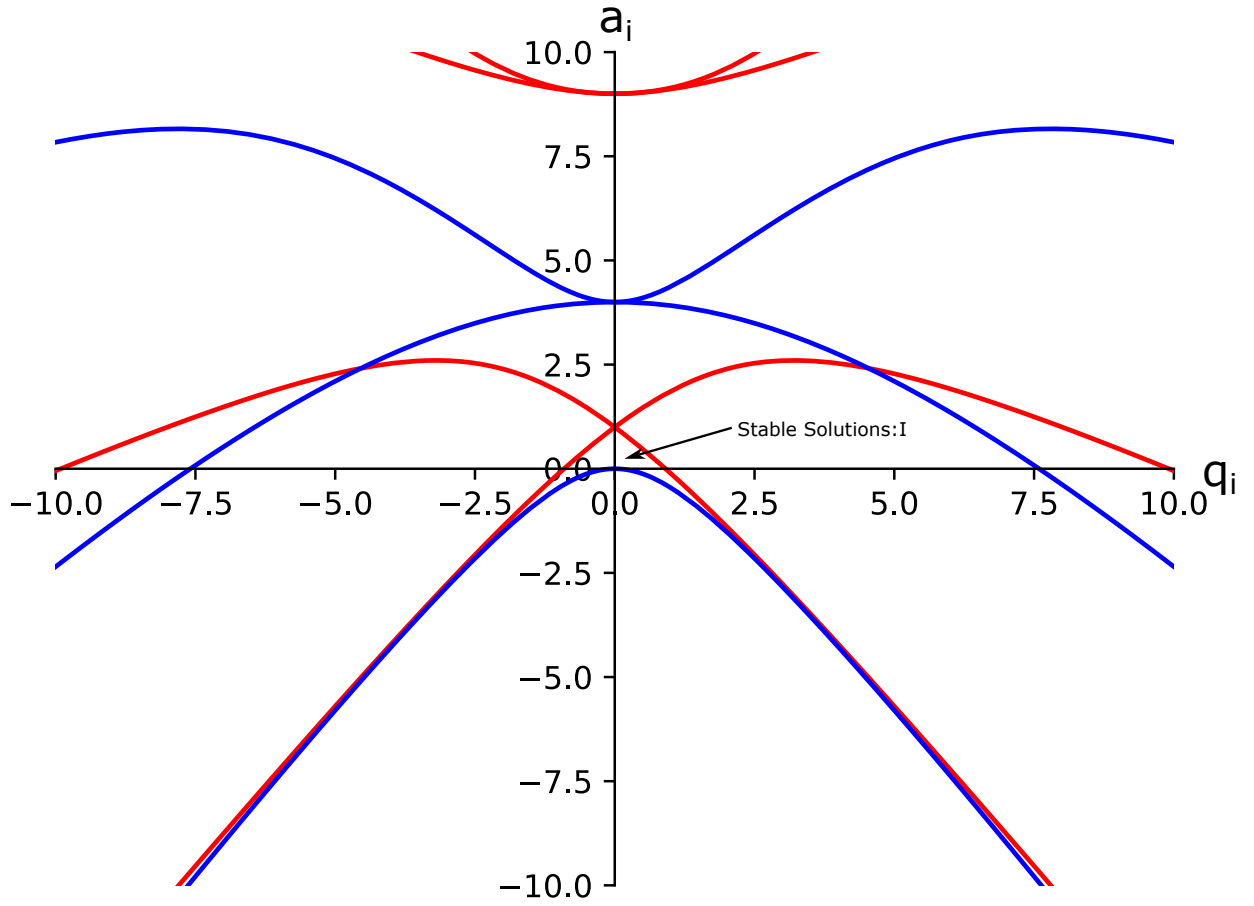


Figure 2.2: Stability Diagram for the Mathieu Equation

The above stability diagram is valid for stability in both radial directions separately. The blue and red curves mark solutions with π and 2π periodicity. The areas completely enclosed within the two curves are the regions of stability.

Where C_x, C_y, ϕ_x , and ϕ_y are given by the initial conditions,

$$\begin{aligned}\omega_x &= \left(\Omega_T \sqrt{a_x + q_x^2/2} \right) / 2, \\ \omega_y &= \left(\Omega_T \sqrt{a_y + q_y^2/2} \right) / 2.\end{aligned}\tag{2.6}$$

Usually $a_{x/y} \ll q_{x/y} \ll 1$, hence $\omega_{x/y} \ll \Omega_T$ and the above trajectories can be interpreted as slow, large-amplitude oscillations at the “secular” frequency $\omega_{x/y}$ and fast, small-amplitude oscillations or “micromotion” at Ω_T . Previously, I mentioned that we add a DC voltage V_r on one pair of diagonally opposite rods, and Eq. (2.6) should make it clear why. The voltage leads to a non-zero $a_{x/y}$ and this allows the trapping frequency in the two radial directions to be nondegenerate. However, nonzero $a_{x/y}$ also means that there is a chance of reaching the unstable trapping region and losing the ions. Fig. 2.3 shows the first stability region in the combined stability diagram for the x and y trajectories in the trap.

Neglecting the micromotion in the X and Y trajectories, one can see that the ion motion corresponds to that of a particle trapped in a harmonic potential and we can write the “pseudopotential” experienced by the ions as

$$q\phi_p = \frac{1}{2}m\omega_x^2 x^2 + \frac{1}{2}m\omega_y^2 y^2.\tag{2.7}$$

Together with the static confining potential in the Z direction, the mechanical potential experienced by the ion in the trap is confining in all 3 directions and is gives as,

$$\phi_{\text{trap}} = \frac{1}{2}m\omega_x^2 x^2 + \frac{1}{2}m\omega_y^2 y^2 + \frac{1}{2}m\omega_z^2 z^2.\tag{2.8}$$

2.1.1 Ion chain dynamics

Entangling operations in a trapped ion system are mediated by the collective motional excitation of the ions. Laser-based forces allow for coupling the internal and the motional degrees of freedom of trapped ions and this is the fundamental interaction that leads to spin-spin and spin-motion entanglement. In this section, we will explore the collective

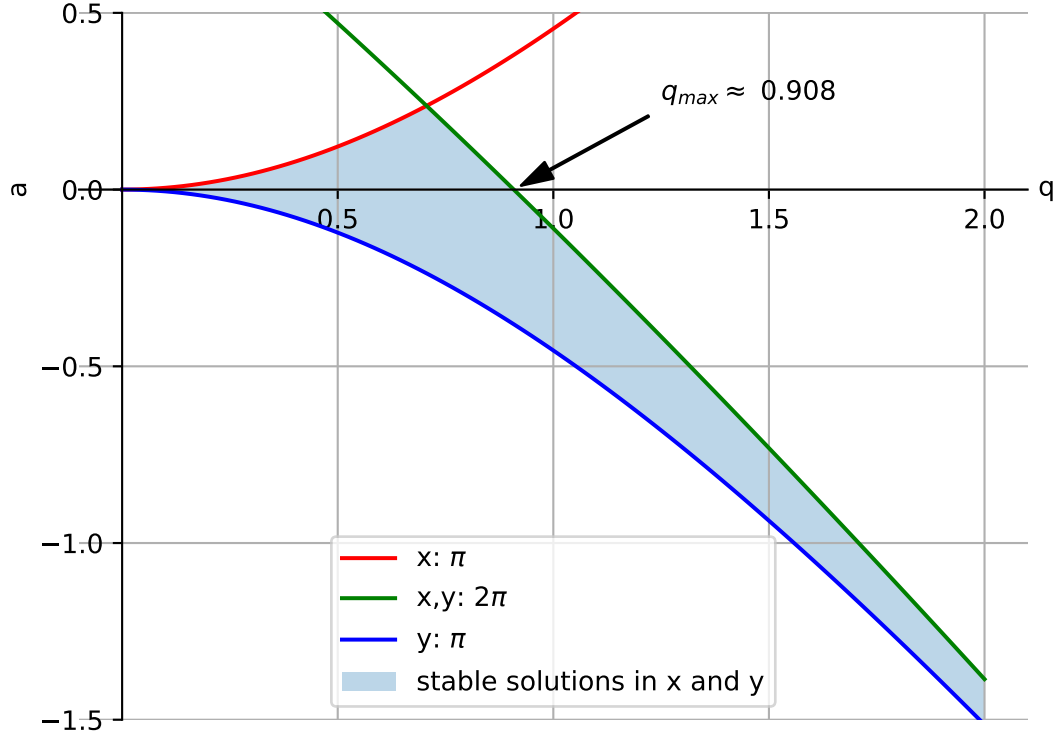


Figure 2.3: Stability diagram for a four-rod paul trap

The labels for the solid curves indicate the periodicity of the solutions that bound the stable region (blue shading) and also the direction. The curves in the stability diagram for a single direction (Fig. 2.2) are symmetric in the q parameter and hence only three distinct lines are visible. For symmetric operation, i.e. $a_{x/y} = 0$, the maximum allowed value of $q_{x/y} \approx 0.908$ marks the maximum radial trapping frequencies although typical values used in experiments are $|q_{x/y}| < 0.4$. The stability diagram helps identify maximum allowed asymmetry in the two radial trap frequencies.

motional dynamics of a system of trapped ions in a harmonic potential. The total energy of a system of trapped ions in a harmonic potential can be written as

$$H = \sum_{i=1}^N \frac{p_i^2}{2m} + V(\vec{r}_i). \quad (2.9)$$

The potential energy term comes from the harmonic confining potential as well as the Coulomb interaction between the ions,

$$V(\vec{r}_i) = m \sum_{i=1}^N (\omega_x^2 x_i^2 + \omega_y^2 y_i^2 + \omega_z^2 z_i^2) + \frac{1}{2} \cdot \frac{1}{4\pi\epsilon_0} \sum_{i=1}^N \sum_{j \neq i}^N \frac{Q^2}{|\vec{r}_i - \vec{r}_j|}. \quad (2.10)$$

We can rescale the ion positions using a length scale, $l_0 = Q^2/(4\pi\epsilon_0 m \omega_z^2)^{1/3}$ and substitute $\vec{r}_i/l_0 \rightarrow \vec{r}_i'$ i.e. $(x_i, y_i, z_i)/l_0 \rightarrow (x_i', y_i', z_i')$ and get the following simplified potential³,

$$V(\vec{r}_i) = V_0 \left(\frac{1}{2} \sum_{i=1}^N (\alpha_x^2 x_i'^2 + \alpha_y^2 y_i'^2 + z_i'^2) + \frac{1}{2} \sum_{i=1}^N \sum_{j \neq i}^N \frac{1}{|\vec{r}_i' - \vec{r}_j'|} \right). \quad (2.11)$$

Here we have defined $V_0 \equiv m \omega_z^2 l_0^2$ and $\alpha_{x/y} \equiv \omega_{x/y}/\omega_z$.

When $\alpha_{x/y} \gg 1$, the potential is strongly confining in the X and Y directions compared to the Z direction, and this leads to chains of ions trapped along the Z direction. To find the equilibrium positions of the ions, we need to minimize $V(\vec{r}_i)$ with respect to all $\vec{r}_i$ and usually this is done numerically. Fig. 2.4 shows the camera image and simulated equilibrium positions of 18 bright $^{171}\text{Yb}^+$ ions.

When laser-based forces are applied to a linear chain of ions, the forces cause fluctuations of the ions about their equilibrium positions. There are two forces at play here: forces external to the chain and the repulsive force that the ions apply on each other because of the Coulomb interaction. The existence of internal forces makes the ion chain behave as a set of coupled harmonic oscillators and, like any coupled system, this system also has its resonances i.e. collective normal modes of oscillations about their equilibrium positions.

We will now explore this collective motion of the ions about their equilibrium positions. I will follow the convention used in [91] with appropriate modifications to accommodate

³The entire section could be presented without the need for rescaling. However, rescaling makes the numerical calculations presented in the following paragraphs easier.

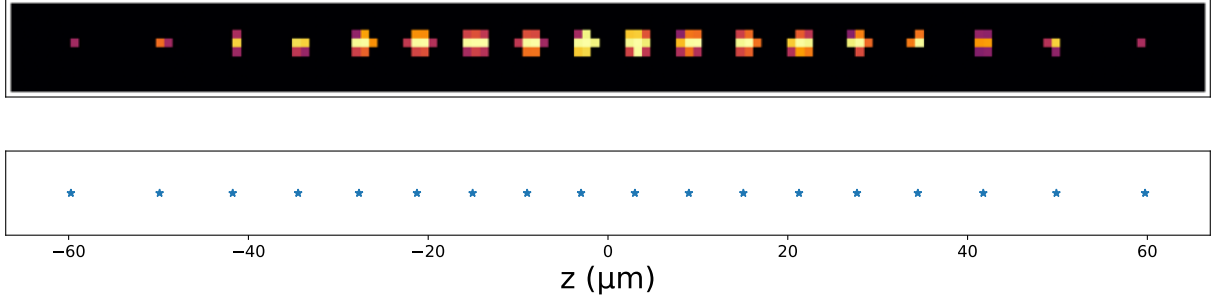


Figure 2.4: Real and Simulated Ion Positions

Top: Camera image of 18 bright $^{171}\text{Yb}^+$ ions in our trap.

Bottom: Simulated equilibrium positions for 18 $^{171}\text{Yb}^+$ ions with $\omega_z = 2\pi \times 80\text{kHz}$.

all 3 spatial dimensions. Let the equilibrium positions of the ions after the potential minimization in the previous paragraphs be denoted by $(\tilde{X}_i, \tilde{Y}_i, \tilde{Z}_i)$. We define the fluctuations of the ions about their mean positions by another set of 3N coordinates q_i such that

$$\begin{aligned} x'_i &= \tilde{X}_i + q_i^x(t), \\ y'_i &= \tilde{Y}_i + q_i^y(t), \\ z'_i &= \tilde{Z}_i + q_i^z(t). \end{aligned} \tag{2.12}$$

The Lagrangian describing the motion about equilibrium positions is

$$\begin{aligned} L = & \frac{ml_0^2}{2} \sum_{m=1}^N (\dot{q}_m^x)^2 + (\dot{q}_m^y)^2 + (\dot{q}_m^z)^2 \\ & - \frac{1}{2} \sum_{n,m=1}^N q_n^x q_m^x \left[\frac{\partial^2 V}{\partial x'_n \partial x'_m} \right]_0 - \frac{1}{2} \sum_{n,m=1}^N q_n^y q_m^y \left[\frac{\partial^2 V}{\partial y'_n \partial y'_m} \right]_0 - \frac{1}{2} \sum_{n,m=1}^N q_n^z q_m^z \left[\frac{\partial^2 V}{\partial z'_n \partial z'_m} \right]_0 \\ & - \frac{1}{2} \sum_{n,m=1}^N q_n^x q_m^y \left[\frac{\partial^2 V}{\partial x'_n \partial y'_m} \right]_0 - \frac{1}{2} \sum_{n,m=1}^N q_n^x q_m^z \left[\frac{\partial^2 V}{\partial x'_n \partial z'_m} \right]_0 \cdots \end{aligned} \tag{2.13}$$

where the subscript 0, in terms like $\left[\frac{\partial^2 V}{\partial x'_n \partial x'_m} \right]_0$, denotes that the derivatives are calculated at the equilibrium positions of the ions that we have calculated previously, that is, at

$(\tilde{X}_i, \tilde{Y}_i, \tilde{Z}_i)$. It is straightforward to show that the cross terms in the last line of Eq.(2.13) are zero⁴ and the Lagrangian can be written as a set of 3 uncoupled systems, one for each spatial dimension.

$$\begin{aligned}
L &= L_x + L_y + L_z, \text{ where,} \\
L_x &= \frac{ml_0^2}{2} \sum_{m=1}^N (\dot{q}_m^x)^2 - \frac{1}{2} \sum_{n,m=1}^N A_{nm}^x q_n^x q_m^x, \\
L_y &= \frac{ml_0^2}{2} \sum_{m=1}^N (\dot{q}_m^y)^2 - \frac{1}{2} \sum_{n,m=1}^N A_{nm}^y q_n^y q_m^y, \\
L_z &= \frac{ml_0^2}{2} \sum_{m=1}^N (\dot{q}_m^z)^2 - \frac{1}{2} \sum_{n,m=1}^N A_{nm}^z q_n^z q_m^z.
\end{aligned} \tag{2.14}$$

With the matrix elements defined as

$$A_{nm}^x = \left[\frac{\partial^2 V}{\partial x'_n \partial x'_m} \right]_0, A_{nm}^y = \left[\frac{\partial^2 V}{\partial y'_n \partial y'_m} \right]_0 \text{ and } A_{nm}^z = \left[\frac{\partial^2 V}{\partial z'_n \partial z'_m} \right]_0.$$

The matrices A^α , for $\alpha \in x, y, z$ are symmetric and non-negative definite with real elements whose values can be calculated explicitly and only depend on the equilibrium positions calculated previously.

Since we have 3 qualitatively identical systems, we shall analyze only the X direction. Notice that the coordinates in L_x are coupled and the equations of motions resulting from these are N coupled differential equations in q_i^x 's. However, we can make a coordinate transformation such that we have a single differential equation for each of the transformed coordinates. Notice that the first term in L_x is diagonal in any basis and hence we only need to concentrate on the second term. The matrices A^x have eigenvalues (ω_p^2) and eigenvectors $(b^{(p)})$ given by

$$\sum_{m=1}^N A_{nm}^x b_m^{(p)} = \omega_p^2 b_n^{(p)} \quad (p = 0, 1, \dots, N) \tag{2.15}$$

We can write a normal mode transformation matrix b_{im} by stacking the eigenvectors horizontally so that the new coordinate transformations are given as follows

⁴The derivatives can be written out explicitly and the cross terms have $(x'_n - x'_m)$ or $(y'_n - y'_m)$ in the numerator. Since the ions are trapped in a chain along the Z-axis these terms are zero.

$$\begin{aligned}
q_i^x &= \sum_{m=1}^N b_{im} \xi_m, \\
\xi_m &= \sum_{i=1}^N b_{im} q_i^x.
\end{aligned}
\tag{2.16}$$

With these new *normal coordinates*, the Lagrangian can be rewritten as

$$\begin{aligned}
L^x &= \frac{m l_o^2}{2} \sum_{m=1}^N \left[(\dot{\xi}_m)^2 - \omega_m^2 \xi_m^2 \right] \\
&= m \sum_{m=1}^N \left[(\dot{Q}_m)^2 - \omega_m^2 Q_m^2 \right].
\end{aligned}
\tag{2.17}$$

From the above expression for the Lagrangian it is clear that the normal modes are uncoupled and is equivalent to N independent harmonic oscillators. In the last line, I have simply absorbed l_o to get the canonical coordinates Q_m 's with the same units as x_i 's. Again the transformations are done using b_{im}

$$x_i = \tilde{X}_i + \sum_{m=1}^N b_{im} Q_m. \tag{2.18}$$

2.1.2 Ion chain dynamics: Quantum

As we will see in the later part of the thesis, ions in the trap are cooled to their motional ground state and hence we need to treat the motion of the ions quantum mechanically. The canonical momenta corresponding to the uncoupled modes Q_m are $P_m = m\dot{Q}_m$. With this definition, we can write the Hamiltonian of each mode as

$$H_p = \frac{P_m^2}{2m} + \frac{1}{2} M \omega_m^2 Q_m^2. \tag{2.19}$$

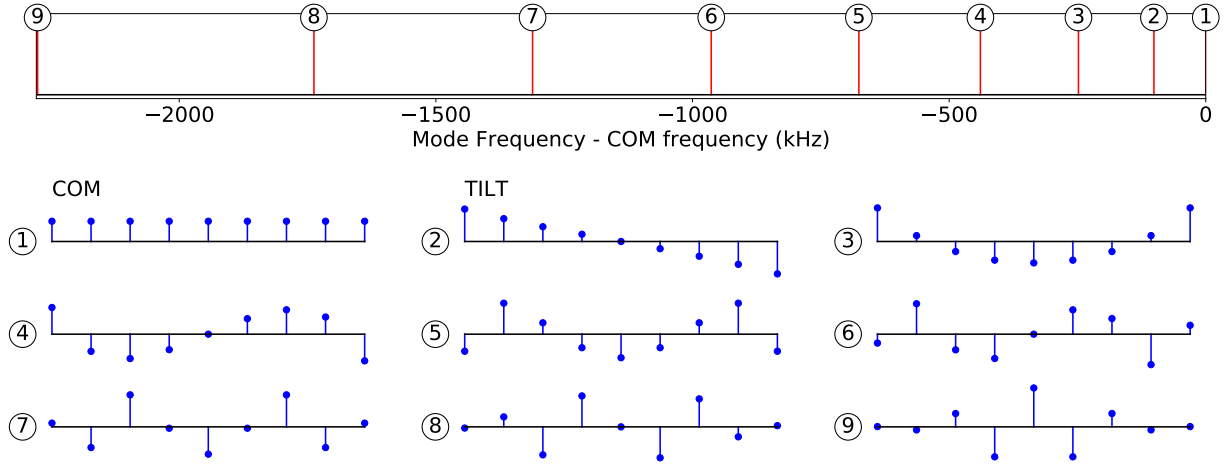


Figure 2.5: Normal Modes for 9 Ions

TOP: The normal mode frequencies in x direction for a chain of 9 ions, in a harmonic trapping potential. The radial trap frequencies $\omega_x \approx \omega_y = 2\pi \times 5$ MHz and axial trap frequency $\omega_z = 2\pi \times 1$ MHz. See Sec.2.1.1 for details.

BOTTOM: Eigenvectors corresponding to each mode.

Now to quantize the system we simply have to make the following replacements,

$$Q_m \rightarrow \hat{Q}_m = \sqrt{\frac{\hbar}{2m\omega_m}} (\hat{a}_m + \hat{a}_m^\dagger),$$

$$P_m \rightarrow \hat{P}_m = i\sqrt{\frac{\hbar m\omega_m}{2}} (\hat{a}_m - \hat{a}_m^\dagger).$$

The operators $\hat{Q}_m$ and $\hat{P}_m$ satisfy the usual canonical commutation relations $[\hat{Q}_m, \hat{P}_n] = i\hbar\delta_{mn}$.

In the previous sections, we denoted the ion's coordinates as x_i 's. In a manner similar to the normal coordinates we can also write operators corresponding to the real space coordinates as $\hat{x}_i$. The coordinate transformations defined in Eq.2.18 are still valid and we can use them to write the real space operators in terms of the quantized normal coordinates as follows.

$$\hat{x}_i = \tilde{X}_i + \sum_{m=1}^N b_{im} \xi_m^{(0)} (a_m^\dagger + a_m) \quad (2.20)$$

2.2 Ion-light interaction: Single Ion

So far we have talked about the motional degrees of freedom of a trapped ion. However, most protocols for quantum information processing utilize the internal degrees of freedom of the trapped ions. Usually, the trapped atomic ions have a large number of internal energy states, which leads to a very high-dimensional Hilbert space. The transition to trapped-ion qubits is done by selecting a set of 2 energy levels and using these as the qubit Hilbert space. In this simplified picture, we can write the Hamiltonian for the ion's internal degrees of freedom using any of the Pauli matrices (for simplicity, I will choose the basis defined by σ_z). For a single ion in a trap and considering motion along only one of the axes of the trap, we have that

$$H_{\text{atom}} = \frac{\omega_{\text{hf}}}{2}\sigma_z; \quad H_{\text{HO}} = \omega_m a^\dagger a; \quad (2.21)$$

Where ω_{hf} is the energy difference between the two qubit states⁵. The two eigenstates of the σ_z operator will be our computational basis states ($|\downarrow_z\rangle, |\uparrow_z\rangle$) and for the motional degrees of freedom we will simply use the Fock (number) basis. For example, $|\downarrow_z, n\rangle$ is a state with spin down and n phonons i.e motional excitations.

To do quantum computation with the ions, we need to be able to induce transitions between the levels that we have chosen to be the qubit levels. Depending on the encoding, this is usually done through coupling of the energy levels via lasers or via a pair of laser beams inducing two-photon Raman transitions (see Fig. 2.6 for a cartoon schematic). In either case, the light-matter interaction Hamiltonian for a single ion takes the following form [21]:

$$H_{\text{lm}} = \Omega \cos(\vec{k} \cdot \vec{r} - \omega_l t + \phi_l) \sigma_x, \quad (2.22)$$

Where Ω is called the Rabi frequency which depends on the intensity of the laser at the ion location, $\vec{k}$ is the laser wavevector such that $|\vec{k}| = 2\pi/\lambda$ where λ is the wavelength of laser⁶, $\vec{r}$ is the position of the ion and ω_l is the angular frequency of the laser. In the following discussion, we will assume that the laser wavevector is aligned along the x-axis and hence $\vec{k} \cdot \vec{r} = k_x x$ where k_x is the x component $\vec{k}$. We will now look at the ion-light

⁵As we will see later, in our choice of the qubit the energy difference comes from the hyperfine splitting of the ground state and hence the choice of subscript in ω_{hf}

⁶Again, for the case of Raman transitions k represents the wavevector difference between the two lasers

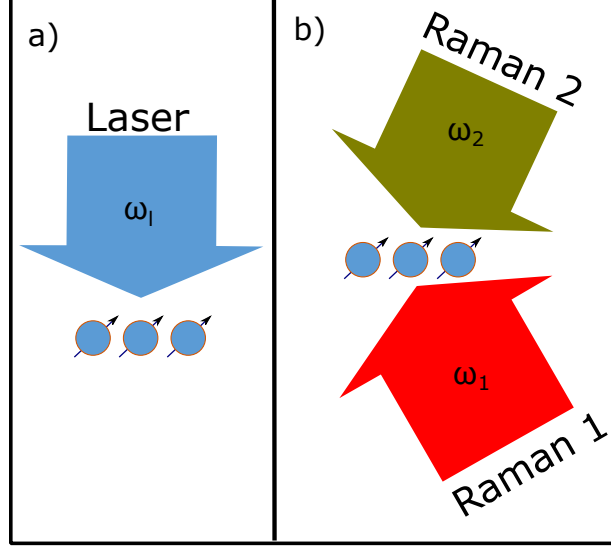


Figure 2.6: Ion Light Interaction Cartoon Schematic

Transitions between qubit levels can be induced by shining laser light on the ions. a) When the qubit levels are chosen such that they can be addressed by optical frequencies, a single laser at frequency ω_l that is resonant with the qubit transition can be used to induce the transition. b) The qubit level can also be chosen such that the transition frequency lies in the microwave regime (as is the case in this work) and in this case a pair of laser beams can be used to induce the transitions between the qubit states. The relevant frequency in this case is the frequency difference between the two laser beams i.e. $|\omega_1 - \omega_2|$.

NOTE: In the text, in order to keep the discussion independent of the qubit encoding, ω_l is used to denote the frequency of interest when addressing ions. For optical transitions ω_l denotes the laser frequency and for the microwave qubits ω_l denotes the frequency difference.

coupling Hamiltonian, H_{lm} , in the interaction picture with respect to $H_{\text{atom}} + H_{\text{HO}}$.

$$\begin{aligned}
H_{\text{int}} &= e^{i(H_{\text{atom}} + H_{\text{HO}})} H_{\text{lm}} e^{-i(H_{\text{atom}} + H_{\text{HO}})} \\
&= \Omega \left\{ e^{\frac{i\omega_{\text{hf}}}{2}\sigma_z} \sigma_x e^{\frac{-i\omega_{\text{hf}}}{2}\sigma_z} \right\} \left\{ e^{i\omega_m a^\dagger a} \cos(k_x x - \omega_l t + \phi_l) e^{-i\omega_m a^\dagger a} \right\} \\
&= \Omega \left\{ \sigma_+ e^{i\omega_{\text{hf}} t} + \sigma_- e^{-i\omega_{\text{hf}} t} \right\} \left\{ \frac{1}{2} e^{i\omega_m a^\dagger a} (e^{i(k_x x - \omega_l t + \phi_l)} + e^{-i(k_x x - \omega_l t + \phi_l)}) e^{-i\omega_m a^\dagger a} \right\}.
\end{aligned} \tag{2.23}$$

Now, we can make the substitution $k_x x = \eta(a + a^\dagger)$ where $\eta = k_x x_0$ and $x_0 = \sqrt{\frac{1}{2m\omega_m}}$ is the spread of the ground state wavefunction of the trapped ion. So the expression in the second curly braces is

$$\begin{aligned}
&\frac{1}{2} e^{i\omega_m a^\dagger a} (e^{i(\eta(a + a^\dagger) - \omega_l t + \phi_l)} + e^{-i(\eta(a + a^\dagger) - \omega_l t + \phi_l)}) e^{-i\omega_m a^\dagger a} \\
&= \frac{1}{2} e^{i(-\omega_l t + \phi_l)} e^{i\eta(ae^{-i\omega_m t} + a^\dagger e^{i\omega_m t})} + \frac{1}{2} e^{-i(-\omega_l t + \phi_l)} e^{-i\eta(ae^{-i\omega_m t} + a^\dagger e^{i\omega_m t})}
\end{aligned}$$

To arrive at the above expression, we have expanded the exponential $e^{i\eta(a + a^\dagger)}$ in Eq. (2.23) and applied the Baker–Campbell–Hausdorff formula on each term and simply summed back the series. Substituting this into Eq. (2.23) and applying a rotating wave approximation i.e neglecting terms containing $e^{\pm(\omega_l + \omega_{\text{hf}})t}$ we get

$$\begin{aligned}
H_{\text{int}} &= \frac{\Omega}{2} \sigma_+ e^{i\eta(ae^{-i\omega_m t} + a^\dagger e^{i\omega_m t})} e^{i((\omega_{\text{hf}} - \omega_l)t + \phi_l)} + \frac{\Omega}{2} \sigma_- e^{-i\eta(ae^{-i\omega_m t} + a^\dagger e^{i\omega_m t})} e^{-i((\omega_{\text{hf}} - \omega_l)t + \phi_l)} \\
&= \frac{\Omega}{2} \sigma_+ e^{i[\eta(ae^{-i\omega_m t} + a^\dagger e^{i\omega_m t}) - \mu t + \phi_l]} + \frac{\Omega}{2} \sigma_- e^{-i[\eta(ae^{-i\omega_m t} + a^\dagger e^{i\omega_m t}) - \mu t + \phi_l]}.
\end{aligned}$$

Here we have $\mu = \omega_l - \omega_{\text{hf}}$. Since we have $\eta \ll 1$ ⁷, we can use the approximation $e^{i\eta(ae^{-i\omega_m t} + a^\dagger e^{i\omega_m t})} \approx 1 + i\eta(ae^{-i\omega_m t} + a^\dagger e^{i\omega_m t})$ in the expression for H_{int}

⁷typical values of η in experiments are below 0.1

$$\begin{aligned}
H_{\text{int}} &= \frac{\Omega}{2} \sigma_+ [1 + i\eta(ae^{-i\omega_m t} + a^\dagger e^{i\omega_m t})] e^{i(-\mu t + \phi_l)} + \frac{\Omega}{2} \sigma_- [1 - i\eta(ae^{-i\omega_m t} + a^\dagger e^{i\omega_m t})] e^{-i(-\mu t + \phi_l)} \\
&= \frac{\Omega}{2} [\sigma_+ e^{i(-\mu t + \phi_l)} + \sigma_- e^{-i(-\mu t + \phi_l)}] \\
&\quad + \frac{\eta\Omega}{2} [\sigma_+ a e^{i(-(\omega_m + \mu)t + \phi_l + \pi/2)} + \sigma_- a^\dagger e^{i((\omega_m + \mu)t - \phi_l - \pi/2)}] \\
&\quad + \frac{\eta\Omega}{2} [\sigma_+ a^\dagger e^{i((\omega_m - \mu)t + \phi_l + \pi/2)} + \sigma_- a e^{i((-\omega_m + \mu)t - \phi_l - \pi/2)}]
\end{aligned} \tag{2.24}$$

Carrier Transitions

When we excite the ion resonantly, i.e. $\mu = 0$ in Eq. (2.24) we get the carrier Hamiltonian (H_{carr}), which is useful for inducing transitions between the two spin states.

$$\begin{aligned}
H_{\text{carr}} &= \frac{\Omega}{2} (\sigma_+ e^{-i\phi_l} + \sigma_- e^{i\phi_l}) \\
&= \frac{\Omega}{2} \left(\frac{1}{2} (\sigma_x + i\sigma_y) e^{-i\phi_l} + \frac{1}{2} (\sigma_x - i\sigma_y) e^{i\phi_l} \right) \\
&= \frac{\Omega}{2} \left(\sigma_x \left(\frac{e^{i\phi_l} + e^{-i\phi_l}}{2} \right) - i\sigma_y \left(\frac{e^{i\phi_l} - e^{-i\phi_l}}{2i} \right) \right) \\
&= \frac{\Omega}{2} (\sigma_x \cos \phi_l + \sigma_y \sin \phi_l) \\
&= \frac{\Omega}{2} \sigma_{\phi_l}
\end{aligned} \tag{2.25}$$

Where we define $\sigma_\theta := (\sigma_x \cos \theta + \sigma_y \sin \theta)$. The evolution operator for the above Hamiltonian is the following.

$$\begin{aligned}
U_{\text{carr}}(t) &= e^{-iH_{\text{carr}}t} \\
&= e^{-i\frac{\Omega t}{2} \sigma_{\phi_l}} \\
&= \left(\cos \frac{\Omega t}{2} \mathbb{I} - i \sin \frac{\Omega t}{2} \sigma_{\phi_l} \right).
\end{aligned}$$

Where $\mathbb{I}$ is the identity operator. This is simply the rotation operator for a spin-1/2 particle, and ϕ_l sets the axis of rotation on the Bloch sphere. As an example, if we set $\phi_l = 0$ i.e $\sigma_{\phi_l} = \sigma_x$ and consider its action on $|\downarrow\rangle$

$$\begin{aligned} U_{\text{carr}}^x |\downarrow\rangle &= \left(\cos \frac{\Omega t}{2} \mathbb{I} - i \sin \frac{\Omega t}{2} \sigma_x \right) |\downarrow\rangle \\ &= \cos \frac{\Omega t}{2} |\downarrow\rangle - i \sin \frac{\Omega t}{2} |\uparrow\rangle. \end{aligned} \quad (2.26)$$

This drives coherent oscillations between the $|\downarrow\rangle$ and $|\uparrow\rangle$.

Sideband Transitions

If we substitute $\mu = -\omega_m$ in Eq. (2.24) we get the red sideband (RSB) transition, and if we substitute $\mu = \omega_m$ in Eq. (2.24) we get the blue sideband transition (BSB).

$$\begin{aligned} H_{\text{RSB}} &= \frac{\eta\Omega}{2} [\sigma_+ a e^{i(\phi_l + \pi/2)} + \sigma_- a^\dagger e^{-i(\phi_l + \pi/2)}] \\ H_{\text{BSB}} &= \frac{\eta\Omega}{2} [\sigma_+ a^\dagger e^{i(\phi_l + \pi/2)} + \sigma_- a e^{-i(\phi_l + \pi/2)}] \end{aligned} \quad (2.27)$$

From the form of the above Hamiltonians we can see that the red sideband transition couples the states $|\downarrow, n\rangle \rightarrow |\uparrow, n-1\rangle$ and the blue sideband transitions couple the $|\downarrow, n\rangle \rightarrow |\uparrow, n+1\rangle$.

2.2.1 Spin Dependent Force

When applied together, the red and blue sidebands lead to a spin-dependent force which forms the basis for simulating spin-spin interactions on trapped ions. However, before we discuss the spin-dependent force, let us take a slight detour and write down the Hamiltonian for a forced quantum harmonic oscillator.

$$H = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2} + F(t)x$$

In the operator formalism this can be written as,

$$H = \omega_m \left(a^\dagger a + \frac{1}{2} \right) + F(t)(a^\dagger + a).$$

If we transform to the interaction picture with respect to the oscillator Hamiltonian i.e $\omega_m(a^\dagger a + 1/2)$ we get the following

$$H_{\text{int}} = F(t)[a^\dagger e^{i\omega t} + a e^{-i\omega t}].$$

This is the Hamiltonian for a forced harmonic oscillator.

A spin-dependent force simply means that the function $F(t)$ has some dependence on the internal degrees of freedom of the ion. In the previous section, we saw that light can couple the internal and external degrees of freedom of the ion using the sideband transitions. The idea of a spin-dependent force takes root from this. If we add two symmetrically detuned sidebands, we get a spin-dependent force. By this, I mean simultaneously applying two laser beams, one tuned to the red side with detuning $\mu_r = -\mu$ and phase ϕ_r and another tuned to the blue side with detuning $\mu_b = \mu$ and phase ϕ_b . Mathematically, this involves adding two copies of Eq. (2.24) where we replace μ by $-\mu$ in one of them. After some simplification, we get

$$H_{\text{SDF}} = \Omega \cos(\mu t + \psi) [\sigma_{\theta-\pi/2} + \eta \sigma_\theta (a e^{-i\omega_m t} + a^\dagger e^{i\omega_m t})],$$

where the spin-phase $\theta = \frac{\phi_r + \phi_b + \pi}{2}$,

and the motional-phase $\psi = \phi_r - \phi_b$.

(2.28)

The first term in the brackets above is an off-resonant carrier term, and the spin-dependent force arises from the second term. Comparing the second term to the expression for the forced harmonic oscillator, we see that $F(t) = \eta \Omega \cos(\mu t + \psi) \sigma_\theta$. The force term is a periodic modulation at frequency μ and its phase changes depending on the internal state of the ion⁸. For example, in the internal state of the ion $|\downarrow_\theta\rangle$ the force is exactly out of phase with the force on the internal state $|\uparrow_\theta\rangle$.

2.3 Ion-light Interactions: Multi-Ion Case

The multi-ion case is quite similar to the single ion case. Assuming a global laser beam incident on all the ions, we can write the following Hamiltonian for the system and ion-light interactions.

⁸In most ion trap literature, including this thesis, a spin-dependent force refers to a periodic spin-dependent force at a modulation frequency μ .

$$\begin{aligned}
H_{\text{system}} &= \sum_i \frac{\omega_{\text{hf}}}{2} \sigma_z^i + \sum_m \omega_m a_m^\dagger a_m \\
H_{\text{lm}} &= \sum_i \Omega_i \cos(k_x x - \omega_l t + \phi_l) \sigma_x^i \\
&= \sum_i \Omega_i \cos\left(k_x [\tilde{X}_i + \sum_m b_{im} \xi_m^0 (a_m + a_m^\dagger)] - \omega_l t + \phi_l\right) \sigma_x^i \\
&= \sum_i \Omega_i \cos\left(\phi_x^i + \sum_m \eta_{im} (a_m + a_m^\dagger) - \omega_l t + \phi_l\right) \sigma_x^i \\
&= \sum_i \frac{\Omega_i}{2} \sigma_x^i [e^{i(\phi_x^i - \omega_l t + \phi_l)} e^{i \sum_m \eta_{im} (a_m + a_m^\dagger)} + e^{-i(\phi_x^i - \omega_l t + \phi_l)} e^{-i \sum_m \eta_{im} (a_m + a_m^\dagger)}]
\end{aligned} \tag{2.29}$$

We note that in the work presented in this thesis, we couple to the radial modes of motion and hence the beam k-vector is in a direction perpendicular to the ion chain direction, leading to $\tilde{X}_i = 0$, $\forall i$, where i is the ion index. We have also assumed that the laser phase is the same on all ions.

In the interaction picture with respect to the system, we have the following Hamiltonian

$$\begin{aligned}
H_{\text{int}} &= e^{iH_{\text{system}}} H_{\text{lm}} e^{-iH_{\text{system}}} \\
&= \sum_i \frac{\Omega_i}{2} \{ \sigma_+^i e^{i\omega_{\text{hf}} t} + \sigma_-^i e^{-i\omega_{\text{hf}} t} \} \{ e^{i(\phi_i - \omega_l t)} e^{i \sum_m \eta_{im} (a_m e^{-i\omega_m t} + a_m^\dagger e^{i\omega_m t})} \\
&\quad + e^{-i(\phi_i - \omega_l t)} e^{-i \sum_m \eta_{im} (a_m e^{-i\omega_m t} + a_m^\dagger e^{i\omega_m t})} \} [\text{with } \phi_i = \phi_x^i + \phi_l] \\
&= \sum_i \frac{\Omega_i}{2} \{ \sigma_+^i e^{i\omega_{\text{hf}} t} + \sigma_-^i e^{-i\omega_{\text{hf}} t} \} \{ e^{i(\phi_i - \omega_l t)} \prod_m [1 + i\eta_{im} (a_m e^{-i\omega_m t} + a_m^\dagger e^{i\omega_m t})] \\
&\quad + e^{-i(\phi_i - \omega_l t)} \prod_m [1 - i\eta_{im} (a_m e^{-i\omega_m t} + a_m^\dagger e^{i\omega_m t})] \} \\
&= \sum_i \frac{\Omega_i}{2} \sigma_+^i e^{i(-\mu t + \phi_i)} [1 + \sum_m i\eta_{im} (a_m e^{-i\omega_m t} + a_m^\dagger e^{i\omega_m t})] \\
&\quad + \sum_i \frac{\Omega_i}{2} \sigma_-^i e^{-i(-\mu t + \phi_i)} [1 - \sum_m i\eta_{im} (a_m e^{-i\omega_m t} + a_m^\dagger e^{i\omega_m t})] \}.
\end{aligned}$$

In the last line we have set $\mu = (\omega_l - \omega_{\text{hf}})$ and retained only the terms linear in η_{im}

The above terms can be reshuffled to give

$$\begin{aligned}
H_{\text{int}} &= \sum_i \frac{\Omega_i}{2} \{ \sigma_+^i e^{i(-\mu t + \phi_i)} + \sigma_-^i e^{-i(-\mu t + \phi_i)} \} \\
&\quad + \sum_{i,m} \frac{\eta_{im} \Omega_i}{2} \{ \sigma_+^i a_m e^{i(-(\mu + \omega_m)t + \phi_i + \pi/2)} + \sigma_-^i a_m^\dagger e^{-i(-(\mu + \omega_m)t + \phi_i + \pi/2)} \} \\
&\quad + \sum_{i,m} \frac{\eta_{im} \Omega_i}{2} \{ \sigma_+^i a_m^\dagger e^{i((-\mu + \omega_m)t + \phi_i + \pi/2)} + \sigma_-^i a_m e^{-i((-\mu + \omega_m)t + \phi_i + \pi/2)} \}
\end{aligned} \tag{2.30}$$

This is the multi-ion analogue of Eq. (2.24) with different values of μ that lead to carrier and sideband transitions. The global carrier is easy to understand since it simply leads to rotations of all the spins on the Bloch sphere. However, a global sideband is more complicated because there are multiple ions and motional modes involved.

2.3.1 Multi-Ion Spin-Dependent Forces: Molmer-Sørensen interaction

One of the most important interactions in trapped ions arises when a periodic spin-dependent force is applied to more than one ion at a time. Like in the single-ion case, the spin-dependent force arises when we apply symmetrically detuned red and blue sidebands. Again, this involves simultaneous interaction with two laser beams and the Hamiltonian for this interaction is

$$H_{\text{RSB}} + H_{\text{BSB}} = \sum_i \Omega_i \cos(k_x x_i - \omega_r t + \phi_r^i) \sigma_x^i + \sum_i \Omega_i \cos(k_x x_i - \omega_b t + \phi_b^i) \sigma_x^i.$$

Since we want symmetrically detuned sidebands to get a spin-dependent force, we set the laser frequencies according to $\omega_r = \omega_{\text{hf}} - \mu$ and $\omega_b = \omega_{\text{hf}} + \mu$. To obtain the Hamiltonian interaction with respect to the system we sum two copies of Eq. (2.30) and apply a rotating wave approximation to get the following result [92].

$$\begin{aligned} H_{\text{SDF}} &= \sum_i \Omega_i \cos(\mu t + \psi_i) \sigma_{\theta_i - \pi/2}^i \\ &\quad + \sum_{im} \eta_{im} \Omega_i \cos(\mu t + \psi_i) (a_m e^{-i\omega_m t} + a_m^\dagger e^{i\omega_m t}) \sigma_{\theta_i}^i \\ \text{where the spin-phase } \theta_i &= \frac{\phi_r^i + \phi_b^i + \pi}{2}, \\ \text{and the motional-phase } \psi_i &= \frac{\phi_r^i - \phi_b^i}{2}. \end{aligned} \tag{2.31}$$

This Hamiltonian is the basis for most of the entangling interactions in a trapped ions system, both spin-spin and spin-phonon interactions.

2.4 Quantum Simulation of Spin-Spin Hamiltonians

In the previous section we derived in detail how a spin dependent force emerges from the simultaneous application of symmetrically detuned red and blue sidebands. Now we can

look into how a spin-dependent force produces large scale spin-spin interactions. While deriving Eq. (2.31), we assumed that the laser phase is different on each ion, and this in turn allows for a different spin phase at each ion's location. While this is fairly general, in most quantum simulations the laser phase is tried to be kept constant over the entire ion chain, i.e. $\phi_r^i = \phi_r \forall i$ and $\phi_b^i = \phi_b \forall i$. From this we get that the spin phase $\theta_i = \theta = \frac{\phi_r + \phi_b + \pi}{2} \forall i$ is constant throughout the ion chain, and so is the motional phase $\psi_i = \psi = \frac{\phi_r - \phi_b}{2} \forall i$.

Making these substitutions in Eq. (2.31), and ignoring the first off-resonant term in the limit $\mu \gg \Omega_i$ leads us to the Molmer-Sørensen Hamiltonian,

$$H_{MS} = \sum_{i,m}^N \eta_{i,m} \Omega_i \cos(\mu t + \psi) (a_m e^{-i\omega_m t} + a_m^\dagger e^{i\omega_m t}) \sigma_\theta^i. \quad (2.32)$$

The evolution operator with respect to the above Hamiltonian can be found using the Magnus expansion,

$$U(t) = \mathcal{T} \left\{ \exp \left(-i \int_0^t dt_1 H(t_1) \right) \right\} = \exp \left(\tilde{\Omega}_1 + \tilde{\Omega}_2 + \tilde{\Omega}_3 + \dots \right),$$

where $\mathcal{T}$ refers to the time ordering operator the operators $\tilde{\Omega}_i$ are given as

$$\begin{aligned} \tilde{\Omega}_1 &= -i \int_0^t dt_1 H(t_1) \\ \tilde{\Omega}_2 &= -\frac{1}{2} \int_0^t dt_1 \int_0^{t_1} dt_2 [H(t_1), H(t_2)] \\ \tilde{\Omega}_3 &= -\frac{i}{6} \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 ([H(t_1), [H(t_2), H(t_3)]] + [H(t_3), [H(t_2), H(t_1)]]) , \end{aligned}$$

and so on. Calculating $\tilde{\Omega}_1$ using the formula above is trivial and we get

$$\tilde{\Omega}_1 = - \sum_{i,m} \sigma_\theta^i (\alpha_{im} a_m^\dagger - \bar{\alpha}_{im} a_m), \quad (2.33)$$

where

$$\alpha_{im} = \frac{i\eta_{im}\Omega_i}{\mu^2 - \omega_m^2} \left(e^{i\omega_m t} (\mu \sin[\mu t + \psi] + i\omega_m \cos[\mu t + \psi]) - (\mu \sin[\psi] + i\omega_m \cos[\psi]) \right).$$

If we concentrate only on the first term, the operator $e^{\tilde{\Omega}_1}$ is very similar to a displacement operator for a harmonic oscillator with displacement in phase space given by α_{im} . The only difference is that there is a spin term along with it making it a spin-dependent displacement operator that entangles the spin and motional degrees of freedom. We can further simplify the above expression by noting that usually $\mu \approx \omega_m$ and $\frac{\mu}{(\mu+\omega_m)} \approx \frac{\omega_m}{(\mu+\omega_m)} \approx \frac{1}{2}$ giving us

$$\alpha_{im} = \frac{\eta_{im}\Omega_i}{2\delta_m} (e^{-i\delta_m t} - 1),$$

where $\delta_m = \mu - \omega_m$. This term can be understood as an oscillatory displacement in the motional phase space with an amplitude of $\frac{\eta_{im}\Omega_i}{2\delta}$. If we operate in the regime $\delta_m \gg \eta_{im}\Omega_i$, the amplitude becomes vanishingly small and the contribution of the first-order term in the Magnus expansion can be neglected⁹.

The commutator in the second term $\tilde{\Omega}_2$ is

$$\begin{aligned} [H(t_1), H(t_2)] &= \\ &\left[\sum_{im}^N \eta_{im}\Omega_i \cos(\mu t_1 + \psi) (a_m e^{-i\omega_m t} + a_m^\dagger e^{i\omega_m t}) \sigma_\theta^i, \right. \\ &\left. \sum_{jn}^N \eta_{jn}\Omega_j \cos(\mu t_2 + \psi) (a_n e^{-i\omega_n t} + a_n^\dagger e^{i\omega_n t}) \sigma_\theta^j \right] \\ &= \sum_{i,j,m}^N \eta_{im}\eta_{jm}\Omega_i\Omega_j \sigma_\theta^i \sigma_\theta^j \\ &\quad \times \cos(\mu t_1 + \psi) \cos(\mu t_2 + \psi) (e^{-i\omega_m(t_1-t_2)} - e^{-i\omega_m(t_2-t_1)}) \end{aligned}$$

The simplification in the last term results from the fact that all spin terms commute and $[a_m, a_n^\dagger] = \delta_{mn}$. After somewhat tedious but straightforward integrals the final result

⁹Ensuring $\delta_m \gg \eta_{im}\Omega_i$ is generally referred as the “slow regime”. The regime in which this inequality is not satisfied is more applicable when applying spin-dependent forces for quantum gates, and light is only applied to a pair of ions, unlike a global beam discussed here. Even in this so-called “fast regime” spin-motion entanglement is undesirable and the gate duration τ is carefully chosen to ensure that $\alpha_{im}(\tau) = 0$.

is

$$\begin{aligned}
\tilde{\Omega}_2 = & i \sum_{i,j,m} \sigma_{\theta}^i \sigma_{\theta}^j \frac{\eta_{im} \eta_{jm} \Omega_i \Omega_j}{\mu^2 - \omega_m^2} \\
& \times \left[-\omega_m t + \frac{\omega_m}{2\mu} \sin(2\psi) - \frac{\omega_m}{2\mu} \sin(2(\mu t + \psi)) \right. \\
& + \mu \sin(\psi) \left(\frac{\cos((\mu + \omega_m)t + \psi)}{\mu + \omega_m} - \frac{\cos((\mu - \omega_m)t + \psi)}{\mu - \omega_m} \right) \\
& \left. + \omega_m \cos(\psi) \left(\frac{\sin((\mu + \omega_m)t + \psi)}{\mu + \omega_m} + \frac{\sin((\mu - \omega_m)t + \psi)}{\mu - \omega_m} \right) \right]
\end{aligned} \tag{2.34}$$

The commutator in the second term was independent of the phonon terms and since all of the spin terms commute with each other, all the higher-order commutators are zero. Note that the first term in the above expression is linear in time, and this term contributes towards the effective Hamiltonian. The rest of the terms are fast oscillating terms that can be safely neglected and the final expression for $\tilde{\Omega}_2$ is simply

$$\tilde{\Omega}_2 = -i \left(\sum_{i,j,m} \sigma_{\theta}^i \sigma_{\theta}^j \frac{\eta_{im} \eta_{jm} \Omega_i \Omega_j}{\mu^2 - \omega_m^2} \omega_m \right) t. \tag{2.35}$$

Finally, when operating in the regime $\delta_m \gg \eta_{im} \Omega_i$ we showed that the first-order term ($\tilde{\Omega}_1$) is negligible and the evolution operator can be written as

$$U(t) = T \left\{ \exp \left(- \int_0^t dt_1 H(t_1) \right) \right\} = \exp \left(\tilde{\Omega}_2 \right).$$

This gives us the effective Hamiltonian,

$$\begin{aligned}
H_{\text{eff}} = & \sum_{i,j} J_{ij} \sigma_{\theta}^i \sigma_{\theta}^j, \\
\text{where, } J_{ij} = & \left(\sum_m \frac{\eta_{im} \eta_{jm} \Omega_i \Omega_j}{\mu^2 - \omega_m^2} \omega_m \right).
\end{aligned} \tag{2.36}$$

A spin-dependent force, along with an additional laser frequency (or Raman beatnote) producing the carrier Hamiltonian in Eq. (2.25) gives the following effective Hamiltonian,

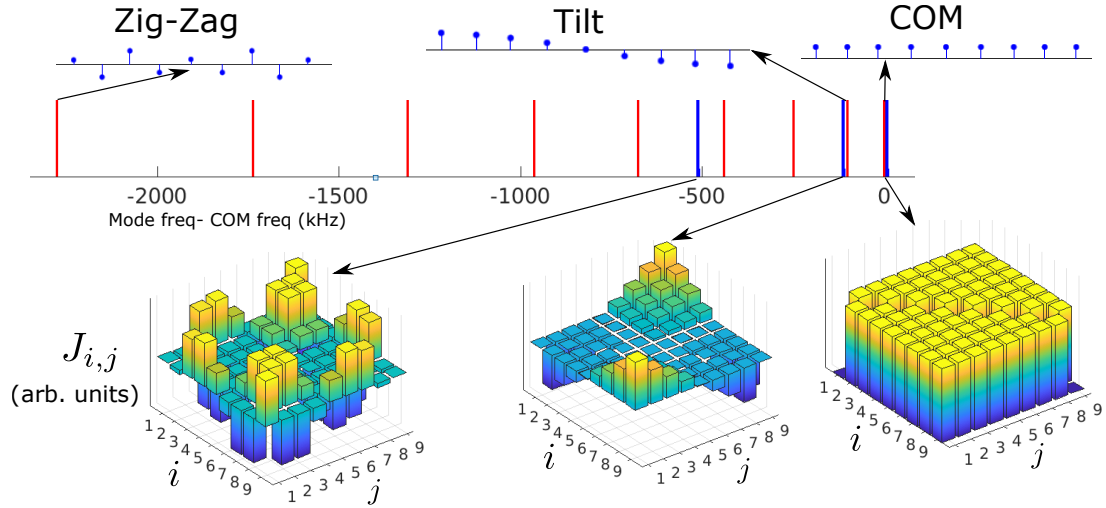


Figure 2.7: Interaction Profiles for Ising Couplings on Trapped Ions

The form of Ising couplings calculated as per Eq. (2.36) with $\Omega_i = 1 \forall i$. The spin dependent force modulation frequency μ determines the form of the coupling matrix J_{ij} . For example, μ is parked close to the center of mass mode, the interaction profile is flat, i.e. all the ion pairs have roughly equal interaction strength. Similarly, the Tilt mode leads to interaction profile where the farthest ions interact the most. In general, all motional modes contribute to the interaction profile as seen in the third plot (leftmost).

$$H_{\text{eff}} = \sum_{i,j} J_{ij} \sigma_{\theta}^i \sigma_{\theta}^j + B_{\text{eff}} \sum_i \sigma_{\theta'}^i \quad . \quad (2.37)$$

In the above equation, B_{eff} is the effective magnetic field and comparing with Eq. (2.25) we have $B_{\text{eff}} = \Omega/2$. Note that θ and θ' can be chosen, by setting the laser phases (Equations (2.31) and (2.25)), to give orthogonal spin axes in the XY plane (in the Bloch sphere) and to give the transverse field Ising model. This effective Hamiltonian has been the backbone of most quantum simulations on trapped ions for over a decade[63, 92].

2.4.1 Ising interaction with a σ_z effective magnetic field

In the previous section the effective magnetic field accompanying the Ising interactions was constrained in the XY plane due to the presence of the $\sigma_{\theta'}$ operators. However, it is also possible to simulate a transverse field that is in the Z direction by simply changing our definition of the carrier, $\omega'_{\text{hf}} = \omega_{\text{hf}} - B_{\text{eff}}$, while applying the symmetrically detuned sidebands. While deriving Eq. (2.30) we went into the interaction picture with respect to the system Hamiltonian H_{system} . If instead we transform in to the interaction frame given by H'_{system} , defined as

$$\begin{aligned} H'_{\text{system}} &= \sum_i \frac{\omega_{\text{hf}} - B_{\text{eff}}}{2} \sigma_z^i + \sum_m \omega_m a_m^\dagger a_m \\ &= \sum_i \frac{\omega_{\text{hf}'}}{2} \sigma_z^i + \sum_m \omega_m a_m^\dagger a_m. \end{aligned} \quad (2.38)$$

The Hamiltonian in the interaction frame is the same as the one in Eq. (2.30) with an added term $\sum_i \frac{B_{\text{eff}}}{2} \sigma_z^i$ and μ is replaced by μ' , defined as $\mu' = \omega_l - (\omega_{\text{hf}} - B_{\text{eff}})$. Hence when we sum the symmetrically detuned red and blue sidebands we recover Eq.(2.31), again with μ replaced by μ' and the added term $\sum_i \frac{B_{\text{eff}}}{2} \sigma_z^i$. The rest of the procedure is the same as described in Sec.2.4, so, in the interaction frame defined by H'_{system} , the effective Hamiltonian is

$$H'_{\text{eff}} = \sum_{i,j} J_{ij} \sigma_\theta^i \sigma_\theta^j + \frac{B_{\text{eff}}}{2} \sum_j \sigma_z^j, \quad (2.39)$$

which is the transverse field Ising model with the transverse field in the Z direction.

There are two important differences here. First, symmetric detunings need to be applied with respect to the new carrier ω'_{hf} . For example, if we want to symmetrically detune by μ_x , we would have to set the new laser frequencies as $\omega_r = \omega'_{\text{hf}} - \mu_x$ and $\omega_b = \omega'_{\text{hf}} + \mu_x$, which can also be thought of as asymmetrically detuned sidebands at $-(\mu_x + B_{\text{eff}})$ and $\mu_x - B_{\text{eff}}$ with respect to ω_{hf} . Second, the Hamiltonian is in an interaction frame different from the lab frame defined by the system Hamiltonian. Hence all other operations, for example, X or Y rotations after the application of the Hamiltonian, need to be applied in the new frame which can be done by shifting the laser/beatnote frequency down by B_{eff} .

2.5 Ytterbium

Ytterbium is a rare earth element with atomic number 70 and electronic configuration $\text{Yb} = [\text{Xe}]4f^{14}6s^2$. It is soft and relatively non-reactive, which makes it easy to handle, especially, for the purpose of breaking into chunks and loading into an atomic oven for atomic physics experiments. A heavy nucleus and existence of a spin 1/2 isotope¹⁰ makes it an ideal candidate for optical clocks [93]. In our experiment, Yb atoms are stored in an oven which is resistively heated, releasing a beam of neutral Yb atoms towards the center of the ion trap. At the trap center, Yb is ionized in a two-photon photoionization process, as shown in Fig. 2.8. The first photon from a 398.9 nm laser is resonant with the $^1\text{S}_0 \rightarrow ^1\text{P}_1$ transition¹¹, and once the atom is excited to $^1\text{P}_1$ a second photon knocks the electron out of the orbit hence ionizing the atom. The $^1\text{S}_0 \rightarrow ^1\text{P}_1$ transition is isotope selective, i.e depending on the frequency of the laser, we can choose which isotope interacts with our laser. Table 2.1 shows the frequency of $^1\text{S}_0 \rightarrow ^1\text{P}_1$ in different isotopes compared to ^{174}Yb , the most naturally abundant isotope.

Fig. 2.9 shows the relevant energy levels of $^{171}\text{Yb}^+$. The ground state of $^{171}\text{Yb}^+$ is $^2\text{S}_{1/2}$ and the ions can be excited to $^2\text{P}_{1/2}$ through an optical dipole transition at 369.5nm. This transition has a natural linewidth of $\Gamma = 2\pi \times 19.6$ MHz and serves as a highly fluorescing transition for laser cooling, qubit state preparation, and detection.

2.5.1 $^{171}\text{Yb}^+$ Clock Qubit

Singly ionized Yb has an electronic configuration of $[\text{Xe}]4f^{14}6s^1$ with only one electron in the outer shell leading to an electron spin quantum number $S = 1/2$ and hence spin angular momentum $\mathbf{S} = \sqrt{S(S+1)}\hbar = \sqrt{3}\hbar/2$. The fine structure in an atom is the result of the coupling between the orbital angular momentum $\mathbf{L}$ and the spin angular momentum $\mathbf{S}$, leading to a total electron angular momentum $\mathbf{J}$

$$\mathbf{J} = \mathbf{L} + \mathbf{S}. \quad (2.40)$$

¹⁰Due to its spin 1/2 the ^{171}Yb has zero tensor polarizability and this makes it more resilient to polarization imperfections, especially for optical lattice clocks where polarization uniformity across sites is difficult to maintain.

¹¹If you are not an atomic physicist or have forgotten the spectroscopic notation for writing the atomic states, for example $^1\text{S}_0$, I will discuss this briefly in the next section when we talk about the internal energy structure of $^{171}\text{Yb}^+$

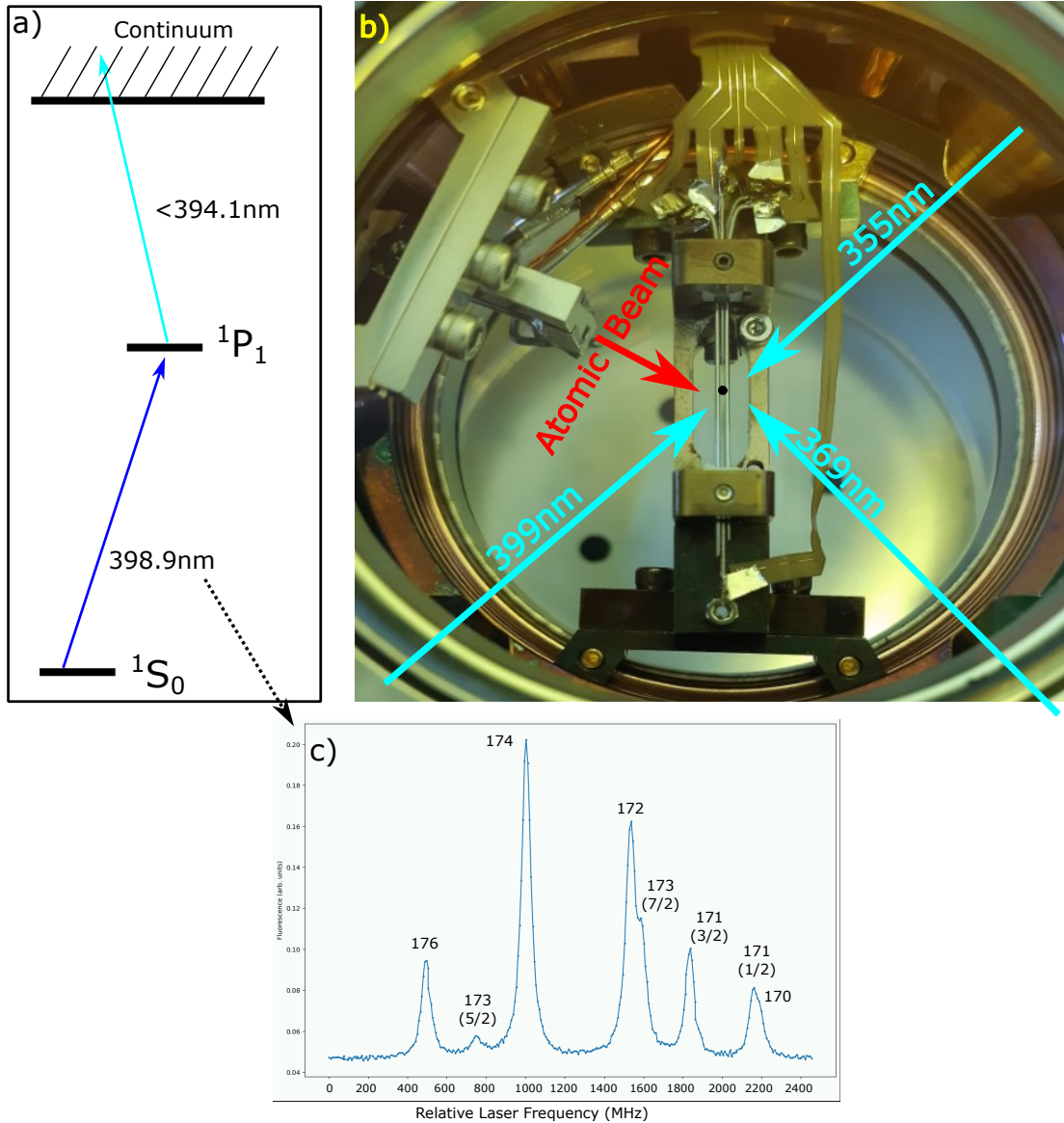


Figure 2.8: Photoionization Beam Orientation

a) Laser frequencies required for ionizing neutral Ytterbium atoms. b) Beam orientations with respect to ion in our experimental apparatus. The isotope selective beam at ≈ 399 nm is roughly perpendicular to minimize Doppler shift. Ion position marked as a black dot in the center of the trap. c) Doppler free spectrum of the isotope selective transition in neutral Ytterbium (data acquired by Siddharth Chawla in a chamber separate from the one in b)).

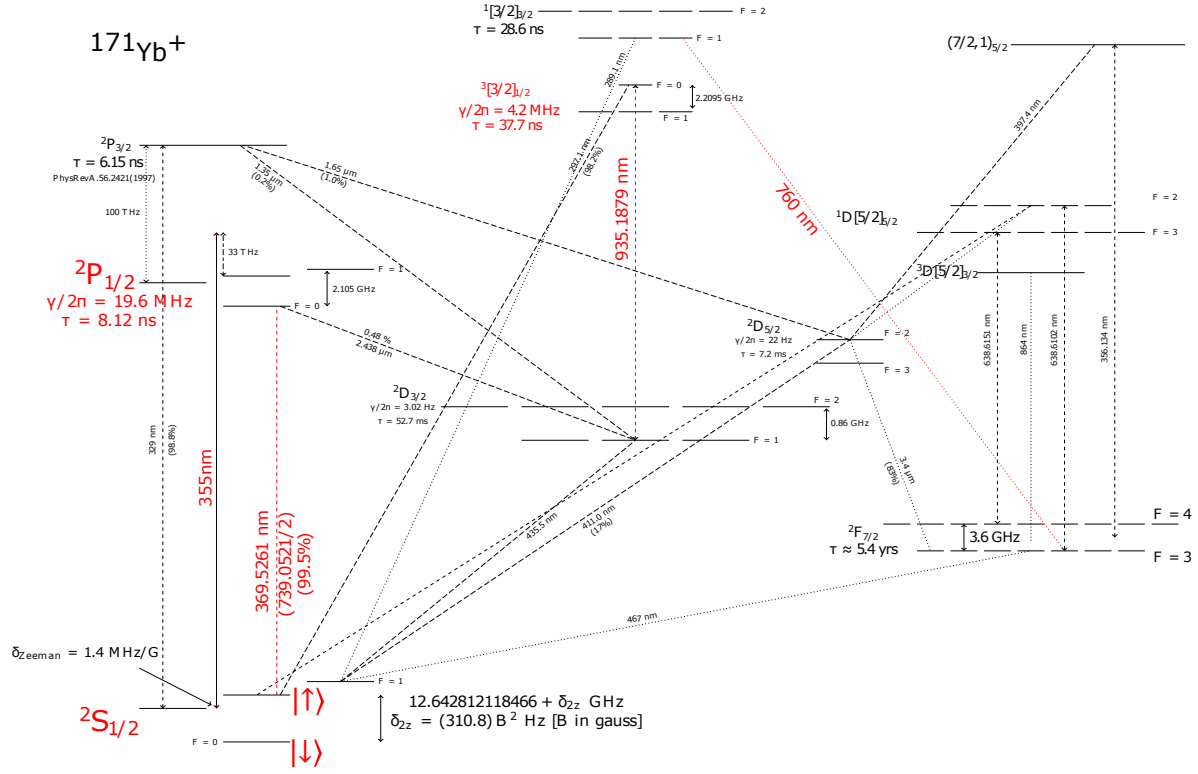


Figure 2.9: Relevant energy levels in $^{171}\text{Yb}^+$.

Optical transitions used in this work are marked in red. For details on the utility of each of these transitions see Sec. 2.5.1.

Isotope	Shift w.r.t ^{174}Yb (MHz)	Wavelength (nm)
^{176}Yb	-509.310(50)	398.91190
$^{173}\text{Yb}(F' = 5/2)$	-253.418(50)	398.91177
$^{173}\text{Yb}(F' = 3/2)$	515.975(200)	398.91136
^{172}Yb	533.309(53)	398.91135
$^{173}\text{Yb}(F' = 7/2)$	587.986(56)	398.91132
$^{171}\text{Yb}(F' = 3/2)$	832.436(50)	398.91119
$^{171}\text{Yb}(F' = 1/2)$	1153.696(61)	398.91102
^{170}Yb	1192.393(66)	398.91100
^{168}Yb	1887.400(50)	398.91063
^{173}Yb (centroid)	291.516(54)	398.91147
^{171}Yb (centroid)	939.523(39)	398.91113

Table 2.1: Isotope shifts and corresponding wavelengths for various Yb isotopes

All the values are for the $^1\text{S}_0 \rightarrow ^1\text{P}_1$ transition in neutral Ytterbium. The odd isotopes have Hyperfine structure and the value is F for the excited state is given in parantheses. Data extracted from Ref. [94].

The total angular momentum $\mathbf{J} = \sqrt{J(J+1)}\hbar$, where J the total angular momentum quantum number must satisfy the following relation

$$|L - S| \leq J \leq |L + S|. \quad (2.41)$$

While S and J are written as numbers, for historical reasons, L has been denoted with alphabets; where $L = 0$ is represented with S , $L = 1$ is represented with P , $L = 2$ is represented with D , $L = 3$ is represented by F , etc. The spectroscopic notation for writing a particular state is $^{2S+1}L_J$.

In the case of $^{171}\text{Yb}^+$ the nucleus has a nonzero nuclear spin, $I = 1/2$, and the hyperfine structure arises from the coupling between the nuclear spin angular momentum $\mathbf{I}$ and the total electron angular momentum $\mathbf{J}$. The total atomic (or ionic) angular momentum $\mathbf{F}$ is then given as

$$\mathbf{F} = \mathbf{I} + \mathbf{J} \quad (2.42)$$

In the case of the ground state $^2S_{1/2}$ and an excited state $^2P_{1/2}$, this leads to splitting into two hyperfine levels given by $F = 0, 1$ as shown in Fig. 2.9. In the presence of an applied magnetic field, the $F = 1$ hyperfine levels further split into three Zeeman levels ($m_F = -1, 0, 1$). Finally, $\sqrt{F(F+1)}\hbar$ is the total angular momentum of the ion and m_F is the projection of the angular momentum along the quantization axis defined by the applied magnetic field. In the presence of a magnetic field, the Zeeman splitting is given as

$$\Delta E_{\text{Zeeman}} = m_F g_F \mu_B |\vec{B}| \quad (2.43)$$

Where the Landé G-factor can be calculated as¹²

$$g_F = g_J \frac{F(F+1) + J(J+1) - S_n(S_n+1)}{2F(F+1)} \quad (2.44)$$

$$g_J = 1 + \frac{J(J+1) - L(L+1) + S(S+1)}{2J(J+1)}, \quad (2.45)$$

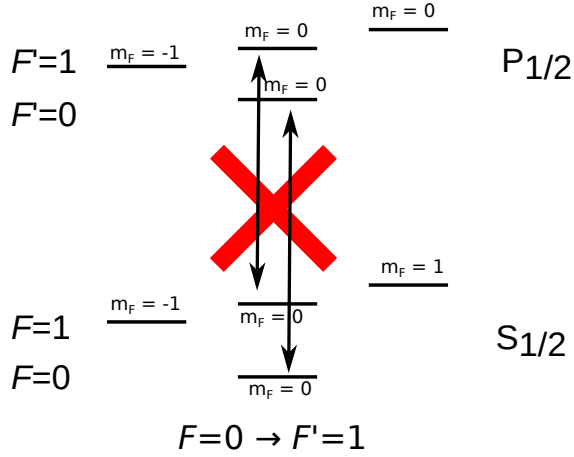
For the ground state this translates to 1.4 MHz/G. In our experiments we use a magnetic field of ≈ 4.8 G which translates to a Zeeman splitting of 6.7 MHz. The two $m_F = 0$ states $|F=0, m_F=0\rangle$ and $|F=1, m_F=0\rangle$ are insensitive to Zeeman shift upto first order and hence we use these “clock states” as our qubit $|\downarrow\rangle$ and $|\uparrow\rangle$ states respectively. The hyperfine splitting of the $^2S_{1/2}$ defines the qubit frequency $\omega_{\text{hf}}/2\pi = 12\,642\,812\,118.5 \text{ Hz} + |\vec{B}|^2 \times 310.8 \text{ (Hz/G}^2\text{)}$.

2.5.2 Doppler cooling

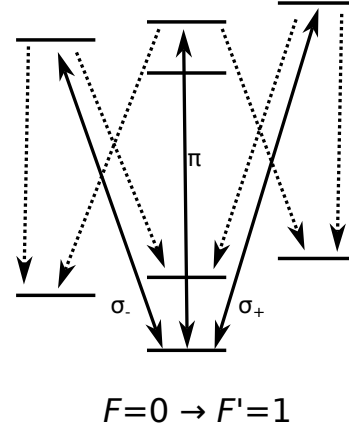
Once the ions are loaded into the trap, we use a laser tuned to the $^2S_{1/2} \rightarrow ^2P_{1/2}$ (Natural linewidth, $\Gamma = 2\pi \times 19.6 \text{ MHz}$) optical transition at 369.5 nm to Doppler cool the ions. The lifetime of $^2P_{1/2}$ is about 8 ns, and each time the atom is excited to $^2P_{1/2}$, it decays back almost immediately. This makes $^2S_{1/2} \rightarrow ^2P_{1/2}$ a highly fluorescing optical dipole transition, which is important for efficient Doppler cooling. We park our laser frequency to about $\Gamma/2$ less than the resonance frequency i.e. ‘red’-detuned. The ions traveling in the opposite direction of the beam see enhanced absorption because the Doppler shift

¹²There is also a term containing g_I however since $g_I \approx -0.0009955$ it can be safely be neglected.

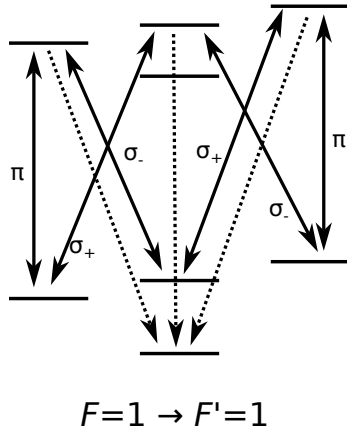
a)



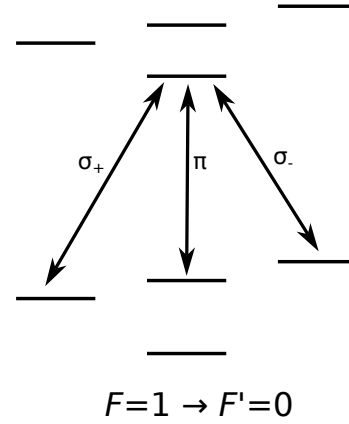
b)



c)



d)



$\longleftrightarrow$ Absorption + Spontaneous Emission
 $\cdots \rightarrow$ Spontaneous Emission

$F=1 \rightarrow F'=1$: Optical Pumping
 $F=1 \rightarrow F'=0$: State Detection
 $F=1 \rightarrow F'=0 + F=0 \rightarrow F'=1$: Doppler Cooling

Figure 2.10: Incoherent operations in $^{171}\text{Yb}^+$

Transitions between the different sublevels in the $2S_{1/2}$ and $2P_{1/2}$. **a)** Dipole forbidden transitions. **b)** $F = 0 \rightarrow F' = 1$. **c)** $F = 1 \rightarrow F' = 1$. **d)** $F = 1 \rightarrow F' = 0$.

(blue) causes the photon to be closer to resonance in the ion's rest frame. Similarly, ions that are traveling in the direction of the beam propagation see reduced absorption because the Doppler shift (red) causes the photon frequency to be further away from resonance in the ion's rest frame. Each time an atom absorbs a photon from the laser, it acquires momentum $\hbar\vec{k}$ from the photon, where $\vec{k}$ is the wavevector of the cooling laser. Because the absorption is enhanced when the ion is traveling opposite to the beam propagation, on average the absorption results in a reduction of the momentum of the ion. When the ion decays from $^2P_{1/2}$ to the ground state $^2S_{1/2}$, the spontaneous emission of fluorescence is isotropic and the average momentum imparted is zero. Hence, the red-detuned laser beam leads to an average reduction in momentum of the ion and causes the ion to be cooled.

In the last section, we saw that the hyperfine splitting of the $^2S_{1/2}$ level is ≈ 12.6 GHz. $^2P_{1/2}$ has a hyperfine splitting of roughly 2.1 GHz, therefore, the transition frequencies for coupling the different F levels in both $^2S_{1/2}$ and $^2P_{1/2}$ are separated by roughly 14.7 GHz. For Doppler cooling, we want to simultaneously drive the $(^2S_{1/2}, F=1) \rightarrow (^2P_{1/2}, F=0)$ and the $(^2S_{1/2}, F=0) \rightarrow (^2P_{1/2}, F=1)$ transitions (see Fig. 2.10). A diode laser has a linewidth that is much narrower than 14.7 GHz, and in our case the 369.5nm laser, tuned to the $(^2S_{1/2}, F=1) \rightarrow (^2P_{1/2}, F=0)$ resonance, cannot excite the transition $(^2S_{1/2}, F=0) \rightarrow (^2P_{1/2}, F=1)$. To remedy this, we modulate the laser at ≈ 14.7 GHz using an electro optic modulator (EOM) so that the blue modulation sideband addresses the $(^2S_{1/2}, F=0) \rightarrow (^2P_{1/2}, F=1)$ transition. Since the linewidth of the $^2S_{1/2} \rightarrow ^2P_{1/2}$ transition is ≈ 20 MHz and the Zeeman splitting in the ground and excited state F=1 levels is much smaller, all the m_F levels are excited/addressed as long as the laser has all components i.e σ_+ , σ_- , π . In our experiment, the 369.5 nm laser is focussed to a spot size of $\approx 100 \mu m$ at the ion location and the beam has a power of roughly $50 \mu W$.

When excited to $^2P_{1/2}$, ion decays mostly to $^2S_{1/2}$ (branching ratio ≈ 99.5 %) but also in $^2D_{3/2}$ (0.5 %) as shown in Fig. 2.9. To bring back the population from the $^2D_{3/2}$ to $^2S_{1/2}$, a $\lambda = 935$ nm laser excites the ion from $^2D_{3/2}$ to the low-lying bracket state $^3[3/2]_{1/2}$ ¹³ which then decays to $^2S_{1/2}$ bringing the ion population back to the ground state. In our experiment the $\lambda = 935$ nm laser is tuned to the $^2D_{3/2}, F=2 \rightarrow ^3[3/2]_{1/2}, F=1$ resonance and an electro-optic modulator is used to modulate the laser at 3.1GHz for addressing the $^2D_{3/2}, F=1 \rightarrow ^3[3/2]_{1/2}, F=2$ transition. The $\lambda = 935$ nm beam has roughly 200 μW of

¹³The $^2D_{3/2}$ to $^3[3/2]_{1/2}$ has a linewidth of $\Gamma = 2\pi \times 4.2$ MHz. The bracket notation is used in reference to an angular momentum coupling scheme that is different from the regular L-S coupling scheme or the jj coupling scheme that occurs in heavier nuclei. I found a very good explanation in this physics stack exchange question (<https://physics.stackexchange.com/questions/229564/what-do-term-symbols-with-a-half-integer-l-like-33-2-1-2-mean>). In case that link disappears when you read this, it is also covered in detail in Ref. [95]

power and at the ion location it is focussed to a waist of about 100 μm .

The $^2\text{S}_{1/2}$ to $^2\text{P}_{1/2}$ transition together with the repump laser coupling the $^2\text{D}_{3/2}$ to the $^3[3/2]_{1/2}$ form a closed cycle and ideally the ion population should not leave these manifolds. However, while the ions are in $^2\text{D}_{3/2}$, a collision with a background gas molecule could decay into $^2\text{F}_{7/2}$ which has a lifetime of approximately 5.4 years. Hence, a second repump laser at 760 nm coupling $^2\text{F}_{7/2}$ to $^3[3/2]_{1/2}$ is used to pump the ion population back into $^2\text{S}_{1/2}$. The two repump lasers are left on during all operations that involve coupling $^2\text{S}_{1/2}$ to $^2\text{P}_{1/2}$.

2.5.3 State reset

Preparing an initial state of ions for quantum simulations begins with optical pumping [96] of all ions into the $|\downarrow\rangle$ ($|F=0, m_F=0\rangle$) state. Fig. 2.10 shows the laser frequencies required for optical pumping. With the 369.5 nm laser tuned to the $^2\text{S}_{1/2} F=1 \rightarrow ^2\text{P}_{1/2} F=1$ transition, all the population is effectively pumped into $|\downarrow\rangle$. This is because $^2\text{P}_{1/2} F=1$ decays into both $^2\text{S}_{1/2} F=0$ and $^2\text{S}_{1/2} F=1$. However, since the laser is off-resonant with $^2\text{S}_{1/2} F=1 \rightarrow ^2\text{P}_{1/2} F=0$ and also $^2\text{S}_{1/2} F=0 \rightarrow ^2\text{P}_{1/2} F=0$ is forbidden by the dipole selection rules [21], the population in $^2\text{S}_{1/2} F=0$ ($|\downarrow\rangle$) is left unaltered by the incident laser. Once the ion is prepared in $|\downarrow\rangle$, the population can be coherently transferred between $|\downarrow\rangle$ and $|\uparrow\rangle$ to create arbitrary initial states.

2.5.4 State detection

As shown in Fig. 2.10 d), exciting the $(^2\text{S}_{1/2}, F=1) \rightarrow (^2\text{P}_{1/2}, F=0)$ transition does not lead to the spillage of the population into $(^2\text{S}_{1/2}, F=0)$. This is because the decay path $(^2\text{P}_{1/2}, F=0) \rightarrow (^2\text{S}_{1/2}, F=0)$ is forbidden by dipole selection rules (see Fig. 2.10 a)). Hence, $(^2\text{P}_{1/2}, F=0)$ only decays into the $(^2\text{S}_{1/2}, F=1)$ manifold, leading to sustained fluorescence, while the laser is incident on the ions prepared in any magnetic sublevel in the $(^2\text{S}_{1/2}, F=1)$ (including $|\uparrow\rangle$). The only requirement for ensuring sustained fluorescence is that the laser has all polarization components (σ_+ , σ_- , π) with respect to the quantization axis defined by the magnetic field hence avoiding a coherent dark state [97]. The same light appears off-resonant in the $|\downarrow\rangle$ state, and hence the ion does not fluoresce. This state-dependent fluorescence is the basis for discriminating between the $|\downarrow\rangle$ and $|\uparrow\rangle$ states, and on a detector the two states appear ‘dark’ and ‘bright’, respectively.

The photons emitted by the ions are collected using an optical setup (Numerical Aperture (NA) = 0.16) described in [98] and imaged on a photomultiplier tube (PMT) or a qCMOS camera depending on the experiment. For an ion in the bright state, the number

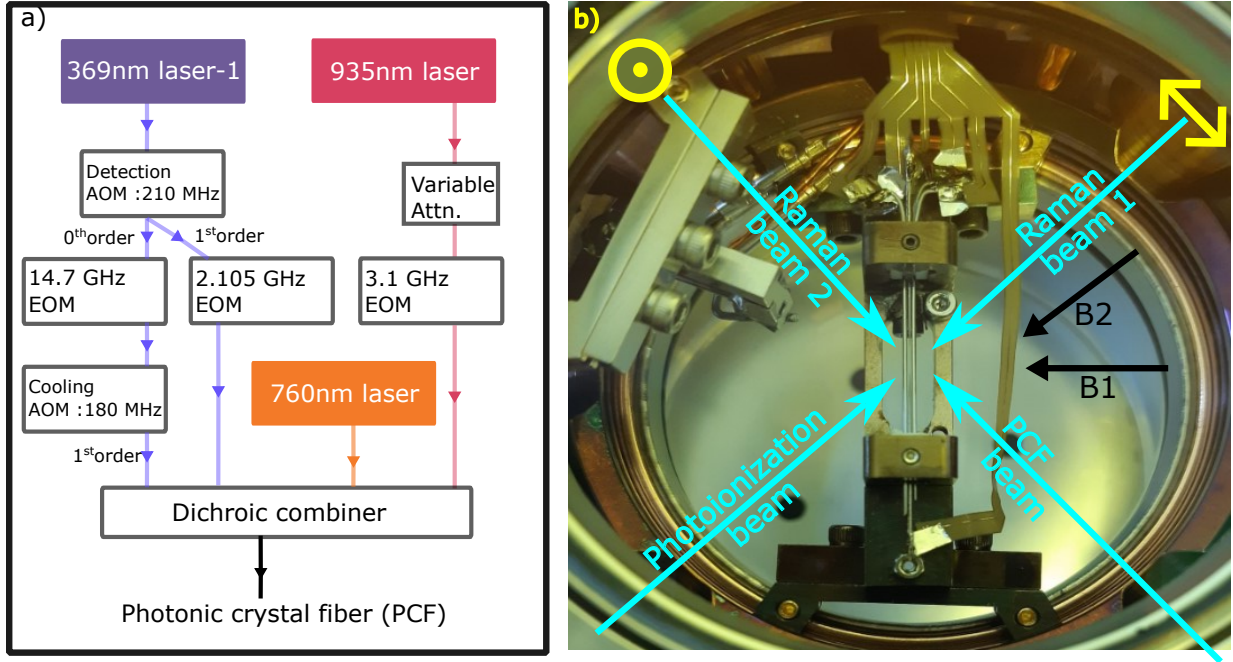


Figure 2.11: Beam Orientations in Four Rod Trap

a) Optical schematic for lasers used in incoherent operations. All frequencies are combined into a single Photonic Crystal Fiber (PCF) from NKT photonics(LMA-PM-10). The signal frequency for the detection Acousto Optic Modulator (AOM) is arbitrarily chosen within the AOM's operating range. The hyperfine splitting in the $\omega_{\text{hf}}^S = 2\pi \times 12.6$ GHz and $\omega_{\text{hf}}^P = 2\pi \times 2.105$ GHz respectively. EOM frequencies, 14.7 GHz and 2.105 GHz are $(\omega_{\text{hf}}^S + \omega_{\text{hf}}^P)$ and ω_{hf}^P respectively to allow for cooling and optical pumping respectively. b) Beam orientations for all optical beams in the experiment. B1 and B2 represent magnetic field directions of two magnetic field coils.

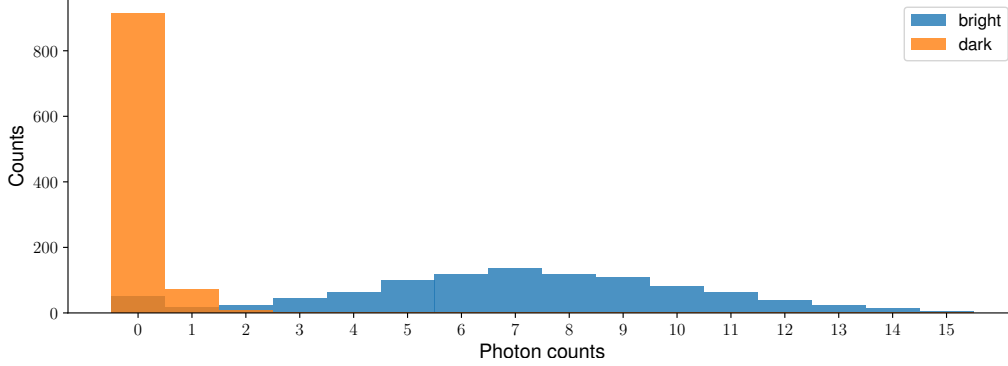


Figure 2.12: Histogram of photon counts in bright and dark states

Histogram of photon counts observed on a photomultiplier tube (Hamamatsu: H10682-210) for 2000 shots, 1000 each for ions prepared in bright and dark state. See Sec.2.5.4 for more details.

of photons in a given time interval satisfies a Poisson distribution. In our system, we usually operate at a detection time of $\approx 400 \mu\text{s}$ and collect an average of 10 photon counts. Fig. 2.12 shows typical histograms of photon counts for an ion prepared in the $|\downarrow\rangle$ and $|\uparrow\rangle$ states. Analyzing the two histograms in Fig. 2.12, the bright state is classified as bright with a probability of $\approx 93.3\%$, the dark state is classified as dark with a probability of $\approx 98.6\%$ and the average detection fidelity is $\approx 95\%$.

2.5.5 Coherent Operations

Microwave driven spin flips

With the application of resonant microwave radiation at $\omega_{mic} \approx \omega_{hf}$ to the ions, the transitions between $F = 0$ to $F = 1$ can be induced. The magnetic moment of the ion couples to the magnetic field with the following Hamiltonian

$$\begin{aligned}
 H_{micro} &= -\boldsymbol{\mu} \cdot \mathbf{B}(t) \\
 &= -\mu_B(g_J \mathbf{J} + g_I \mathbf{I}) \cdot \mathbf{B}(t) \\
 &\approx \mu_B g_J (\mathbf{J} \cdot \mathbf{B}(t))
 \end{aligned} \tag{2.46}$$

We neglected the nuclear magnetic moment coupling because g_I is more than three orders of magnitude smaller than g_J . The Rabi frequency for the transition between the $F=0$ and a specific hyperfine level m_1 in $F=1$ is given as

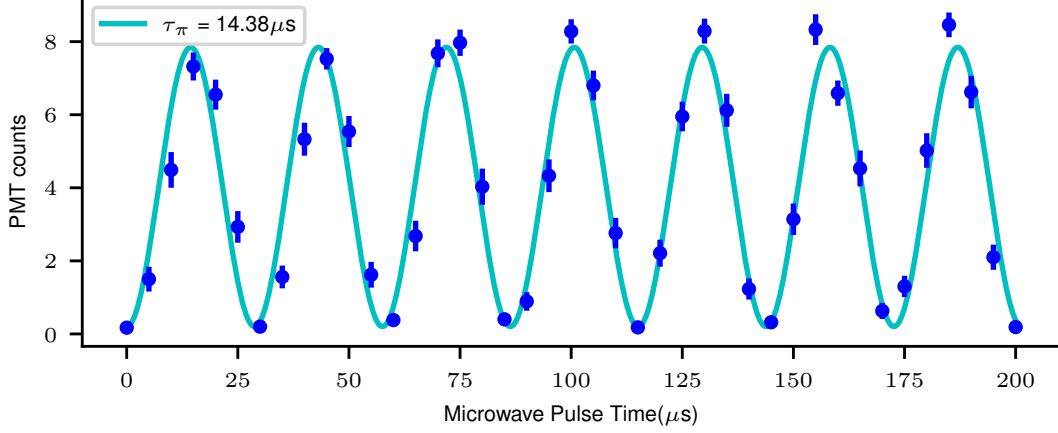


Figure 2.13: Coherent oscillations using microwave radiation

Detected fluorescence from a single $^{171}\text{Yb}^+$ ion with respect to microwave pulse time. The microwave radiation is resonant with the $|\downarrow\rangle \rightarrow |\uparrow\rangle$ transition. Each point is the average of 100 shots, with error bars showing the standard error. See Sec.2.5.5 for more details.

$$\Omega_{F=0}^{F=1,m_1} = \frac{gJ\mu_B}{\hbar} \langle 1, m_1 | \mathbf{B} \cdot \mathbf{J} | 0, 0 \rangle \quad (2.47)$$

The magnetic field at the ion location can be written as $\mathbf{B}(t) = \frac{1}{2} [\tilde{B}e^{-i\omega t} + \tilde{B}^*e^{i\omega t}]$, where the complex phasor $\tilde{B}$ is given as

$$\tilde{B} \equiv \begin{pmatrix} B_x e^{-i\phi_x} \\ B_y e^{-i\phi_y} \\ B_z e^{-i\phi_z} \end{pmatrix}. \quad (2.48)$$

With this definition, we can write the dot product in the Hamiltonian as follows:

$$\begin{aligned} \mathbf{B} \cdot \mathbf{J} &= B_x J_x e^{-i\phi_x} + B_y J_y e^{-i\phi_y} + B_z J_z e^{-i\phi_z} \\ &= \frac{1}{2} (B_x e^{-i\phi_x} - iB_y e^{-i\phi_y}) J_+ + \frac{1}{2} (B_x e^{-i\phi_x} + iB_y e^{-i\phi_y}) J_- \\ &\quad + B_z e^{-i\phi_z} J_z \\ &= B_+ J_+ + B_- J_- + B_z J_z \end{aligned} \quad (2.49)$$

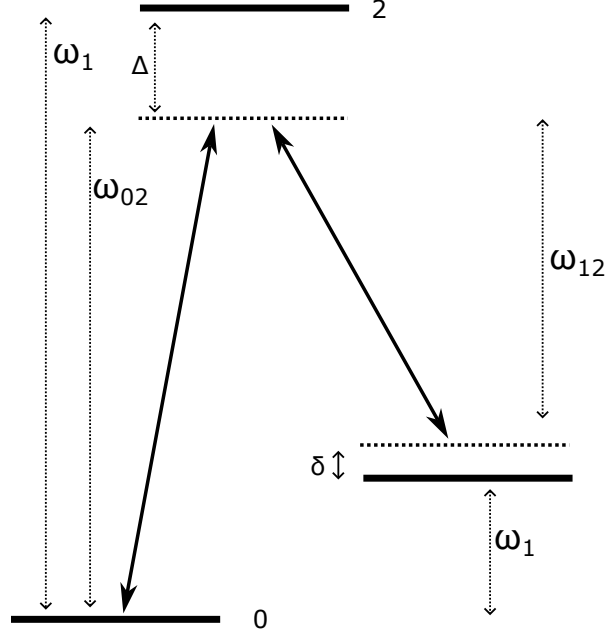


Figure 2.14: Two Photon Raman Transitions

Energy level schematic for driving two-photon raman transitions between levels $|0\rangle$ and $|1\rangle$, mediated by virtually exciting $|2\rangle$. $\hbar\omega_1$ and $\hbar\omega_2$ are the energies of levels $|0\rangle$ and $|1\rangle$ respectively. ω_{01} and ω_{02} are the laser frequencies coupling $|0\rangle$ and $|1\rangle$ off resonantly to $|2\rangle$ respectively.

Where $J_{\pm} = J_x \pm iJ_y$, $B_+ = (B_x e^{-i\phi_x} - iB_y e^{-i\phi_y})$, $B_- = (B_x e^{-i\phi_x} + iB_y e^{-i\phi_y})$. Plugging the expression from Eq.(2.49) into the matrix element in Eq.(2.47) it can be shown that the B_+ , B_- , B_z components of the magnetic field induce transitions to $|F=1, m_1=1\rangle$, $|F=1, m_1=-1\rangle$, $|F=1, m_1=0\rangle$ respectively. In our experimental setup the microwave radiation is sent onto the ions through a microwave Horn and the radiation has all the above three components of polarization. The linewidth of each of these transitions is much narrower compared to the Zeeman splitting (≈ 6.7 MHz) and hence tuning the microwave frequency to the correct transition allows selective addressing of any of the $|F=1, m_f\rangle$ levels from the ground state $|F=0, m_0=0\rangle$. Fig. (2.13) shows coherent oscillations between $|\downarrow\rangle$ and $|\uparrow\rangle$ in our experimental apparatus.

Coherent operations using two photon Raman transitions

Transitions between the clock states can also be accomplished using two-photon Raman transitions by virtual excitation to a higher energy level. This is the most common way that such transitions are accomplished because the photons at optical frequencies have much more momentum, and hence we can also induce motional excitation with these. Let us first go through the theory behind how transitions between two ground-state energy levels can be mediated through an excited state [99]. We assume two metastable ground states $|0\rangle$, $|1\rangle$ and an excited state $|2\rangle$ and start with writing the Hamiltonian of the three-level system with zero energy assigned to $|0\rangle$.

$$H_{\text{atom}} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & \omega_1 & 0 \\ 0 & 0 & \omega_2 \end{bmatrix}. \quad (2.50)$$

Now we assume that the light couples the levels $|0\rangle$ to $|2\rangle$ and $|1\rangle$ to $|2\rangle$ off-resonantly through optical dipole transitions as shown in Fig. (2.14). The Hamiltonian of the light-atom interaction can be written as

$$H_{\text{lm}} = -\vec{d} \cdot \vec{E}(\vec{r}, t) \quad (2.51)$$

Since we have two lasers, $\vec{E} = \vec{E}_{01} \cos(\vec{k}_1 \cdot \vec{r} - \omega_{01}t) + \vec{E}_{12} \cos(\vec{k}_2 \cdot \vec{r} - \omega_{02}t)$. Now the dipole operator can be shown to be off-diagonal¹⁴ and hence, the light atom interactions, after a rotating wave approximation, can be shown to be

¹⁴The dipole moment operator d can be shown to be off-diagonal from parity arguments. Let Π be the parity operator with the following action $\Pi r \Pi^\dagger = -r$; also, $\Pi = \Pi^{-1} = \Pi^\dagger$ and $\Pi^2 = I$. Since $\Pi^2 = I$, the two eigenvalues are ± 1 which correspond to the even and odd parity states. The atomic Hamiltonian is isotropic, hence Π and H commute and have simultaneous eigenstates. For any two levels $|a\rangle$ and $|b\rangle$,

$$\begin{aligned} \langle a | r | b \rangle &= \langle a | \Pi^2 r \Pi^2 | b \rangle \\ &= \pi_a \pi_b \langle a | \Pi r \Pi^\dagger | b \rangle \\ &= -\pi_a \pi_b \langle a | r | b \rangle. \end{aligned}$$

Hence we have that for $\pi_a = \pi_b$, $\pi_b \langle a | r | b \rangle = 0$ i.e. the position operator does not couple states with the same parity. Now, obviously, the diagonal elements $\langle a | \Pi r | a \rangle = 0$. Since the dipole operator is proportional to the position operator, the same arguments hold for it.

$$H_{light} = \begin{bmatrix} 0 & 0 & \frac{\Omega_{02}}{2} e^{i\omega_{02}t - i\vec{k}_1 \cdot \vec{r}} \\ 0 & 0 & \frac{\Omega_{12}}{2} e^{i\omega_{12}t - i\vec{k}_2 \cdot \vec{r}} \\ \frac{\Omega_{02}^*}{2} e^{-i\omega_{02}t + i\vec{k}_1 \cdot \vec{r}} & \frac{\Omega_{12}^*}{2} e^{-i\omega_{12}t + i\vec{k}_2 \cdot \vec{r}} & 0 \end{bmatrix} \quad (2.52)$$

Here we have defined $\Omega_{02} = \frac{\langle 0|d \cdot E_{01}|2 \rangle}{\hbar}$ and $\Omega_{12} = \frac{\langle 1|d \cdot E_{12}|2 \rangle}{\hbar}$.

The total Hamiltonian of the system is then given as follows.

$$H_{total} = \begin{bmatrix} 0 & 0 & \frac{\Omega_{02}}{2} e^{i\omega_{02}t - i\vec{k}_1 \cdot \vec{r}} \\ 0 & \omega_1 & \frac{\Omega_{12}}{2} e^{i\omega_{12}t - i\vec{k}_2 \cdot \vec{r}} \\ \frac{\Omega_{02}^*}{2} e^{-i\omega_{02}t + i\vec{k}_1 \cdot \vec{r}} & \frac{\Omega_{12}^*}{2} e^{-i\omega_{12}t + i\vec{k}_2 \cdot \vec{r}} & \omega_2 \end{bmatrix}. \quad (2.53)$$

To remove the time dependence, we define the following Unitary

$$U = \begin{bmatrix} 1 & 0 & 0 \\ 0 & e^{it(\omega_{02} - \omega_{12})} & 0 \\ 0 & 0 & e^{i\omega_{02}t} \end{bmatrix}. \quad (2.54)$$

In the interaction frame of U (See Appendix 1) we have the transformed Hamiltonian given as

$$H_U = \begin{bmatrix} 0 & 0 & \frac{\Omega_{02}}{2} e^{-i\vec{k}_1 \cdot \vec{r}} \\ 0 & \omega_1 - \omega_{02} + \omega_{12} & \frac{\Omega_{12}}{2} e^{-i\vec{k}_2 \cdot \vec{r}} \\ \frac{\Omega_{02}^*}{2} e^{i\vec{k}_1 \cdot \vec{r}} & \frac{\Omega_{12}^*}{2} e^{i\vec{k}_2 \cdot \vec{r}} & \omega_2 - \omega_{02} \end{bmatrix}. \quad (2.55)$$

After substituting $\Delta = \omega_2 = \omega_{01}$ and $\delta = \omega_2 - \omega_{12} - \Delta$, we get

$$H_U = \begin{bmatrix} 0 & 0 & \frac{\Omega_{02}}{2} e^{-i\vec{k}_1 \cdot \vec{r}} \\ 0 & -\delta & \frac{\Omega_{12}}{2} e^{-i\vec{k}_2 \cdot \vec{r}} \\ \frac{\Omega_{02}^*}{2} e^{i\vec{k}_1 \cdot \vec{r}} & \frac{\Omega_{12}^*}{2} e^{i\vec{k}_2 \cdot \vec{r}} & -\Delta \end{bmatrix} \quad (2.56)$$

To study the time evolution under the above Hamiltonian we define the following wavefunction where c_i is the amplitude for the state $|i\rangle$.

$$\psi = \begin{bmatrix} c_0 \\ c_1 \\ c_2 \end{bmatrix} \quad (2.57)$$

The Schrodinger's equation is now given as

$$i \begin{bmatrix} \dot{c}_0 \\ \dot{c}_1 \\ \dot{c}_2 \end{bmatrix} = \begin{bmatrix} \frac{\Omega_{02}}{2} c_2 e^{-i\vec{k}_1 \cdot \vec{r}} \\ \frac{\Omega_{12}}{2} c_2 e^{-i\vec{k}_2 \cdot \vec{r}} - c_1 \delta \\ -\Delta c_2 + \frac{\Omega_{02}^*}{2} c_0 e^{i\vec{k}_1 \cdot \vec{r}} + \frac{\Omega_{12}^*}{2} c_1 e^{i\vec{k}_2 \cdot \vec{r}} \end{bmatrix} \quad (2.58)$$

Since $|2\rangle$ is only off-resonantly coupled, its population grows very slowly, and hence we can set $\dot{c}_2 = 0$ and from the last equation we get

$$c_2 = \frac{\Omega_{02}^* c_0 e^{i\vec{k}_1 \cdot \vec{r}}}{2\Delta} + \frac{\Omega_{12}^* c_1 e^{i\vec{k}_2 \cdot \vec{r}}}{2\Delta}. \quad (2.59)$$

Putting this back in Eq.(2.58),

$$i \begin{bmatrix} \dot{c}_0 \\ \dot{c}_1 \end{bmatrix} = \begin{bmatrix} \frac{\Omega_{02}\Omega_{02}^*}{4\Delta} & \frac{\Omega_{02}\Omega_{12}^*}{4\Delta} e^{-i(\vec{k}_1 - \vec{k}_2) \cdot \vec{r}} \\ \frac{\Omega_{12}\Omega_{02}^*}{4\Delta} e^{i(\vec{k}_1 - \vec{k}_2) \cdot \vec{r}} & \delta + \frac{\Omega_{12}\Omega_{12}^*}{4\Delta} \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \end{bmatrix} \quad (2.60)$$

Since we want resonant coupling we can choose $\delta = 0$. The diagonal terms are stark shifts on $|0\rangle$ and $|1\rangle$ and if we assume equal rabi frequencies ($\Omega_{02} = \Omega_{12}$) then upto the first order the differential stark shifts cancel and we can neglect the diagonal terms.

$$i \begin{bmatrix} \dot{c}_0 \\ \dot{c}_1 \end{bmatrix} = \begin{bmatrix} 0 & \frac{|\Omega_{02}|^2}{4\Delta} e^{-i(\vec{k}_1 - \vec{k}_2) \cdot \vec{r}} \\ \frac{|\Omega_{02}|^2}{4\Delta} e^{i(\vec{k}_1 - \vec{k}_2) \cdot \vec{r}} & 0 \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \end{bmatrix} \quad (2.61)$$

The above Hamiltonian is precisely the Hamiltonian in Eq.(2.25) and induces transitions between $|0\rangle$ and $|1\rangle$. Note the presence of $e^{-i(\vec{k}_1 - \vec{k}_2) \cdot \vec{r}}$ in the exponentials. $(\vec{k}_1 - \vec{k}_2)$ is the difference in wavevector of the two Raman beams and r is the atom's position vector. The Raman beams can also impart momentum to the atom, and this allows us to excite the carrier, red-sideband, and blue-sideband transitions that were discussed in Sec.2.2.

In $^{171}\text{Yb}^+$ we use a pulsed 355 nm laser to excite two-photon Raman transitions between $|\downarrow\rangle$ and $|\uparrow\rangle$. The precise details of using pulsed lasers for exciting such transitions can be found in [100]. As shown in Fig. 2.15 we can detune the beatnote between the two arms to excite the carrier, red, and blue sidebands.

2.6 Typical Experimental Sequence

Prior to conducting experiments with trapped ions, a number of external factors must be optimized. DC and radio frequency voltages need to be applied to the ion trap electrodes to allow trapping. To ensure that we can faithfully perform the operations discussed in the previous sections, the different lasers being used need to be locked to their respective frequency. Once the trapping fields are present and the lasers are locked, the ion trapping begins with turning on the atomic oven and allowing it to reach an appropriate temperature. The photoionization beams discussed in Fig. 2.8 are then turned ON and the required number of ions is trapped. The trapping of ions is followed by Doppler cooling, and the calibration of various other experimental parameters with respect to the ions, for example, the microwave and Raman flop times. For more details on the apparatus, please refer to the recent master's and Ph.D. theses from our group[88, 101, 98].

Once trapping¹⁵ and calibrations have been performed, a quantum simulation experiment comprises of state preparation, evolution, and measurement. To study dynamics, the following sequence of operations is performed, N times, at each value of evolution time.

- Doppler cooling
- Prepare initial state (usually $|\downarrow\rangle_z^{\otimes N}$)
- Raman sideband cooling
- Global microwave operations + local resets (For example a π pulse to create $|\uparrow\rangle_z^{\otimes N}$ and then local resets only on selected qubits to create arbitrary initial states)
- Coherent evolution under simulated Hamiltonian using Raman laser pulses
- Measurement: detection of site dependent fluorescence while applying detection laser beam

¹⁵Often we do not need to trap if the ions are still in the trap from a previous experiment or even the previous day

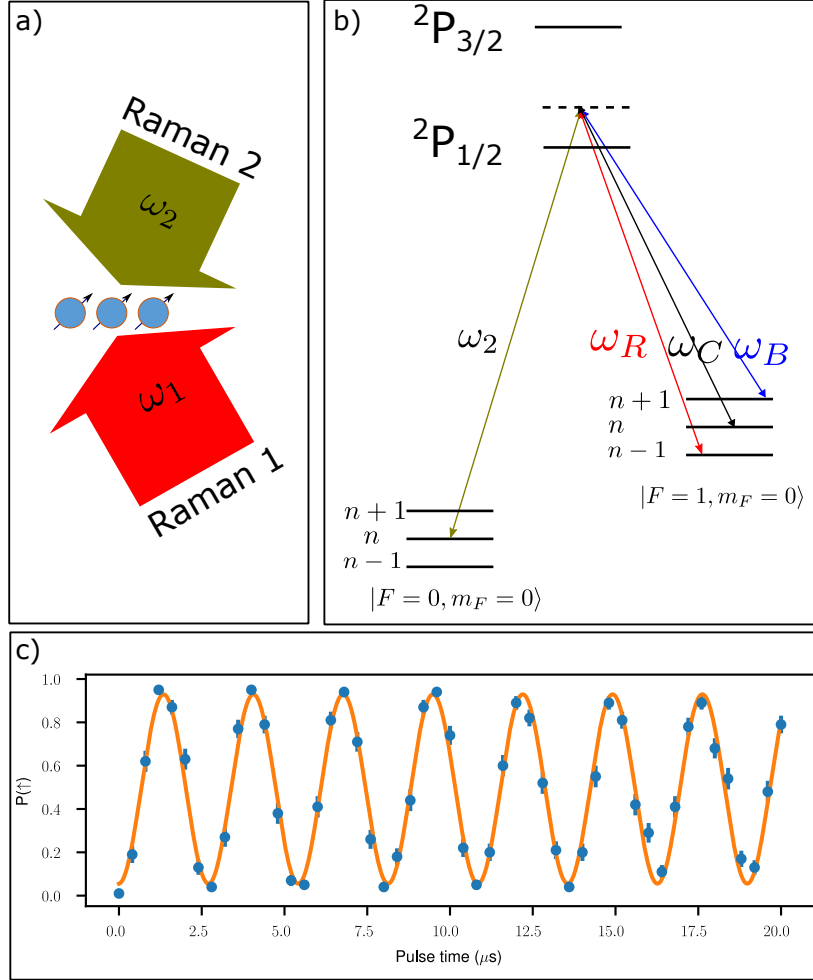


Figure 2.15: Two Photon Raman Transitions

a) Cartoon schematic showing two raman beams shining on a chain of ions. **b)** The frequency difference between the two raman beams can be chosen to excite the carrier, red sideband and blue sideband transitions described in Equations (2.25) and (2.27) **c)** Coherent oscillations between $|\downarrow\rangle$ and $|\uparrow\rangle$ while exciting the carrier transition. Plot shows the probability of detecting ion in $|\uparrow\rangle$ with respect to the raman pulse duration. Each point is the average of 100 shots, with error bars showing the standard error. See Sec.2.5.5 for more details.

The number of times the above steps are repeated at each evolution time depends on precision requirements on the extracted quantities, and we usually repeat operations in the regime $N \approx \mathcal{O}(10^2)$.

Chapter 3

Tunable XY Interactions on trapped ions

Author contributions: Most of the results discussed in this chapter have been published in Ref. [102]. Exploration of tunable XY interactions on trapped ions started after discussions with Prof. Rajibul Islam. The idea of applying multiple spin-dependent forces on the same motional modes of trapped ions was conceived by the author, and subsequent theory and numerical simulations were also developed by the author, who benefitted from helpful discussions with Prof. Rajibul Islam. Dr. Chung-You Shih added an arbitrary waveform generator to the experimental apparatus that was useful for creating waveforms allowing dual spin-dependent forces, and the author added the capability to generate waveforms for generating dual spin-dependent forces. The author performed the experiments and data analysis.

3.1 Overview

In the last chapter, we went in detail how trapped ions can be used as programmable simulators of connected spin Hamiltonians by using laser-based spin dependent forces. Further, the setup also allows for simulating an added magnetic field (B_{eff}) along with the tunable long-range spin-spin couplings to yield an effective Hamiltonian.

$$H_{\text{eff}} = \sum_{i < j} J_{ij} \sigma_{\theta}^i \sigma_{\theta}^j + B_{\text{eff}} \sum_i \sigma_{\theta}^i \quad (3.1)$$

where J_{ij} are the matrix elements that determine the interaction strength between the i -th and the j -th spin $\sigma_\theta = (\sigma_x \cos \theta + \sigma_y \sin \theta)$ and B_{eff} is the effective magnetic field. Note that θ and θ' can be chosen, by setting the laser phases (Equations (2.31) and (2.25)), to give orthogonal spin axes in the XY plane (in the Bloch sphere).

Long-range interactions¹ are a unique feature native to the trapped ions platform and for more than a decade, this technique has been used to study a wide variety of physical phenomena. Some prominent examples include the simulation of magnetic ordering[103, 104], preparation of ground and equilibrium states of complicated magnetic systems[105, 106, 107, 108, 104], and phase transitions in magnetic systems[108, 109]. Further, these techniques have also been used to study dynamical phenomena in quantum magnetism[110, 74], entanglement dynamics and information propagation in large systems[111], quantum thermalization[112] and inhibitors to thermalization, etc.

All the examples quoted above involved the quantum simulation of the Hamiltonian in equation 3.1, and even though this allows the exploration of a wide variety of physical phenomena, adding more complexity to the models is important. For example, it is desirable to simulate models where long-range interactions exist along multiple axes of the spins. The most general of such models is the Heisenberg model with a Hamiltonian.

$$H = \sum_{i < j} J_{ij}^x \sigma_x^i \sigma_x^j + J_{ij}^y \sigma_y^i \sigma_y^j + J_{ij}^z \sigma_z^i \sigma_z^j \quad (3.2)$$

The Heisenberg model appears naturally in physics[113], for example, in modeling 3D magnetic interactions. Moreover, standard transformations[114, 115] directly map fermionic Hubbard models to spin models such as the XXZ ($J_{ij}^x = J_{ij}^y$) and the XY model ($J_{ij}^z = 0$). The XY model and the anisotropic XY model ($J_{ij}^x \neq J_{ij}^y, J_{ij}^z = 0$) also open avenues for studying exotic quantum phases such as spin liquids, superconductivity, etc. Despite the wide implications, very few quantum simulation experiments on trapped ions have explored such interactions in the past decade². This is because existing proposals make use of orthogonal sets [116] of phonon modes, with each set mediating an independent Ising term (such as $\sigma_x^i \sigma_x^j$ or $\sigma_y^i \sigma_y^j$). This requires selective excitation of phonon modes along different spatial directions, and the beams that excite phonon modes along one trap axis, must not excite the other orthogonal set of phonon modes. However, exciting multiple

¹For example, one can, in principle, simulate a system with all to all couplings with the matrix J_{ij} having roughly equal entries on the off-diagonal elements

²Even when such interactions have been implemented, it was almost always using the large B-field method discussed shortly. Furthermore, these simulations were limited to the isotropic case ($J_{ij}^x = J_{ij}^y, J_{ij}^z = 0$) due to the large B-field method

sets of orthogonal phonon modes ‘selectively’ requires additional laser beams, electronic controls, and complex optical design beyond the scope of current experimental setups. Further, this scheme may not produce the same form and range of interactions along different spin axes [63], limiting the usefulness of such simulations.

In this chapter, I will go over some existing techniques that allow for simulating tunable XY couplings, discuss their limitations, and present our results on a new method that bypasses these limitations and allows parallel and tunable XX and YY Ising interactions on trapped ions. Although spin-dependent forces leading to an effective Hamiltonian in Equation 3.1 have been used in trapped ions experiments for over two decades, their parallel application with separate spin phases was not considered even though the experimental overhead is minimal. This was most likely due to the known existence of cross-couplings between the two forces on the same set of motional modes (cross-terms in the Magnus expansion). The experimentally demanding theoretical proposals for simulating parallel Ising interactions, such as in [116], mainly tried to bypass this limitation by requiring selective excitation of orthogonal modes. The key insight is that the same set of motional modes can mediate multiple Ising interactions through the application of parallel spin-dependent forces with different spin phases.

3.2 Existing Techniques for generating effective XY dynamics

3.2.1 Large B-field method

The most common method used to simulate the XY model on trapped ions is to apply a large transverse magnetic field along with the Ising couplings in the limit where the magnetic field strength is much larger than the strength of the Ising terms. The Hamiltonian that is simulated is the following³

$$\begin{aligned} H_{\text{eff}} &= \sum_{i < j} J_{ij} \sigma_x^i \sigma_x^j + \frac{B_{\text{eff}}}{2} \sum_i \sigma_z^i \\ &= \frac{1}{4} \sum_{i < j} J_{ij} (\sigma_+^i \sigma_+^j + \sigma_+^i \sigma_-^j + \sigma_-^i \sigma_+^j + \sigma_-^i \sigma_-^j) + \sum_i \frac{B_{\text{eff}}}{2} \sigma_z^i. \end{aligned} \tag{3.3}$$

³The transverse field does not necessarily have to be σ_z . The field just has to be transverse; that is, σ_y also works.

Where $\sigma_{\pm} = \sigma_x \pm i\sigma_y$ and hence $\sigma_x^i \sigma_x^j + \sigma_y^i \sigma_y^j = (\sigma_+^i \sigma_-^j + \sigma_-^i \sigma_+^j)/2$. Now, if we go into the interaction frame of $\frac{B_{\text{eff}}}{2}\sigma_z^i$, the Hamiltonian is

$$H_{\text{rot}} = \frac{1}{4} \sum_{i < j} J_{ij} \left(\sigma_+^i \sigma_+^j e^{iB_{\text{eff}}t} + \sigma_+^i \sigma_-^j + \sigma_-^i \sigma_+^j + \sigma_-^i \sigma_-^j e^{-iB_{\text{eff}}t} \right). \quad (3.4)$$

Since we made the assumption that $B_{\text{eff}} \gg \max(J_{ij})$, the terms oscillatory terms containing $e^{\pm iB_{\text{eff}}t}$ can be discarded, leading to an effective Hamiltonian

$$\begin{aligned} H_{\text{rot}} &\approx \frac{1}{4} \sum_{i < j} J_{ij} (\sigma_+^i \sigma_-^j + \sigma_-^i \sigma_+^j) \\ &= \sum_{i < j} \frac{J_{ij}}{2} (\sigma_x^i \sigma_x^j + \sigma_y^i \sigma_y^j) \end{aligned} \quad (3.5)$$

This approach works well whenever the rotating wave approximation is valid and separate tunability of the XX, and the YY terms are not required. However, the mapping is stroboscopic since the frame rotates at the Larmor frequency $\omega_L = 2\pi B_{\text{eff}}$, and therefore the measurements must be properly timed at specific intervals. This has been further analyzed by Kiely et al. in Ref. [117], and they numerically benchmarked this technique with five spins. They plot the overlap of the wave functions of the states $|\psi_{\text{Ising}}\rangle$ and $|\psi_{XY}\rangle$ with respect to the evolution time where $|\psi_{\text{Ising}}\rangle$ is the state evolving under H_{eff} and $|\psi_{XY}\rangle$ is the state evolving under H_{rot} both with the initial state $|\downarrow_z\rangle^{\otimes 5}$. They find that the optimal frequency where the wavefunction overlap is maximized is not at the Larmor frequency but at another optimized frequency that depends on the form of J_{ij} , the initial state, and the strength of the magnetic field. Regarding this optimized frequency, they also conclude that “it is not easy to know what it would be without solving the problem *a priori*”. Due to this, the only option is to time the stroboscopic measurements at the Larmor frequency, and hence, the approximation breaks down for large simulation times. Given these limitations and the lack of separate tunability for the $\sigma_x^i \sigma_x^j$ and $\sigma_y^i \sigma_y^j$ terms, this approach is limited in its applicability.

3.2.2 Spin dependent forces on orthogonal motional modes

The problems in the previous approach are, in principle, circumvented using spin-dependent forces along the three transverse axes of the trap and mediating three separate Ising interactions, one along each axis on the Bloch sphere to generate the Heisenberg model in Eq.

(3.2). The issue with this approach is that the beams that excite the motional modes in one direction (trap axis) should not excite the motional modes along the other trap axes. Theoretically, this might seem possible; however, practically this is very challenging. For example, a highly cited theoretical proposal [116] for simulating lattice gauge theories with trapped ions proposes doing so with several optical beams incident on the ions in various directions. The idea is to selectively address motional modes along different directions (trap principal axes) to generate the different Ising interactions; however, the optical engineering required to produce the beam configuration is quite daunting. Such configurations are not being used as of writing this thesis.

It may occur to the reader that the same optical beams could overlap with two trap axes and apply spin-dependent forces to orthogonal sets of motional modes, and if these orthogonal modes are separated in frequency, selective addressing could be achieved. This is in principle possible; however, the radial modes have to be highly separated and this is not always possible without pushing the trap out of the stability region. Moreover, the more ions that are added to the trap, the modes occupy more frequency “real estate”. Fig. 3.1 shows the simulated interaction profile for two separate Ising interactions (XX and YY) mediated on ten ions. The two detunings, μ_1, μ_2 , for the two spin-dependent forces, are chosen to mediate the power law interaction profiles through their respective modes; however, the cross-coupling of the interactions leads to a significant deviation from power law interaction profiles, especially in those mediated by the lower frequency motional modes. See Fig. 3.1 for more details.

3.2.3 Floquet Engineering

Before we start on Floquet engineering, let us first revisit an important formula for obtaining the exponential of the sum of non-commuting operators, the Lie formula,

$$e^{A+B} \neq e^A + e^B = \lim_{n \rightarrow \infty} (e^{A/n} e^{B/n})^n. \quad (3.6)$$

For quantum simulation, this means that if we want to simulate a Hamiltonian $H = \sum_k H_k$, then we have the following.

$$\begin{aligned} e^{iHt} &\approx \lim_{n \rightarrow \infty} \left(e^{iH_1 t/n} e^{iH_2 t/n} e^{iH_3 t/n} \dots e^{iH_k t/n} \right)^n \\ &= \left(e^{iH_1 t/n} e^{iH_2 t/n} e^{iH_3 t/n} \dots e^{iH_k t/n} \right)^n + \sum_{i,j}^k [H_i, H_j] t^2 / 2n. \end{aligned} \quad (3.7)$$

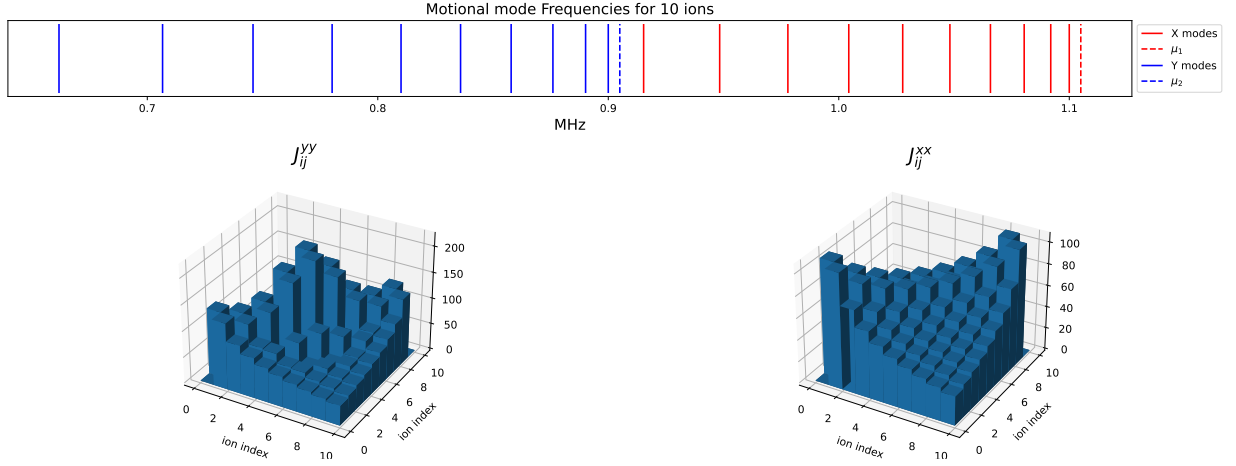


Figure 3.1: Two spin-dependent forces on orthogonal modes from the same beam

TOP: The solid lines represent normal mode frequencies for the two radial directions of the trap. μ_1 and μ_2 are the spin-dependent force frequencies in the X and Y direction, respectively. μ_1 , μ_2 are chosen to generate interaction profiles with power-law decay and are placed 5 kHz from the respective COM modes. Trap frequencies: $\omega_x = 2\pi \times 1.1$, $\omega_y = 2\pi \times 0.9$ MHz and $\omega_z = 2\pi \times 132.7$ kHz.

BOTTOM: Simulated interaction profiles for the X and Y directions with $\Omega_i = 2\pi \times 20$ kHz for all ions. Note that there is a significant contribution to the J_{ij}^y from the X modes that results in visibly different interaction profile.

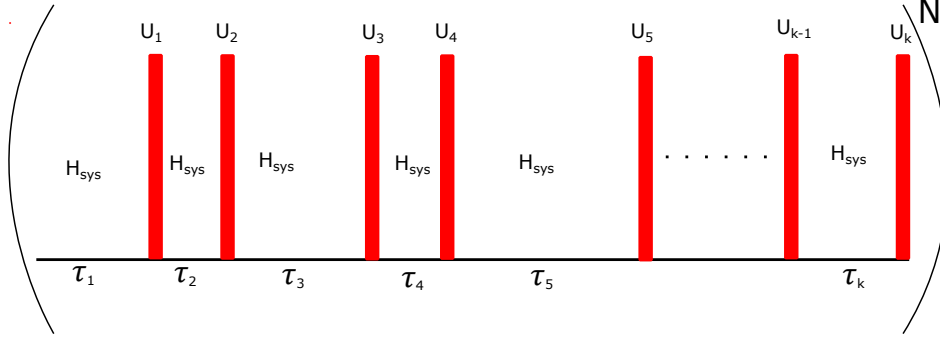


Figure 3.2: Floquet Sequence Schematic

The typical Floquet sequence comprises infinitesimally short pulses applied at times $t_1, t_2, \dots, t_k$, which implement unitaries $U_1, U_2 \dots U_k$. The whole sequence is repeated N times with the effective Hamiltonian being valid at times $t = NT_f$, where the Floquet time T_f is given as $T_f = \sum_n^k \tau_k$.

Here, the last line is valid for finite n [14]. This means that the evolution under H can be broken down into a sequential evolution under its constituents H_1, H_2 , etc., up to H_k and repeating n times. This idea was presented by Seth Lloyd in his seminal paper in 1996 [14] in the context of what is now referred to as digital quantum simulation, simulating a large many-body Hamiltonian, H by breaking down its evolution into sequential evolution under its local parts, i.e., H_k . Note that the Trotter error ($\epsilon \propto (t/n) \times t = \Delta t \times t$) grows linearly with simulation time t and decreases linearly with step size Δt .

The same idea of sequential evolution under different Hamiltonians is exploited in Floquet engineering. Here, operators in $\{H_k\}$ are not necessarily local and are generally transformed versions of the same Hamiltonian. The Hamiltonian for a Floquet system is

$$H(t) = H_{\text{sys}} + H_{\text{drive}} \quad (3.8)$$

Here, H_{sys} is the time-independent system Hamiltonian and H_{drive} is a periodic drive Hamiltonian such that $H_{\text{drive}}(t + NT) = H_{\text{drive}}$. Usually H_d is a set of pulses, very often $\pi/2$ -pulses, as shown in Fig. 3.2 and the evolution occurs under the system Hamiltonian in between the pulses. If each pulse performs a unitary U_n then the unitary of the control Hamiltonian, given as $U_{\text{drive}}(t)$, is

$$U_{drive}(t) = \begin{cases} U_0 & \text{if } t < t_1 \\ U_1 & \text{if } t_1 \leq t < t_2 \\ \vdots & \vdots \\ U_{k-1} \cdots U_0 & \text{if } t_{k-1} \leq t < t_k \\ U_k \cdots U_0 & \text{if } t = t_k \end{cases}. \quad (3.9)$$

For the sequence considered here, there is no zeroeth pulse, and hence $U_0 = \mathcal{I}$. We now transform into the interaction picture with respect to the Hamiltonian H_{drive} leading to an interaction Hamiltonian $\tilde{H}_{sys}(t)$ given as $\tilde{H}_{sys}(t) = U_{drive}(t)^\dagger H_{sys} U_{drive}(t)$.

$$\tilde{H}_{sys} = \begin{cases} U_0^\dagger H_{sys} U_0 & \text{if } t < t_1 \\ (U_1 U_0)^\dagger H_{sys} (U_1 U_0) & \text{if } t_1 \leq t < t_2 \\ \vdots & \vdots \\ (U_{k-1} \cdots U_0)^\dagger H_{sys} (U_{k-1} \cdots U_0) & \text{if } t_{k-1} \leq t < T \\ (U_k \cdots U_0)^\dagger H_{sys} (U_k \cdots U_0) & \text{if } t = T \end{cases}. \quad (3.10)$$

Note that the interaction Hamiltonian is time dependent and to calculate the evolution under this Hamiltonian, we need to calculate the following time-ordered exponential.

$$\begin{aligned} \tilde{U}_{sys}(T) &= \mathcal{T} \exp \left[-i \int_0^T \tilde{H}_{sys}(t) dt \right] \\ &\approx \exp \left[-\frac{i}{T} \int_0^T \tilde{H}_{sys}(t) dt \right] \\ &= \exp \left[-\frac{i}{T} \int_0^{t_1} \tilde{H}_{sys}(t) dt - \frac{i}{T} \int_{t_1}^{t_2} \tilde{H}_{sys}(t) dt \cdots - \frac{i}{T} \int_{t_{k-1}}^T \tilde{H}_{sys}(t) dt \right] \\ &= \exp \left[-i \sum_{n=0}^k \tilde{H}_{sys}^n \tau_n \right]. \end{aligned} \quad (3.11)$$

In the second line above, we have truncated to the first order in the Magnus expansion for calculating the time-ordered exponential. And $\tilde{H}_{sys}^n = (U_{n-1} \cdots U_0)^\dagger H_{sys} (U_{n-1} \cdots U_0)$ and $\tau_n = (t_n - t_{n-1})$.

From the last line, we can see that the effective Hamiltonian for the sequence at time T is

$$H_f = \frac{1}{T} \sum_{n=0}^k \tilde{H}_{sys}^n \tau_n \quad (3.12)$$

So, the Floquet system behaves as if evolving under the effective Hamiltonian H_f at times $t = NT$, which are the chosen times for performing measurements. Usually, the sequence of pulses is chosen such that $\prod_{n=1}^k U_n = \mathcal{I}$, which ensures that the system is back in the lab frame when the measurements are performed. A simple example of such a protocol for a system that has an inherent XX interaction is four pulses $(Y, \pi/2)$, $(X, \pi/2)$, $(X, -\pi/2)$, $(Y, -\pi/2)$, and it is easy to see that this would simulate the Heisenberg model given in Eq. (3.2).

The ideas behind the Floquet engineering approach come from the decades-old concepts of average Hamiltonian theory (AHT) [118] and composite pulses [119, 120, 121], developed in the nuclear magnetic resonance (NMR) literature. Trapped ions offer a unique advantage for programmable simulations using Floquet methods; unlike NMR or Rydberg atom systems, the system Hamiltonian can also be changed over time, and few implementations of this technique on trapped ions have utilized this feature [122, 123]. However, the Floquet method has not been widely adopted on the trapped ion platform primarily because of the inadvertent motional heating that comes as a side effect of these periodic drives. Since this is the only close to feasible method for simulating the anisotropic XY model that allows tunable anisotropy, we made a comparison of the Floquet method with our approach, and this comparison is presented towards the end of the chapter. We, too, concluded that the Floquet drives lead to high motional excitation, leading to a breakdown of the quantum simulation, and it is difficult to predict when such excitation occurs.

3.3 Parallel spin-dependent forces on same motional modes

3.3.1 Theory

In this section, I will derive how two parallel spin dependent forces on trapped ions lead to parallel XY-type couplings. The idea is to apply two spin-dependent forces with different spin phases, one generating XX-Ising interactions and the other generating YY-Ising interactions. We start with the system and motional modes in one direction.

$$H_{\text{system}} = \sum_i^N \frac{\omega_{hf}}{2} \sigma_z^i + \sum_{m=1}^N \omega_m a_m^\dagger a_m$$

Again, ω_{hf} is the frequency difference between the qubit states, and ω_m is the frequency of the m^{th} motional mode. To study the action of parallel spin-dependent forces of spin, we proceed with applying two symmetrically detuned red and blue sidebands, i.e., four different frequencies of light. The Hamiltonian for the light-ion interaction is as follows:

$$\begin{aligned} H_{\text{lm}} &= H_{\text{RSB}}^1 + H_{\text{BSB}}^1 + H_{\text{RSB}}^2 + H_{\text{BSB}}^2 \\ \text{where,} \\ H_{\text{RSB}}^1 + H_{\text{BSB}}^1 &= \sum_i \Omega_i^x \cos(k_x x_i - \omega_r^1 t + \phi_r^1) \sigma_x^i + \sum_i \Omega_i^x \cos(k_x x_i - \omega_b^1 t + \phi_b^1) \sigma_x^i \\ H_{\text{RSB}}^2 + H_{\text{BSB}}^2 &= \sum_i \Omega_i^y \cos(k_x x_i - \omega_r^2 t + \phi_r^2) \sigma_y^i + \sum_i \Omega_i^y \cos(k_x x_i - \omega_b^2 t + \phi_b^2) \sigma_y^i. \end{aligned} \quad (3.13)$$

Here, k_x is the x component of the laser wavevector⁴, x_i is the x coordinate of the i^{th} ion, $\phi_r^1, \phi_b^1, \phi_r^2, \phi_b^2$ are the respective laser phases, laser frequencies⁵ $\omega_r^1 = \omega_{hf} - \mu_1$, $\omega_b^1 = \omega_{hf} + \mu_1$, $\omega_r^2 = \omega_{hf} - \mu_2$, $\omega_b^2 = \omega_{hf} + \mu_2$ and μ_1, μ_2 are the detunings used for spin-dependent forces 1 and 2.

Going into the interaction picture with respect to the H_{system} and proceeding in a similar way as in the derivation of Eq. (2.31), we get

$$\begin{aligned} H_{2\text{SDF}} &= - \sum_i \Omega_i^x \cos(\mu_1 t) \sigma_y^i \\ &\quad + \sum_i \Omega_i^y \cos(\mu_2 t) \sigma_x^i \\ &\quad + \sum_{im} \eta_{im} \Omega_i^x \cos(\mu_1 t) (a_m e^{-i\omega_m t} + a_m^\dagger e^{i\omega_m t}) \sigma_x^i \\ &\quad + \sum_{im} \eta_{im} \Omega_i^y \cos(\mu_2 t) (a_m e^{-i\omega_m t} + a_m^\dagger e^{i\omega_m t}) \sigma_y^i. \end{aligned} \quad (3.14)$$

The above Hamiltonian is the result of the specific choice $\phi_r^1 = -\pi/2$, $\phi_b^1 = -\pi/2$, $\phi_r^2 = 0$, $\phi_b^2 = 0$ in Eq. (3.13). This results in the spin phase for the first spin-dependent force to be zero, and we get a σ_x^i dependent force. Similarly, for the second spin-dependent force, we get a spin phase of $\pi/2$, resulting in a σ_y^i dependent force. The last two terms

⁴In the case of two-photon Raman transitions this is the difference between the k vectors of the two Raman beams

⁵For Raman transitions these are the beatnote frequencies

represent the spin-dependent forces that we are interested in, and the first two terms are the associated off-resonant carrier excitation that accompanies the forces (see derivation of Eq. (2.31)). The σ_x^i dependent force causes off-resonant excitation of the spins along σ_y^i , and the σ_y^i dependent force causes off-resonant excitation of the spins along σ_x^i , which is a direct consequence of the $\pi/2$ phase shift in the carrier and sideband terms.

We assume that the application of the two spin-dependent forces occurs in the regime such that $\Omega_i^{x/y} \ll \mu_{1/2}$ and we can safely dismiss the first two off-resonant carrier terms leading to the final Hamiltonian,

$$\begin{aligned}
H &= H_x + H_y, \\
\text{where,} \\
H_x &= \sum_{i,m} \eta_{im} \Omega_i^x \cos(\mu_1 t) (\hat{a}_m e^{-i\omega_m t} + \hat{a}_m^\dagger e^{i\omega_m t}) \sigma_x^i, \\
H_y &= \sum_{i,m} \eta_{im} \Omega_i^y \cos(\mu_2 t) (\hat{a}_m e^{-i\omega_m t} + \hat{a}_m^\dagger e^{i\omega_m t}) \sigma_y^i.
\end{aligned} \tag{3.15}$$

To calculate the effective Hamiltonian from this beam configuration, we use the Magnus expansion and proceed in a similar way as in the derivation of Eq. (2.36).

$$U(t) = \mathcal{T} \left\{ \exp \left(-i \int_0^t dt_1 H(t_1) \right) \right\} = \exp \left(\tilde{\Omega}_1 + \tilde{\Omega}_2 + \tilde{\Omega}_3 + \dots \right)$$

where $\mathcal{T}$ is the time ordering operator and the operators $\tilde{\Omega}_i$ are given as

$$\begin{aligned}
\tilde{\Omega}_1 &= -i \int_0^t dt_1 H(t_1) \\
\tilde{\Omega}_2 &= -\frac{1}{2} \int_0^t dt_1 \int_0^{t_1} dt_2 [H(t_1), H(t_2)] \\
\tilde{\Omega}_3 &= -\frac{i}{6} \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 ([H(t_1), [H(t_2), H(t_3)]] + [H(t_3), [H(t_2), H(t_1)]])
\end{aligned}$$

And so on.

As before, the first-order terms lead to spin phonon entanglement where the phonon part has the form of a displacement operator.

$$\tilde{\Omega}_1 = - \sum_{i,m} \sigma_x^i (\alpha_{i,m}^x a_m^\dagger - \overline{\alpha_{i,m}^x} a_m) - \sum_{i,m} \sigma_y^i (\alpha_{i,m}^y a_m^\dagger - \overline{\alpha_{i,m}^y} a_m) \tag{3.16}$$

Where

$$\alpha_{im}^x = \frac{\eta_{im}\Omega_i^x}{2\delta_m^x} (e^{-i\delta_m^x t} - 1)$$

and

$$\alpha_{im}^y = \frac{\eta_{im}\Omega_i^y}{2\delta_m^y} (e^{-i\delta_m^y t} - 1),$$

where $\delta_m^x = \mu_1 - \omega_m$ and $\delta_m^y = \mu_2 - \omega_m$. In the limit where $\delta_m^{x/y} \gg \eta_{im}\Omega_i^{x/y}$ the displacements become negligible, and the contribution of the first-order term in the Magnus expansion, $\tilde{\Omega}_1$, can be safely ignored.

In the analysis of a single spin-dependent force (see Eq. 2.31), it was the second term that led to the spin-spin interactions. Here too, the second-order term gives the required XX and YY couplings, however, there are several unwanted terms that appear.

$$\begin{aligned} [H(t_1), H(t_2)] &= [H_x(t_1) + H_y(t_1), H_x(t_2) + H_y(t_2)] \\ &= [H_x(t_1), H_x(t_2)] + [H_y(t_1), H_y(t_2)] \\ &\quad + [H_x(t_1), H_y(t_2)] + [H_y(t_1), H_x(t_2)]. \end{aligned} \tag{3.17}$$

The first two terms lead to expressions similar to those seen before (See Eq. (2.4))

$$\begin{aligned} &[H_x(t_1), H_x(t_2)] + [H_y(t_1), H_y(t_2)] \\ &= \sum_{ijm} \eta_{im}\eta_{jm}\Omega_i^x\Omega_j^x\sigma_x^i\sigma_x^j \\ &\quad \times \cos(\mu_1 t_1) \cos(\mu_1 t_2) (e^{-i\omega_m(t_1-t_2)} - e^{-i\omega_m(t_2-t_1)}) \\ &+ \sum_{ijm} \eta_{im}\eta_{jm}\Omega_i^y\Omega_j^y\sigma_y^i\sigma_y^j \\ &\quad \times \cos(\mu_2 t_1) \cos(\mu_2 t_2) (e^{-i\omega_m(t_1-t_2)} - e^{-i\omega_m(t_2-t_1)}). \end{aligned} \tag{3.18}$$

To simplify the analysis for analyzing the next two terms, we first begin by applying a

rotating wave approximation to Eq. (3.15). Expanding the cosine in Eq. (3.15) we get,

$$H = H_x + H_y,$$

where,

$$\begin{aligned} H_x &= \sum_{i,m} \frac{\eta_{im} \Omega_i^x}{2} (\hat{a}_m (e^{i(\mu_1 - \omega_m)t} + e^{-i(\mu_1 + \omega_m)t}) + \hat{a}_m^\dagger (e^{i(\mu_1 + \omega_m)t} + e^{-i(\mu_1 - \omega_m)t})) \sigma_x^i, \\ H_y &= \sum_{i,m} \frac{\eta_{im} \Omega_i^y}{2} (\hat{a}_m (e^{i(\mu_2 - \omega_m)t} + e^{-i(\mu_2 + \omega_m)t}) + \hat{a}_m^\dagger (e^{i(\mu_2 + \omega_m)t} + e^{-i(\mu_2 - \omega_m)t})) \sigma_y^i. \end{aligned} \quad (3.19)$$

Now substituting $\delta_m^x = \mu_1 - \omega_m$ and $\delta_m^y = \mu_2 - \omega_m$ and discarding the terms with exponentials oscillating at $(\mu_{x/y} + \omega_m)$ we get

$$\begin{aligned} H &= H_x + H_y, \\ \text{where,} \\ H_x &= \sum_{i,m} \eta_{im} \Omega_i^x (a_m e^{i\delta_m^x t} + a_m^\dagger e^{-i\delta_m^x t}) \sigma_x^i, \\ H_y &= \sum_{i,m} \eta_{im} \Omega_i^y (a_m e^{i\delta_m^y t} + a_m^\dagger e^{-i\delta_m^y t}) \sigma_y^i. \end{aligned} \quad (3.20)$$

With this simplified Hamiltonian, the cross terms in Eq. (3.17) are

$$\begin{aligned} &[H_x(t_1), H_y(t_2)] + [H_y(t_1), H_x(t_2)] \\ &= \left[\sum_{i,m} \eta_{im} \Omega_i^x (a_m e^{i\delta_m^x t_1} + a_m^\dagger e^{-i\delta_m^x t_1}) \sigma_x^i, \sum_{j,n} \eta_{jn} \Omega_j^y (a_n e^{i\delta_n^y t_2} + a_n^\dagger e^{-i\delta_n^y t_2}) \sigma_y^j \right] \\ &+ \left[\sum_{i,m} \eta_{im} \Omega_i^y (a_m e^{i\delta_m^y t_1} + a_m^\dagger e^{-i\delta_m^y t_1}) \sigma_y^i, \sum_{j,n} \eta_{jn} \Omega_j^x (a_n e^{i\delta_n^x t_2} + a_n^\dagger e^{-i\delta_n^x t_2}) \sigma_x^j \right] \end{aligned}$$

$$\begin{aligned}
&= \sum_{i,m,n} \eta_{im} \eta_{in} \Omega_i^x \Omega_i^y (a_m e^{i\delta_m^x t_1} + a_m^\dagger e^{-i\delta_m^x t_1}) (a_n e^{i\delta_n^y t_2} + a_n^\dagger e^{-i\delta_n^y t_2}) [\sigma_x^i, \sigma_y^j] \\
&+ \sum_{i,m,n} \eta_{im} \eta_{in} \Omega_i^x \Omega_i^y (a_m e^{i\delta_m^x t_2} + a_m^\dagger e^{-i\delta_m^x t_2}) (a_n e^{i\delta_n^y t_1} + a_n^\dagger e^{-i\delta_n^y t_1}) [\sigma_y^i, \sigma_x^j] \\
&+ \sum_{i,j,m} \eta_{im} \eta_{jm} \Omega_i^x \Omega_i^y \left[(a_m e^{i\delta_m^x t_1} + a_m^\dagger e^{-i\delta_m^x t_1}), (a_m e^{i\delta_m^y t_2} + a_m^\dagger e^{-i\delta_m^y t_2}) \right] \sigma_x^i \sigma_y^j \\
&+ \sum_{i,j,m} \eta_{im} \eta_{jm} \Omega_i^x \Omega_i^y \left[(a_m e^{i\delta_m^y t_1} + a_m^\dagger e^{-i\delta_m^y t_1}), (a_m e^{i\delta_m^x t_2} + a_m^\dagger e^{-i\delta_m^x t_2}) \right] \sigma_x^i \sigma_y^j \\
&= 2i \sum_{i,m,n} \eta_{im} \eta_{in} \Omega_i^x \Omega_i^y (a_m e^{i\delta_m^x t_1} + a_m^\dagger e^{-i\delta_m^x t_1}) (a_n e^{i\delta_n^y t_2} + a_n^\dagger e^{-i\delta_n^y t_2}) \sigma_z^i \\
&- 2i \sum_{i,m,n} \eta_{im} \eta_{in} \Omega_i^x \Omega_i^y (a_m e^{i\delta_m^x t_2} + a_m^\dagger e^{-i\delta_m^x t_2}) (a_n e^{i\delta_n^y t_1} + a_n^\dagger e^{-i\delta_n^y t_1}) \sigma_z^i \\
&+ \sum_{i,j,m} \eta_{im} \eta_{jm} \Omega_i^x \Omega_i^y \left(e^{i(\delta_m^x t_1 - \delta_m^y t_2)} - e^{-i(\delta_m^x t_1 - \delta_m^y t_2)} \right) \sigma_x^i \sigma_y^j \\
&+ \sum_{i,j,m} \eta_{im} \eta_{jm} \Omega_i^x \Omega_i^y \left(e^{i(\delta_m^y t_1 - \delta_m^x t_2)} - e^{-i(\delta_m^y t_1 - \delta_m^x t_2)} \right) \sigma_x^i \sigma_y^j \\
&= 2i \sum_{i,m,n} \eta_{im} \eta_{in} \Omega_i^x \Omega_i^y (a_m e^{i\delta_m^x t_1} + a_m^\dagger e^{-i\delta_m^x t_1}) (a_n e^{i\delta_n^y t_2} + a_n^\dagger e^{-i\delta_n^y t_2}) \sigma_z^i \\
&- 2i \sum_{i,m,n} \eta_{im} \eta_{in} \Omega_i^x \Omega_i^y (a_m e^{i\delta_m^x t_2} + a_m^\dagger e^{-i\delta_m^x t_2}) (a_n e^{i\delta_n^y t_1} + a_n^\dagger e^{-i\delta_n^y t_1}) \sigma_z^i \tag{3.21} \\
&+ 2i \sum_{i,j,m} \eta_{im} \eta_{jm} \Omega_i^x \Omega_i^y \sigma_x^i \sigma_y^j (\sin(\delta_m^x t_1 - \delta_m^y t_2) + \sin(\delta_m^y t_1 - \delta_m^x t_2)).
\end{aligned}$$

Now that we have evaluated the commutators in Eq. (3.17), we simply have to integrate these to find $\tilde{\Omega}_2$. Looking at the form of the commutators we can write $\tilde{\Omega}_2$ as the following

$$\begin{aligned}
\tilde{\Omega}_2 = \exp & \left(-it \sum_{i < j} J_{ij}^x \sigma_x^i \sigma_x^j - it \sum_{i < j} J_{ij}^y \sigma_y^i \sigma_y^j \right. \\
& \left. + \sum_{i,j} \Lambda_{ij}(t) \sigma_x^i \sigma_y^j + \sum_i \hat{\zeta}_i(t) \sigma_z^i \right). \tag{3.22}
\end{aligned}$$

The first two terms above come from integrating Eq. (3.18) and are exactly the same as those performed in the last chapter (Eq. (2.34)). These lead to two “secular terms” i.e. terms proportional to t that contribute to the effective Hamiltonian giving parallel XX and YY Ising interactions. The last two terms come from integrating Equation 3.21 and contain pure spin-spin and spin-phonon terms.

We first note that all the terms in $\Lambda_{ij}(t)$ and $\hat{\zeta}_i(t)$ are oscillatory in nature and do not have any linear term in t . Moreover, all terms have an amplitude that is small in the limit $\delta_m^{x/y} \gg \eta_{im}\Omega_i^{x/y}$. The only terms that could have a large amplitude and hence offset the expected dynamics are in $\Lambda_{ij}(t)$ and these come from the last term in Eq. (3.21). Evaluating the integrals, we see that.

$$|\Lambda_{ij}(t)| \propto \left| \frac{J_{ij}^x J_{ij}^y}{\delta_m^x - \delta_m^y} \right| = \left| \frac{J_{ij}^x J_{ij}^y}{\mu_1 - \mu_2} \right|. \quad (3.23)$$

Hence, in the limit where $|\mu_1 - \mu_2| \gg \max_{i,j}(|J_{ij}^x|)$ and $|\mu_1 - \mu_2| \gg \max_{i,j}(|J_{ij}^y|)$, the contribution from the cross terms to $\tilde{\Omega}_2$ can be neglected and only the first two terms in Eq. (3.23) contribute to the effective Hamiltonian.

$$H_{\text{eff}} = \sum_{i < j} J_{ij}^x \sigma_x^i \sigma_x^j + \sum_{i < j} J_{ij}^y \sigma_y^i \sigma_y^j, \quad (3.24)$$

with,

$$J_{ij}^x = \sum_m \frac{\eta_{im}\eta_{jm}\Omega_i^x\Omega_j^x}{\mu_1^2 - \omega_m^2} \omega_m, \quad J_{ij}^y = \sum_m \frac{\eta_{im}\eta_{jm}\Omega_i^y\Omega_j^y}{\mu_2^2 - \omega_m^2} \omega_m.$$

When,

$$|\mu_1 - \mu_2| \gg \max_{i,j}(|J_{ij}^x|), \quad |\mu_1 - \mu_2| \gg \max_{i,j}(|J_{ij}^y|). \quad (3.25)$$

It should be noted that the constraint in Eq. (3.25) should be satisfied on top of the constraint for applying each of the two spin-dependent forces in the slow regime, i.e. $\delta_m^x \gg \eta_{im}\Omega_i^x$ and $\delta_m^y \gg \eta_{im}\Omega_i^y \forall i$ (see Sec. 2.4). In the single spin-dependent force case, the commutators in the higher-order terms in the magnus expansion were zero, but in the case with multiple spin-dependent forces this is not the case. For the multiple spin dependent case the magnus expansion does not terminate; however, looking at second-order terms, the higher-order terms are expected to be oscillatory. In the next section, we will perform numerical simulations to test the accuracy of the effective Hamiltonian derived above.

3.3.2 Numerical simulations

The main insight of the above analysis is that the same set of motional modes can mediate parallel Ising interactions through two spin-dependent forces applied simultaneously. To test the veracity of this finding, we decided to simulate the action of such forces on a system of ions. The smallest system that can be used to test this is two ions and one motional mode, and in this section I will present numerical simulations of the Hamiltonian in Eq. (3.15) for two ions and a single motional mode.

The simulation package was written in Python and makes use of the Python package qutip [124] for time evolutions of the time-dependent Hamiltonian. It allows the simulation of multiple spin-dependent forces on an arbitrary number of ions within the limitation of the device RAM and processing resources. As a test, we shall look at the time evolution under a single spin-dependent force that generates only the XX Ising terms. The simulation parameters used for this test were $\omega_m = 2\pi \times 1$ MHz, $\mu = 2\pi \times 1.02$ MHz, and $\eta_i = 0.1 \forall i$. We assume an equal rabi frequency at all the ions, and the motional mode corresponds to a center of mass mode. Under the action of such a force, we expect the dynamics to be determined by the effective Hamiltonian in Eq. (2.36), which is the same as Eq. (3.24) with $\Omega_i^y = 0 \forall i$. The effective Hamiltonian for the two-ion case is

$$H_{\text{eff}} = J_{12}^x \sigma_x^1 \sigma_x^2 = \frac{\eta^2 \Omega^2 \omega_m}{\mu^2 - \omega_m^2} \sigma_x^1 \sigma_x^2. \quad (3.26)$$

The dynamics expected from the Hamiltonian is the following:

$$\begin{aligned} U_{XX} |\downarrow\downarrow\rangle &= \cos(J_{12}^x t) |\downarrow\downarrow\rangle - i \sin(J_{12}^x t) |\uparrow\uparrow\rangle \\ U_{XX} |\uparrow\uparrow\rangle &= \cos(J_{12}^x t) |\uparrow\uparrow\rangle - i \sin(J_{12}^x t) |\downarrow\downarrow\rangle \\ U_{XX} |\downarrow\uparrow\rangle &= \cos(J_{12}^x t) |\downarrow\uparrow\rangle - i \sin(J_{12}^x t) |\uparrow\downarrow\rangle \\ U_{XX} |\uparrow\downarrow\rangle &= \cos(J_{12}^x t) |\uparrow\downarrow\rangle - i \sin(J_{12}^x t) |\downarrow\uparrow\rangle. \end{aligned} \quad (3.27)$$

If we initialize the ions in $|\downarrow\downarrow\rangle$ we expect coherent oscillations between $|\downarrow\downarrow\rangle$ and $|\uparrow\uparrow\rangle$. Fig. 3.3 shows the dynamics for two ions initialized in $|\downarrow\downarrow\rangle$ under the action of a σ_x spin-dependent force. The phonon Hilbert space is truncated to 5 quanta since the off resonant driving of the motion only virtually excites the $n > 0$ levels and higher occupation of motional levels is not expected. Dynamics for both the effective Hamiltonian and the spin-phonon Hamiltonian are plotted where the initial state for the effective Hamiltonian simulation is $|\downarrow\downarrow\rangle$, and the initial state for the spin-phonon Hamiltonian is $|\downarrow\downarrow\rangle \otimes |n=0\rangle$

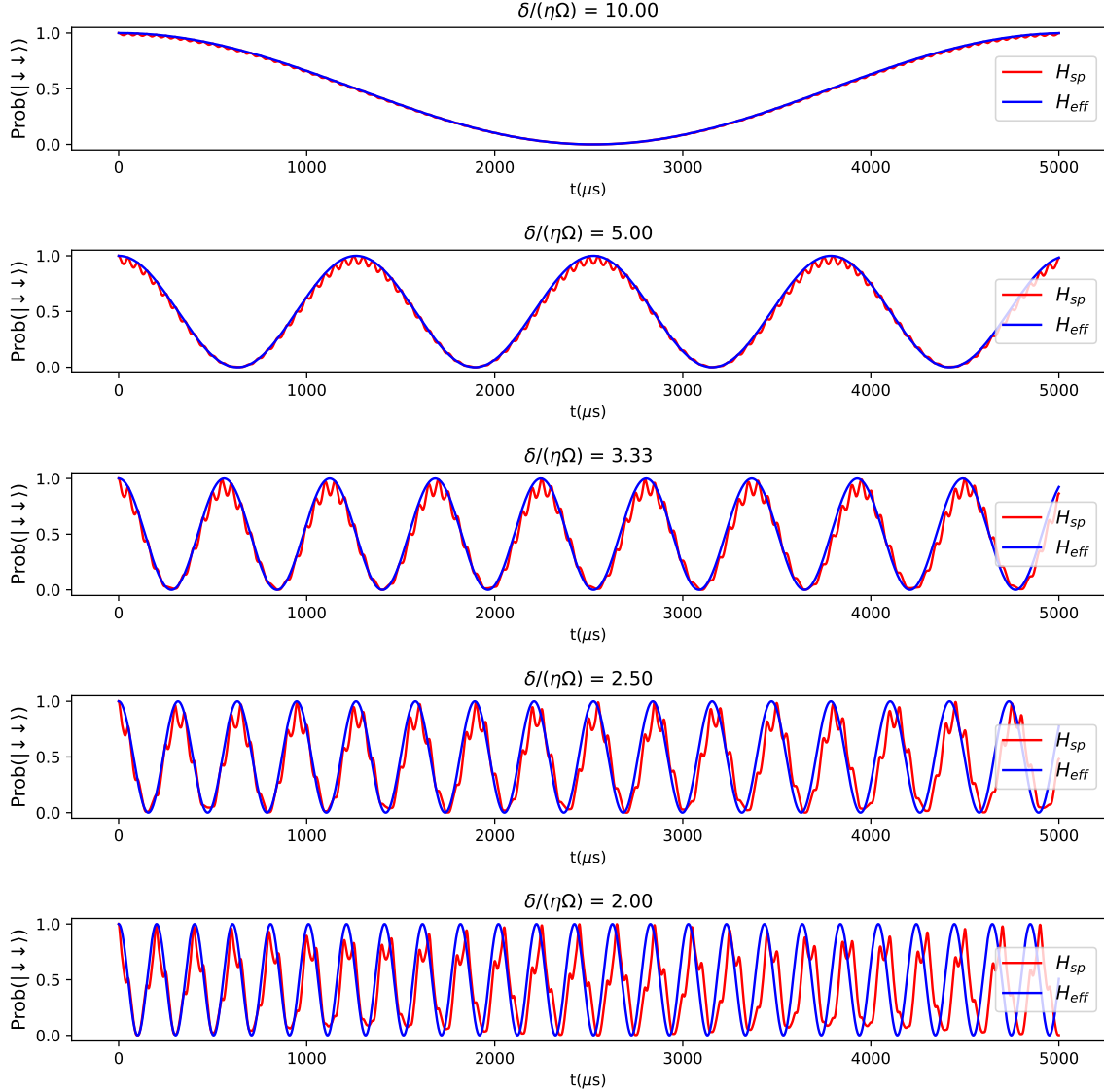


Figure 3.3: Testing simulation with single σ_x spin-dependent force

Numerical simulations of a single spin-dependent force on two ions and one motional mode; see text for simulation parameters. For $\delta = |\mu - \omega_m| = 10 \times \eta\Omega$, the behavior is almost exactly the same as predicted from the effective Hamiltonian in Eq. (2.36). As $\delta/(\eta\Omega)$ decreases, the dynamics deviate from that of the effective Hamiltonian as expected. This is because the requirement for applying the spin-dependent force in the slow regime is not satisfied anymore (See Sec. 2.4).

where $|n = 0\rangle$ is the ground state of motion. The probabilities for $|\downarrow\downarrow\rangle$ state plotted in Fig. 3.3 are the expectation value of $|\downarrow\downarrow\rangle\langle\downarrow\downarrow|$ for the effective Hamiltonian and $|\downarrow\downarrow\rangle\langle\downarrow\downarrow| \otimes \mathbb{I}$ for the spin-phonon case. The Rabi frequency on the two ions is varied from low to $2\pi \times 20$ kHz to $2\pi \times 100$ kHz, so we start in the slow regime given by $\delta = |\mu - \omega_m| = 10 \times \eta\Omega$ and increase to $\delta = 2 \times \eta\Omega$. When $\delta = 10 \times \eta\Omega$, the time evolution is almost exactly as expected from the effective Hamiltonian, and as $\delta/(\eta\Omega)$ decreases, in this case increasing Ω , we see the high-frequency wiggles appear in the population dynamics because the contribution of the first order term in the Magnus expansion (see Eq. (2.33)) becomes non-negligible.

The above behavior is well known, and the purpose of these simulations was simply to ensure that the numerical simulation package captured the expected dynamics observed in the experiments. We will now see the simulation results for the case of two spin-dependent forces, one mediating the XX-Ising interaction and the other mediating a YY-Ising interaction. Based on the discussion in the previous section, we expect the effective Hamiltonian in the slow regime ($|\mu_1 - \omega_m| \gg \eta_{im}\Omega_i^x$, $|\mu_2 - \omega_m| \gg \eta_{im}\Omega_i^y$) to be as follows.

$$\begin{aligned} H_{\text{eff}}^{\text{XY}} &= J_{12}^x \sigma_x^1 \sigma_x^2 + J_{12}^y \sigma_y^1 \sigma_y^2 \\ &= \frac{\eta\Omega_1^x \Omega_2^x \omega_1}{\mu_1^2 - \omega_1^2} \sigma_x^1 \sigma_x^2 + \frac{\eta\Omega_1^y \Omega_2^y \omega_1}{\mu_2^2 - \omega_1^2} \sigma_y^1 \sigma_y^2 \end{aligned} \quad (3.28)$$

Where ω_1 is the frequency of the single motional mode included in the simulations, and $\eta = \eta_{11} = \eta_{21} = \delta k_x \sqrt{\hbar/2m\omega_1}$. The expected dynamics from the above Hamiltonian, with $U_{XY} = e^{-iH_{\text{eff}}^{\text{XY}}t}$, are the following.

$$\begin{aligned} U_{XY} |\downarrow\downarrow\rangle &= \cos(\tau(J_{12}^x - J_{12}^y)) |\downarrow\downarrow\rangle - i \sin(\tau(J_{12}^x - J_{12}^y)) |\uparrow\uparrow\rangle \\ U_{XY} |\uparrow\uparrow\rangle &= \cos(\tau(J_{12}^x - J_{12}^y)) |\uparrow\uparrow\rangle - i \sin(\tau(J_{12}^x - J_{12}^y)) |\downarrow\downarrow\rangle \\ U_{XY} |\downarrow\uparrow\rangle &= \cos(\tau(J_{12}^x + J_{12}^y)) |\downarrow\uparrow\rangle - i \sin(\tau(J_{12}^x + J_{12}^y)) |\uparrow\downarrow\rangle \\ U_{XY} |\uparrow\downarrow\rangle &= \cos(\tau(J_{12}^x + J_{12}^y)) |\uparrow\downarrow\rangle - i \sin(\tau(J_{12}^x + J_{12}^y)) |\downarrow\uparrow\rangle \end{aligned} \quad (3.29)$$

Looking at the above equations, we see that the Hamiltonian drives the oscillations between $|\downarrow\downarrow\rangle$ and $|\uparrow\uparrow\rangle$ and also between $|\downarrow\uparrow\rangle$ and $|\uparrow\downarrow\rangle$. Note that the population in $\{ |\downarrow\downarrow\rangle, |\uparrow\uparrow\rangle \}$ subspace does not leak into the $\{ |\downarrow\uparrow\rangle, |\uparrow\downarrow\rangle \}$ subspace under the action of $H_{\text{eff}}^{\text{XY}}$. When initialized in $|\downarrow\downarrow\rangle$ or $|\uparrow\uparrow\rangle$, the oscillations occur at a frequency of $(J_{12}^x - J_{12}^y)$, similarly initializing in $|\downarrow\uparrow\rangle$ or $|\uparrow\downarrow\rangle$ the oscillations occur at a frequency $(J_{12}^x + J_{12}^y)$. The rate of oscillations in these two subspaces yields a simple qualitative benchmark for testing the dynamics under this Hamiltonian. If we have $(J_{12}^x = J_{12}^y)$, the population oscillations with

the initial state $|\downarrow\downarrow\rangle$ ($|\uparrow\uparrow\rangle$) will be suppressed; however, when initialized in $|\downarrow\uparrow\rangle$ ($|\uparrow\downarrow\rangle$), the population oscillations will persist.

Fig. 3.4 a) shows the schematic of the applied drives, i.e., two symmetrically detuned red and blue sideband beat notes. At the level of Eq. (3.15), it does not matter; however, we call these beat notes instead of laser frequencies because the experiments in the next section were done with Raman transitions, and the frequency of the beat note is the quantity of interest from the point of view of the spins/qubits. The applied beat notes generate spin-dependent forces at frequencies μ_1 (for coupling to σ_x spin components) and μ_2 (for coupling to σ_y spin components)⁶. The time evolution shown in (b) - (d) is calculated for the initial state $|\downarrow\downarrow\rangle \otimes |n=0\rangle$ and the probability is calculated as the expectation value of $|\downarrow\downarrow\rangle \langle\downarrow\downarrow| \otimes \mathbb{I}$. Here, $\omega_1 = 2\pi \times 1.1$ MHz, $\mu_1 = 2\pi \times 1.108$ MHz, $\psi_i^x = \psi_i^y = 0$, $\eta_{i1} = 0.0648$, and $\Omega_i^x = 2\pi \times 15$ kHz ($i = 1, 2$). Ω_i^x is chosen to generate $J_{12}^x \approx 2\pi \times 60$ Hz (calculated from Eq. 3.24 and we truncate the motional Hilbert space to up to four phonons (five levels)).

The values for the specific numerical simulations presented here were chosen to align with the experimental results shown in the next section. Fig. 3.4 (b) shows the time evolution for $\mu_1 = \mu_2$ and $\Omega_i^x = \Omega_i^y$ for $i = 1, 2$. When $\mu_1 = \mu_2$, the dynamics correspond to that of a single spin-dependent force, and we observe oscillations between $|\downarrow\downarrow\rangle$ and $|\uparrow\uparrow\rangle$. The high-frequency oscillations are again from the contribution of the first-order term in the Magnus expansion as seen before in the case of the single spin-dependent force in Fig. 3.3.

Fig. 3.4 (c) shows the time evolution for $\Omega_i^x = \Omega_i^y$ and $|\mu_1 - \mu_2| \approx J_{12}^x$. This is chosen to specifically violate the constraint, Eq. (3.25), in the derivation of the effective Hamiltonian in Eq. (3.25). Since the constraint for the validity of the effective Hamiltonian is not satisfied, we see deviations from the dynamics under the effective Hamiltonian. When $|\mu_1 - \mu_2| \approx J_{12}^x$, the amplitude $|\Lambda_{12}(t)|$ in Eqs. (3.22) and (3.23) is non-negligible and significant contributions from terms like $\sigma_x^1 \sigma_y^2$ are expected. Note that the high-frequency oscillations, from the first-order terms in the magnus expansion, are not expected to grow when $|\mu_1 - \mu_2| \approx J_{12}^x$ and this is evident from the similar scale of these oscillations in (b) and (c).

Finally, Fig. 3.4 (d) shows the time evolution for $|\mu_1 - \mu_2| \gg J_{12}^x$ ($\mu_2 = 2\pi \times 1.105$ MHz) where the constraint (Eq. (3.25)) for the validity of our effective Hamiltonian is satisfied. We set $\Omega_i^y = 2\pi \times 12.2$ kHz for $i = 1, 2$ to set $J_{12}^x = J_{12}^y$ and observe the dynamics

⁶To align with the theory presented above, I chose $\phi_r^x = \phi_b^x = 0$, $\phi_r^y = \phi_b^y = -\pi/2$ yielding zero motional phases for both forces and spin phases of 0 and $\pi/2$ respectively for the σ_x dependent force and the σ_y dependent force.

of the effective XY Hamiltonian, i.e. the lack of oscillations between $|\downarrow\downarrow\rangle$ and $|\uparrow\uparrow\rangle$ and when initialized in $|\downarrow\uparrow\rangle$ or $|\uparrow\downarrow\rangle$ (not shown here), the population oscillations recover. We note that the exact value of Ω_i^y required to set $J_{12}^x = J_{12}^y$ deviates from the value calculated from Eq. (3.24) at about 5% level based on several simulations performed. This deviation is again attributed to the non-negligible contribution of the first order term in the magnus expansion causing AC stark shifts and hence shifting the qubit frequency used in Eq. (3.24) to calculate the strengths of the couplings⁷.

3.3.3 Experimental Results

To validate the findings in the previous sections, we tested the protocol experimentally on two $^{171}\text{Yb}^+$ ions. The application of spin-dependent forces and coherent operations are performed through 2-photon Raman transitions with a 355 nm pulsed laser with a repetition rate of 80 MHz [100]⁸. Fig. 3.5 shows the relative orientation of the trap axes with respect to the Raman beams. The two trap axes (X' and Y') are aligned at 45 degrees with respect to the wave-vector difference of the two Raman beams, $\delta\vec{k}$, which is along the X axis. The inset in Fig. 3.5 shows a cross-sectional view of the trap, showing the above axes with respect to the four rods, depicted as black dots. The relative orientation of the $\delta\vec{k}$ allows the Raman beams to apply spin-dependent forces to motional modes along both the X' and Y' directions.

The trap frequencies at the time of the experiment were $\omega_X \approx 2\pi \times 1.135$ MHz, $\omega_Y \approx 2\pi \times 0.920$ MHz and $\omega_Z \approx 2\pi \times 201$ kHz. Fig. 3.5 b) shows the blue sideband spectrum showing the four motional modes, two each corresponding to the X' and Y' directions. The higher frequency modes correspond to the X' direction. We have, $\omega_{\text{COM}}^{X'} = 2\pi \times 1.135$ MHz, $\omega_{\text{TILT}}^{X'} = 2\pi \times 1.117$ MHz, $\omega_{\text{COM}}^{Y'} = 2\pi \times 0.920$ MHz, $\omega_{\text{TILT}}^{Y'} = 2\pi \times 0.899$ MHz. The four-beat notes for the spin-dependent forces are created by adding four harmonic tones on the Raman 1 beam. This results in two spin-dependent force modulation frequencies $\mu_1 = \omega_{\text{TILT}}^{X'} - 2\pi \times 8$ kHz, $\mu_2 = \omega_{\text{TILT}}^{X'} - 2\pi \times 5$ kHz. This way both Ising interactions are primarily mediated by the X'-TILT mode which has significantly low heating rates compared to the X'-COM mode.

The experimental sequence is as follows. We apply 1.5 ms of Doppler cooling and 8 ms of Raman sideband cooling to cool all transverse modes to $\bar{n} < 1$ to be in the Lamb-Dicke

⁷The effect gets even stronger when we include the off-resonant carrier terms in the numerical simulation, i.e., Eq. (3.14). I am currently working on accounting for these effects while calculating the coupling matrices

⁸We use a slightly modified version of the protocol for coherent addressing using pulsed laser. For more information please refer to the masters thesis of Anthony Vogliano [125]

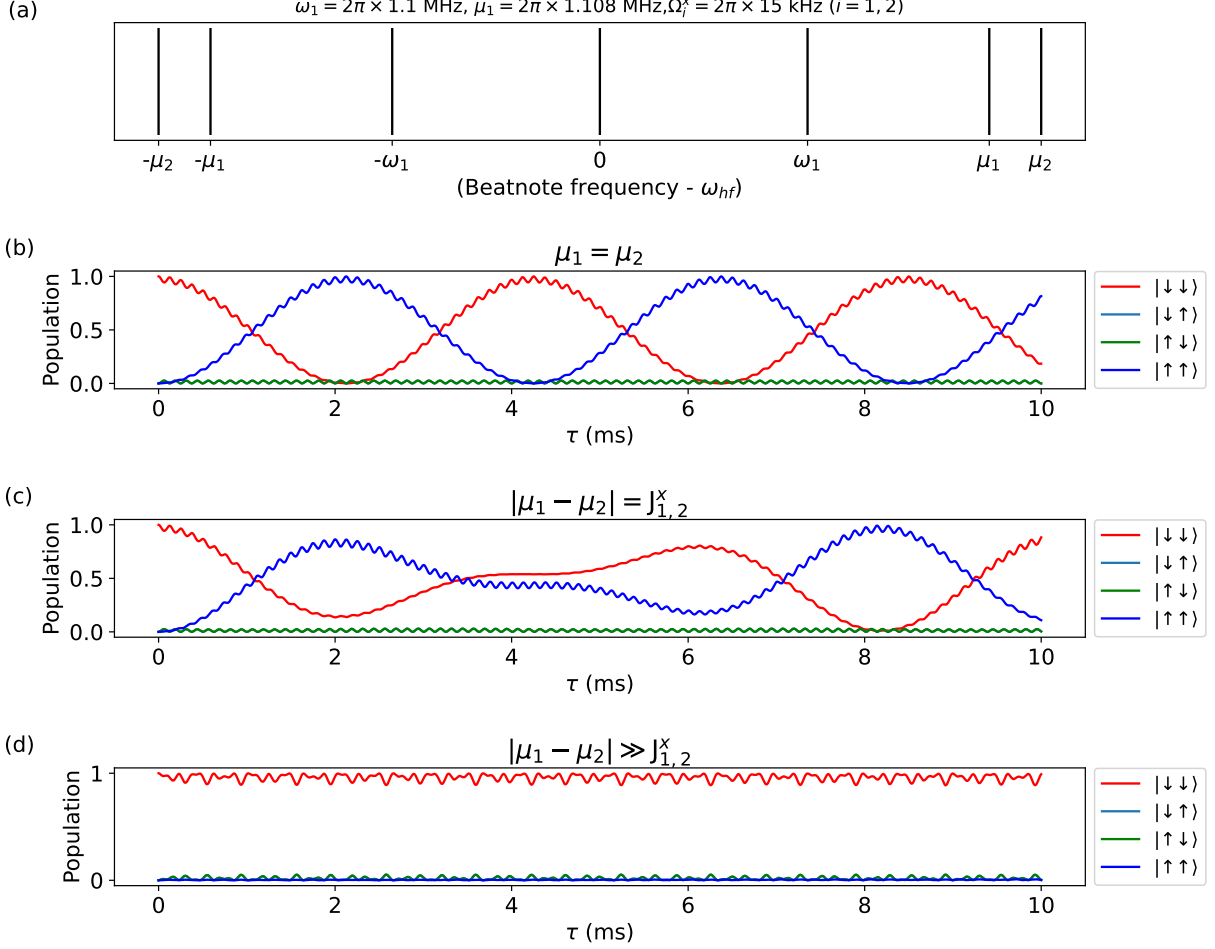


Figure 3.4: Schematic and numerical simulation of the parallel spin-dependent forces

(a) Schematic of the applied beatnotes generating SDFs at frequencies μ_1 (for coupling to σ_x spin components) and μ_2 (for coupling to σ_y spin components). The frequency axis is not drawn to scale. (b) Evolution for $\mu_1 = \mu_2$ and $\Omega_i^x = \Omega_i^y$ for $i = 1, 2$. This corresponds to a single spin-dependent force with a rotated spin axis. (c) Evolution for $|\mu_1 - \mu_2| \approx J_{12}^x$ and $\Omega_i^x = \Omega_i^y$ for $i = 1, 2$. This corresponds to the violation of the constraint in Eq. (3.25) and contribution from terms like $\sigma_x^1 \sigma_y^2$ in the evolution operator. (d) Evolution for $|\mu_1 - \mu_2| \gg J_{12}^x$ ($\mu_2 = 2\pi \times 1.105$ MHz) where the constraint in Eq. (3.25) is satisfied and dynamics under XY Hamiltonian are observed. See text for more details.

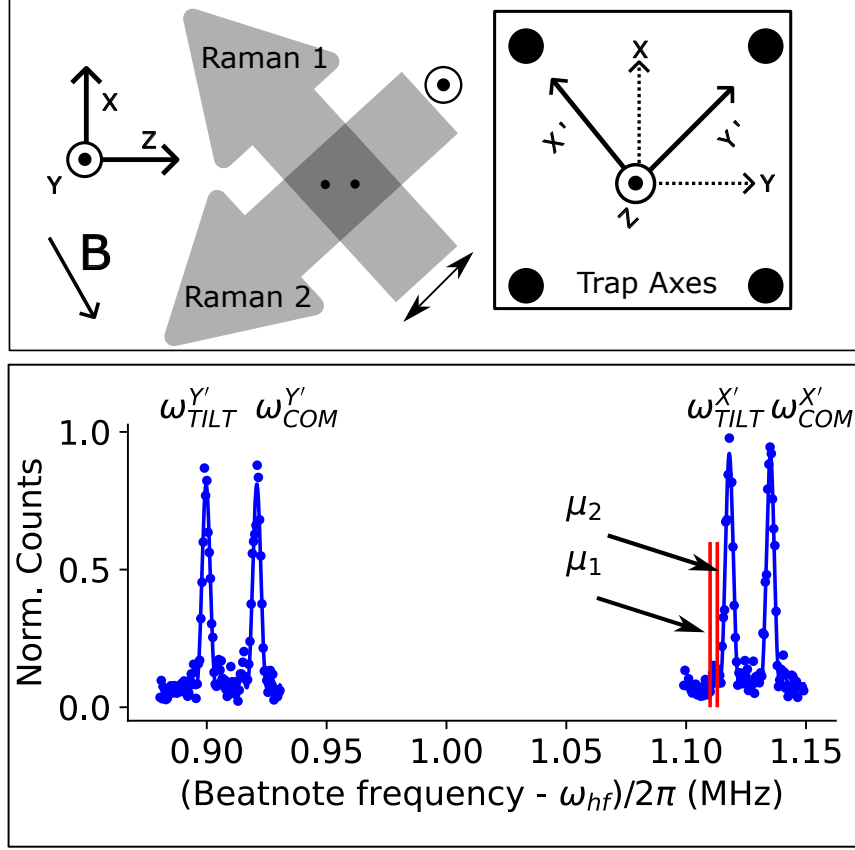


Figure 3.5: Experimental schematic

(a) Relative orientations of 2 Raman beams w.r.t. ions (black dots), magnetic field, and beam polarization. The inset shows the transverse trap axes, X' and Y' , in the XY plane, with the circles representing the electrode (rod) positions. The k -vector difference $\delta\vec{k}$ between the Raman beams lies along the X -axis, and hence, the Raman beams can excite both X' and Y' motional modes. Experimental data are presented in (b)-(d), where the fluorescence counts are normalized w.r.t. the counts from the $|\uparrow\uparrow\rangle$ state in each experimental repetition, and each point is the average of 100 experimental repetitions. (b) Raman beatnote frequency scan with two ions showing the blue sidebands. The higher frequency modes correspond to the X' direction. We have, $\omega_{\text{COM}}^{X'} = 2\pi \times 1.135$ MHz, $\omega_{\text{TILT}}^{X'} = 2\pi \times 1.117$ MHz, $\omega_{\text{COM}}^{Y'} = 2\pi \times 0.920$ MHz, $\omega_{\text{TILT}}^{Y'} = 2\pi \times 0.899$ MHz, $\mu_1 = \omega_{\text{TILT}}^{X'} - 2\pi \times 8$ kHz, $\mu_2 = \omega_{\text{TILT}}^{X'} - 2\pi \times 5$ kHz.

regime[63], and global optical pumping for 20 μs to initialize in the $|\downarrow\downarrow\rangle$ state. An optional global π -pulse driven by microwave radiation (at frequency ω_{hf}) and a site-selective optical pumping (that maintains the coherence of the neighboring ion with $\sim 99.9\%$ fidelity [126]) can alternatively prepare the initial states $|\downarrow\uparrow\rangle$ and $|\uparrow\downarrow\rangle$. Spin-dependent forces are then applied for a pulse duration τ , leading to the effective Hamiltonian in Eq. (3.24) during the application of the pulse. For data taken at each value of τ , we use an average of 100 experimental repetitions of the above sequence.

We finally measure the spin states by state-dependent fluorescence on a photomultiplier tube (PMT) for 1.5 ms. We calibrate the fluorescence counts by preparing the spins in $|\uparrow\uparrow\rangle$ with a microwave π -pulse in a separate experiment and obtain approximately 80 PMT counts for this state. Since global fluorescence measurements cannot distinguish between $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$ states, we apply a local optical pumping pulse on the first ion just before the measurement to convert it to a single ion measurement when necessary.

Fig. 3.6(a) shows the spin dynamics when initialized in $|\downarrow\downarrow\rangle$ state. As in the numerical simulations in Fig. 3.4, we tune the Rabi frequencies to achieve $J_{12}^x \approx J_{12}^y$ to get an effective XY model when the interactions are mediated simultaneously. We set the Rabi frequencies, $\Omega_i^x = 2\pi \times 15$ kHz and $\Omega_i^y = 2\pi \times 11.5$ kHz (approximately equal between the two ions). We first test the dynamical evolution for the two spin-dependent forces separately. This is equivalent to the separate application of H_x and H_y from Eq. (3.15). With H_x and H_y applied separately, we observe oscillations between $|\downarrow\downarrow\rangle$ and $|\uparrow\uparrow\rangle$, as expected. We estimate $J_{12}^x = 2\pi \times 77(2)$ Hz and $J_{12}^y = 2\pi \times 80(3)$ Hz based on the frequency of the oscillations extracted by fitting to $f(\tau)_{T,\alpha,\beta,\phi,C} = \sin^2(\omega\tau + \phi)(\alpha e^{-\tau/T}) + \beta(1 - e^{-\tau/T}) + C$. When H_x and H_y applied simultaneously, we find no observable oscillations, which is the signature of the XY Hamiltonian, since $(\sigma_x^1 \sigma_x^2 + \sigma_y^1 \sigma_y^2)|\downarrow\downarrow\rangle = 0$. The slow increase in the fluorescence counts for the XY Hamiltonian is likely due to the decoherence in the system and slow drifts in the intensity of the laser and the trap frequency (estimated to contribute $< 15\%$ drift in J_{12}^x or J_{12}^y) over the duration of the data run.

To further validate that the $\sigma_x^i \sigma_x^j$ and the $\sigma_y^i \sigma_y^j$ couplings are present simultaneously, we initialize the ions in the $|\downarrow\uparrow\rangle$ state and repeat the experiment. Here, we expect oscillations between the $|\downarrow\uparrow\rangle$ and the $|\uparrow\downarrow\rangle$ states, at frequency $J_{12}^x + J_{12}^y$ based on the evolution operator in Eq. (3.29). With global detection, we expect the fluorescence counts to be flat, as observed in Fig. 3.6 (b). This is because both $|\downarrow\uparrow\rangle$ and $|\uparrow\downarrow\rangle$ produce the same amount of fluorescence on the PMT. However, with an individual detection on ion 1 (i.e., by pumping one ion before detection), we observe oscillations in the fluorescence counts as expected from oscillations between the $|\downarrow\uparrow\rangle$ and $|\uparrow\downarrow\rangle$. From the data in Fig. 3.6 (b), we observe oscillations at $2\pi \times 178(2)$ which is within the expected 15% fluctuations of the extracted $J_{12}^x + J_{12}^y$ from previous experiments. The drifts also lead to a reduction in contrast of the

coherent oscillations and with stabilization of both the intensity ($\Omega_i^{x(y)}$) and trap frequency ($\omega_{\text{COM}}^{X'}$ and $\omega_{\text{TILT}}^{X'}$) we expect an order of magnitude improvement in the coherent oscillations.

Having validated the efficacy of the two spin dependent force protocol to create parallel Ising interactions we wish to test the scalability. The inherent full-connectivity of trapped ions allows the scheme to be easily scalable to a large number of ions, as in the case of tunable Ising interactions with a single spin-dependent force [63]. For example, an interaction profile with a power law decay that has been widely studied for quantum Ising models [63] can be extended to XY interactions. To achieve this interaction profile, the Rabi frequencies (Ω_i^x) and the detuning (μ_1) can be chosen first to obey an approximate power law in the coupling matrix J^x in Eq. (3.24). This is done by parking μ_1 to the blue side of the motional modes, and the difference between μ_1 and the COM mode determines the power law exponent α . Then, μ_2 can be chosen to satisfy Eq. (3.25) while keeping it close to μ_1 to maintain the same form for J^x and J^y . Further, if $J^x = J^y$ is desired, then Ω_i^y s can be calculated using a global scaling with respect to Ω_i^x to compensate for the unequal μ_1 and μ_2 . Fig. 3.7 shows that the interaction profiles along the x and y -directions match better than 99% with just global scaling of Rabi frequencies, even when $|\mu_1 - \mu_2|$ is chosen to be 30 times higher than $\max(J^x)$.

We find that this approach of scaling the Rabi frequencies works well whenever $\mu_1(\mu_2)$ is parked close to any motional mode since the contribution to the J_{ij}^x (J_{ij}^y) is dominated by a single motional mode. This makes the two-spin-dependent force approach directly extendable to arbitrary interaction profile generation algorithms [127, 128]. Thus, by simultaneously applying a pair of SDFs near each motional mode, the full spin-spin interaction profile can be engineered arbitrarily. However, it should be noted that the calculation of the coupling matrix should take into account any AC Stark shift induced by the spin-dependent forces when a highly precise knowledge of the coupling matrices (J_{ij}^x, J_{ij}^y) is required.

In the end, a discussion on the effect of the constraint in Eq. (3.25) is warranted since it might appear, at first glance, to set the energy scale for the effective Hamiltonian, i.e., the values in the coupling matrices (J_{ij}^x, J_{ij}^y). This is however not true, and it should be noted that the constraint in Eq. (3.25) is weaker than the constraint for applying each of the forces in the slow regime ($|\mu_{1(2)} - \omega_m| \gg \eta_{im}\Omega_i^{x(y)}$) which is applicable even while applying a single spin-dependent force. This is because, in the slow regime, individual matrix elements J_{ij}^x (J_{ij}^y) are an order of magnitude smaller than $|\mu_{1(2)} - \omega_m|$ and hence leave enough freedom to satisfy Eq. (3.25). For state-of-the-art trapped ion quantum simulators, typical values of radial trap frequencies, ω_m here, are about $2\pi \times 5$ MHz. While operating in the slow regime, typical values of Jmax are close to $2\pi \times 100$ Hz even for a single spin-dependent-force in the weak regime. The spacing between the radial modes is on the order of 10s of kHz, and hence, there is “plenty of room to park” μ_1 and μ_2 close to

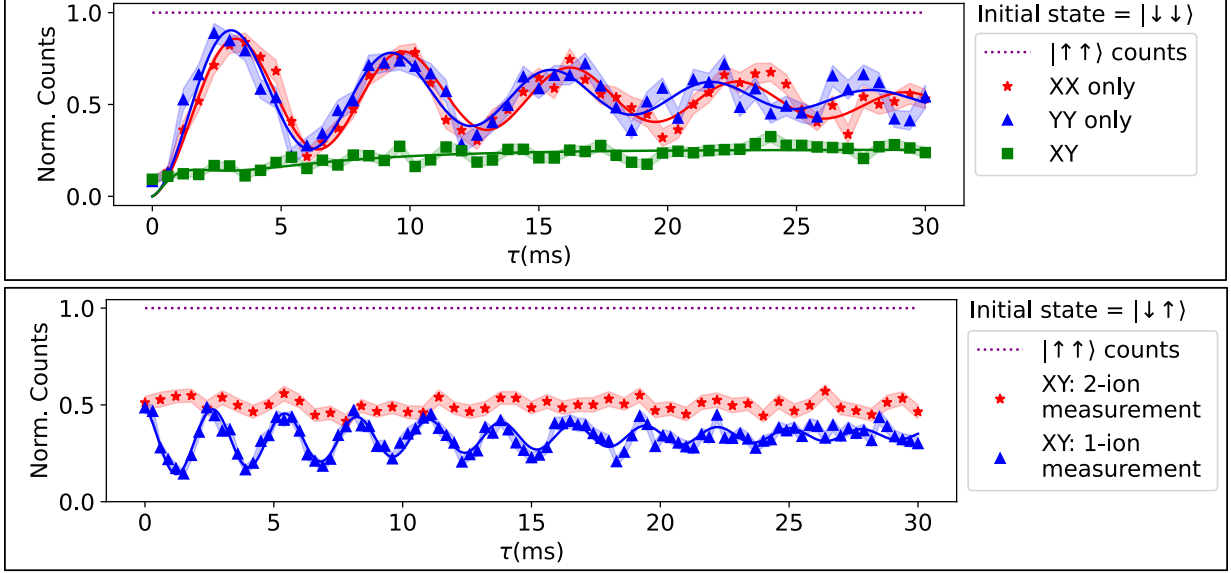


Figure 3.6: Experimental demonstration: XY model on trapped ions

(a) Relative orientations of 2 Raman beams w.r.t. ions (black dots), magnetic field, and beam polarization. For both (a) and (b), solid lines represent fit to $f(\tau)_{T,\alpha,\beta,\phi,C} = \sin^2(\omega\tau + \phi)(\alpha e^{-\tau/T}) + \beta(1 - e^{-\tau/T}) + C$ and the shaded regions represent standard error. $\Omega_i^x \approx 2\pi \times 15$ kHz ($i = 1, 2$) and $\Omega_i^y \approx 2\pi \times 11.5$ kHz ($i = 1, 2$). (c) When initialized in $|\downarrow\downarrow\rangle$, we observe oscillations in the fluorescence counts when either of the two spin-dependent forces is applied separately (red and blue plots). From the fit parameter ω , we estimate $J_{12}^x = 2\pi \times 77(2)$ Hz and $J_{12}^y = 2\pi \times 80(3)$ Hz. When the two forces are applied simultaneously (green plots), we observe no appreciable oscillations, as expected from the XY Hamiltonian (see text). (d) Observation of dynamics under the XY Hamiltonian when initialized in $|\downarrow\uparrow\rangle$. The normalized total fluorescence counts from both ions are nearly constant over the evolution time, as the spin states of the ions oscillate out of phase with each other (between $|\downarrow\uparrow\rangle$ and $|\uparrow\downarrow\rangle$). Oscillations are recovered with a 1-ion fluorescence measurement (see text). We observe oscillations at $2\pi \times 178(2)$ Hz, which is consistent with the expected oscillation frequency of $J_{12}^x + J_{12}^y$, counting for $\approx 15\%$ drifts in the couplings over the timescale of the data run. The drifts also lead to a reduction in contrast of the coherent oscillations and with stabilization of both the intensity ($\Omega_i^{x(y)}$) and trap frequency ($\omega_{\text{COM}}^{X'}$ and $\omega_{\text{TILT}}^{X'}$) we expect an order of magnitude improvement in the coherent oscillations.

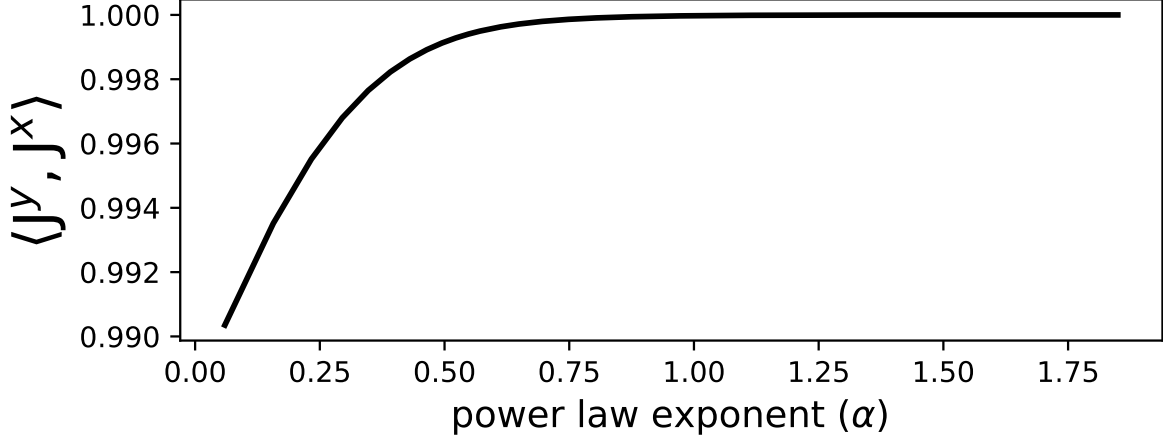


Figure 3.7: Calculated proximity of J^x and J^y while engineering power law decay in XY couplings for $N = 25$ ions.

To have a linear chain of $N = 25$ ions, we assume trap frequencies of $\omega'_X = 2\pi \times 5$ MHz, $\omega'_Y = 2\pi \times 4.8$ MHz and $\omega_Z = 2\pi \times 400$ kHz. J^x is calculated using Eq. (3.24), assuming equal Ω_i^x on all ions operating in the regime where $\max(\{J_{ij}^x\}) \approx 2\pi \times 100$ Hz. μ_1 is varied from $\omega_x + 2\pi \times 1$ kHz to $\omega_x + 2\pi \times 1$ MHz to achieve the approximate power scaling, i.e., $J_{ij}^x \approx 1/|i-j|^\alpha$ with $\alpha \in (0.1, 1.8)$. To get the $J_{ij}^x = J_{ij}^y$, we set $\mu_2 = \mu_1 + 2\pi \times 3$ kHz and calculate Ω_i^y from Eq. (3.24) by assuming only participation of the closest motional mode i.e., COM. To compare J^x and J^y we use the Frobenius norm, $\langle \mathbf{A}, \mathbf{B} \rangle_F = \text{Tr}(\mathbf{A}^\dagger \mathbf{B})$ after appropriate normalization.

each other while not getting too close to other modes. In Fig. 3.7 we conservatively chose $|\mu_1 - \mu_2| = 2\pi \times 3$ kHz, however $|\mu_1 - \mu_2| = 10 \times \max(J^{x(y)})$ is enough. Hence, Eq. (3.25) does not limit the scale of the couplings any more than the limit imposed by being in the weak regime.

3.3.4 Comparison with Floquet method

The XY-model (and the Heisenberg model) can also be implemented on trapped ions via Floquet engineering [123, 122]. Repeated application of a pulse sequence comprising of a σ_x spin-dependent force for time $T_f/2$ followed by a σ_x spin-dependent force with the same interaction profile for time $T_f/2$ leads to the XY model in the high-frequency limit ($T_f \ll 1/\max_{i,j}(|J_{ij}^{x(y)}|)$) [129], where Trotter errors are negligible. Assuming no addi-

tional spin-motion coupling, varying the Floquet period T_f in this regime should leave the effective Hamiltonian unchanged, except for the residual Trotter errors. However, Floquet drives can be viewed as two separate spin-dependent forces that are further modulated at the Floquet frequency (and harmonics), potentially leading to complicated dynamics and additional spin-motion coupling. To assess these effects, we numerically simulate the evolution of 2 ions (and one motional mode) under a sequence designed to simulate the effective Hamiltonian $H_{\text{eff}} = J\sigma_x^1\sigma_x^2 + J\sigma_y^1\sigma_y^2$ (see Fig. 3.8). We incorporate a Blackman pulse shape [123] at the beginning and end of the pulses with 40% of the pulse time evenly split in the rIsing and falling edges to avoid broadening of the pulses in the frequency domain due to sharp rIsing/falling edges as shown in Fig. 3.8. We observe that the time evolution is highly dependent on $N_f = (\frac{1}{T_f \times J})$ and most values of N_f lead to high motional excitation. Figures 3.8 b) c) and d) show the average phonon occupation for the entire duration of the applied sequence for different values of μ . The average phonon occupation, a function of the Rabi frequencies, and the detuning μ are higher than the native two-spin dependent force approach for most values of N_f and for values of $N_f > 800$, the quantum simulation deviates from the intended even with low phonon occupation.

We observe that the time-averaged phonon occupation serves as a good predictor for when the time evolution matches that of the target Hamiltonian, for $N_f \lesssim 800$. These are the values N_f marked in Fig. 3.9 a). For low N_f values, the Trotter errors are significant (Fig. 3.9 b)), even when the phonon errors are low. The ‘good’ N_f values (Fig. 3.9 c), where both the Trotter and additional spin-motion coupling errors are low, depend on the Rabi frequency and the detuning applied to create the XX and YY pulses. Beyond $N_f \gtrsim 800$, the residual phonon occupation goes below the level expected from our two-spin-dependent force approach to creating the XY model, presented here. However, in this regime, the evolution becomes more complex and deviates from expectations despite the low occupancy of phonons (Fig. 3.9 d)).

For larger systems, numerical simulations are intractable, and experimentally finding an appropriate N_f is also challenging, as this would require thermometry of all the motional modes at multiple times in the evolution. Further, a good N_f with low Trotter error might require reducing the overall magnitude of the J -couplings pushing the dynamical timescale beyond the coherence time. A good value of N_f may not even exist due to the number of motional modes that participate in mediating the spin-spin couplings. Furthermore, creating arbitrary interaction graphs [128] may not be possible because the optimal N_f for different detunings will be different. The two spin-dependent force approach of creating the XY interaction presented here provides a viable way to scale up quantum simulations.

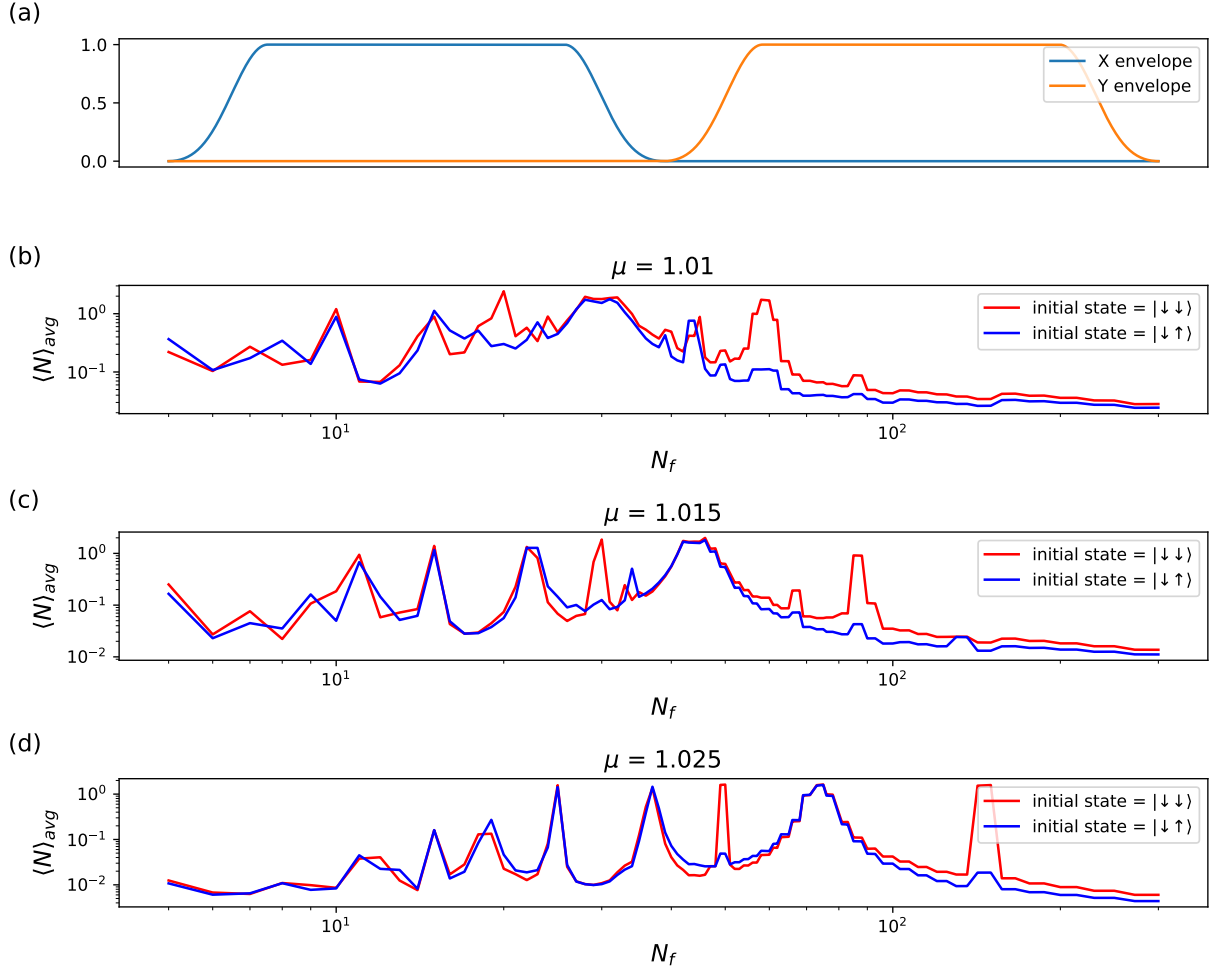


Figure 3.8: Phonon excitations from Floquet drives

Numerically calculated time evolution of 2 ions initialized in the $|\downarrow\downarrow\rangle$ state under a Floquet pulse sequence intended to generate XY-couplings (see text). All the frequencies are scaled to this mode frequency, i.e., $\omega_m = 2\pi \times 1$, $\mu = 2\pi \times 1.02$ and $\eta\Omega = 2\pi \times 0.003$ for both XX and YY pulses, intended to simulate the effective Hamiltonian $H_{\text{eff}} = J_{12}^x \sigma_x^1 \sigma_x^2 + J_{12}^y \sigma_y^1 \sigma_y^2$ with $J_{12}^x = J_{12}^y = J \approx 2\pi \times 8 \times 10^{-5}$. The resulting time evolution depends on $N_f = (\frac{1}{T_f \times J})$ where T_f is the Floquet period.

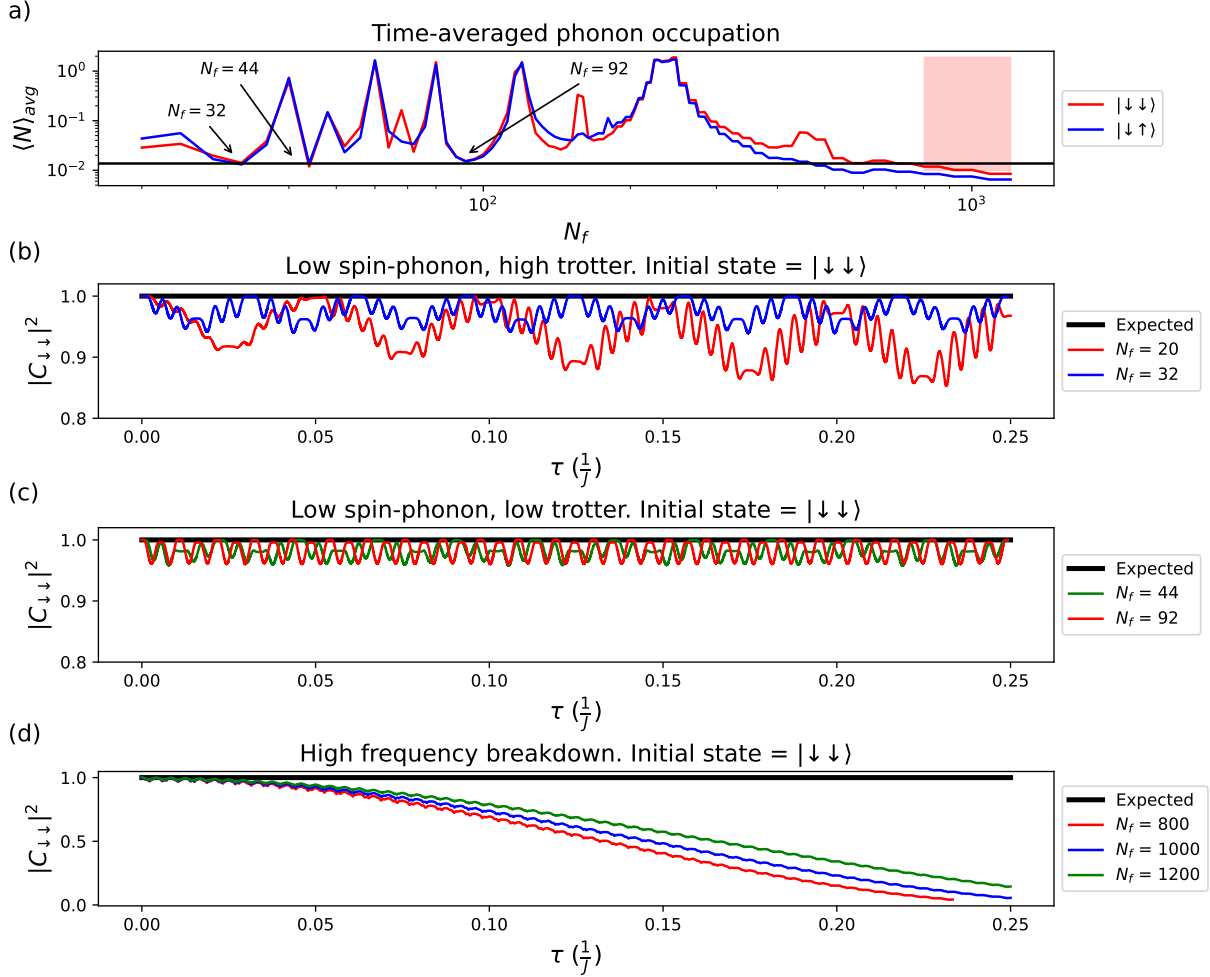


Figure 3.9: Comparison with Floquet Engineering

(a) time averaged phonon population, $\langle N \rangle_{avg}$ during the length of the quantum simulations when initialized in either $|\downarrow\downarrow\rangle$ or $|\downarrow\uparrow\rangle$. Most values of N_f lead to inadvertent spin-motion coupling of the ions. The ideal N_f values are the ones where the average phonon number is comparable to the native ‘2-SDF’ approach (black line) used in this work, for example, $N_f = 32, 44$ and 92 here. The population in the $|\downarrow\downarrow\rangle$ state as a function of time is shown for various values of N_f in (b), (c), and (d). (b) For low values of N_f , the Trotter errors limit the efficacy of the simulation as evidenced by the slow oscillations at $1/T_f$. (c) The best values of N_f are where the Trotter error and the spin-motion coupling are both small. (d) For sufficiently large values, $N_f \geq 800$ here (shaded red in (a)), the time evolution deviates from the expected significantly despite low phonon occupation.

3.4 Conclusion and Outlook

In summary, we have demonstrated tunable long-range XY-type couplings ($J_{ij}^x \sigma_x^i \sigma_x^j + J_{ij}^y \sigma_y^i \sigma_y^j$) by the parallel application of two spin-dependent forces on the same motional modes. Our approach allows for analog quantum simulations of the XY and anisotropic XY models, as the effective Hamiltonian (Eq. (3.24)) is valid in continuous time. The technique inherits the scalability and programmability of existing techniques to generate Ising interactions on trapped ions [63, 128, 130] and does not require additional experimental enhancements of the current generation devices. This opens possibilities for studying ground state order of frustrated XY-type models in large 2D arrays of ions [131], and in principle on programmable lattice geometries [128, 127], to investigate exotic quantum phases, such as spin liquids [132]. Further, evolution under the XY Hamiltonian can be interspersed with single spin quantum gates in analog-digital hybrid quantum simulations [133] to investigate dynamical phase transitions, Hamiltonian quenches, and quantum transport.

The demonstration of parallel spin-dependent forces on the same motional modes can further be extended to simulate XYZ-type Hamiltonians by adding a σ_z - spin-dependent force. This could be done using either the light-shift scheme [134] or using the approach of choosing one of the detunings μ to be close to half the motional mode frequencies [135]. It should be noted that the addition of a σ_z - spin-dependent force using the second method does not allow for neglecting the off-resonant carrier term that results from the application of the red and blue sidebands and accounting for effects from this term while calculating the coupling matrices is important.

Chapter 4

A Single Ion Optical Sensor

Author Contributions: The requirement for characterizing the polarization of light shining on the ions arose due to trying to calculate the operational fidelities of local reset and readout operations shown in [126]. The two theoretical models for characterizing ion-light interactions, in Sections 4.3 and 4.4, were developed by the author. The experimental data shown in Fig. 4.7 was taken by Dr. Sainath Motlakunta, and the data analysis that led to Fig. 4.8 was performed by the author. The author conceived the idea of using a neural network to solve the inverse problem of extracting light properties from the ion population dynamics curves and wrote the subsequent implementation. The work discussed in this chapter is part of a manuscript in preparation, and the author and Prof. Rajibul Islam are actively working on it.

4.1 Overview

At first glance, this chapter might seem unrelated to the rest of the work described in this thesis. However, low-light sensing is crucial for atom- and ion-based quantum computers/simulators. This is because local operations, i.e., operations on select qubits without disturbing the neighbors, require light to be confined to a very tight spatial extent such that light addressing one ion in the chain does not spill over to the neighbor. The spilled-over light causes unwanted effects on the neighboring qubits, and this ‘crosstalk error’ is an important source of error in quantum devices. Thorough characterization of such errors is required to enhance the usability of large-scale quantum devices. Note that quantum operations are sensitive to both the intensity and the polarization of light, and any char-

acterization tool should be able to characterize both. Hence, the characterization of these crosstalk errors can be considered quantum light sensing when the control fields are optical.

This work is an extension of modeling the ion-light interactions for our recently published results [126] on preserving the information in a neighbor ‘asset’ qubits while performing state reset and readout on a ‘process’ qubit using tightly focused optical beams produced using Fourier holography [136]. Fig. 4.1 a) shows a pictorial representation of crosstalk errors in ion trap quantum simulators/computers. The inadvertent addressing of the asset qubit could result from leaked light from the optical addressing of the process qubit, or the photons scattered by the process qubit could be absorbed by the neighboring asset qubit. In essence, there is a finite probability P_{AQM} that the neighbor qubit is accidentally measured due to the addressing of the process qubit, and the fundamental limit to this probability comes from the probability of absorption of the photons scattered by the process qubit P_{AQM}^* . Estimation of P_{AQM} and bounding P_{AQM}^* requires a model of ion-light interactions to calculate the scattering rate of the addressed qubit and the absorption rate of the asset qubit. Moreover, experiments do not directly measure P_{AQM} , rather the coherence time of the asset qubit in the presence of the addressing light, and hence, a model of light ion interactions is necessary to extract P_{AQM} from the experimental observations. For this reason, a model of the ion-light interactions was developed for the ions interacting with light resonant with the $^2\text{S}_{1/2} \rightarrow ^2\text{P}_{1/2}$ transition and a microwave field resonant with the qubit clock transition.

In this chapter, I present our results on sub-wavelength characterization of optical intensity and polarization using a single ion as a sensor of light. The technique utilizes the intensity and polarization-dependent optical pumping of $^{171}\text{Yb}^+$ ions as a signature to extract the light parameters. The spatial extent of the ion is much smaller than the absorption cross-section of a point-like resonant detector ($\lambda^2/2\pi$), and hence the resolution is only limited by this fundamental limit.

Two separate methods for modeling the ion-light interactions are presented. In the first method, the full atomic density matrix for the relevant atomic energy levels interacting with light is evolved, and in the second method only the incoherent population dynamics of the ground state is taken into account. The models are verified by comparing results between the two models and also fitting experimental data. An important insight provided in this work is that these interactions can also be ‘learned’ in some restricted sense. A deep neural network can be used to learn the functional form of the output-to-input relationship, i.e. the inverse of the model, for some specifically chosen set of initial states of the ion. Learning the inverse of this function allows for an extremely efficient means of ‘intelligent sensing’, i.e., directly extracting the intensity and polarization from optical pumping curves without the need for fitting. This makes the approach readily field deployable owing to

the minimal computational overhead in light-parameter extraction.

4.2 Single ions for sensing light

Optical systems capable of creating sub-micrometer features of light have become standard in science and engineering research and industry. Pertinent examples include experimental setups in atomic and nuclear physics, atom- and ion-based quantum computers, and optical lithography setups. Although such setups are widely used, direct characterization of the optical fields produced by these devices is not yet possible because of the limited spatial resolution offered by modern detectors. For example, the smallest available pixel size for a polarization-sensitive detector is $\approx 3.45 \mu\text{m}$ ¹. However, optical lithography setups routinely create feature sizes below $0.1 \mu\text{m}$, and atom/ion-based quantum computers often use sub-micrometer beam sizes.

Note that the fundamental limit for high-resolution light detection is set by the absorption cross-section of the detector. The absorption cross-section for an ideal point-like detector, a two-level atom with no spatial extent absorbing resonant radiation, is $\lambda^2/2\pi$, therefore assuming a circular cross-section, sub-wavelength characterization of optical features is not disallowed by the fundamental limit. The spatial extent of a trapped ion is given by the spread of its spatial wavefunction, and even for Doppler-cooled ions, this is much smaller than the spatial extent required for sub-wavelength characterization of light. For example, in our experimental apparatus for trapping $^{171}\text{Yb}^+$ ions, we usually set our trapping potential so that the three harmonic oscillator frequencies are $(\omega_x, \omega_y, \omega_z)/2\pi = (1.1, 0.9, 0.22)$ MHz. The ions have a position spread of $\Delta = \sqrt{2\bar{n} + 1}x_0$ where $x_0 = \sqrt{\hbar/2m\omega}$ is the zero point spread of a quantum harmonic oscillator, $\bar{n}$ is the mean thermal phonon occupation number and ω is the harmonic oscillator frequency. The minimum position spread is along the X-direction of around 5 nm, and the largest spread is along the Z direction of about 120 nm. Hence, from any direction, the spatial extent of the ion is much smaller than the absorption cross section for resonant absorption of the light resonant with the $^2\text{S}_{1/2}$ to $^2\text{P}_{1/2}$ transition at 369.5 nm.

Fig. 4.2 shows a pictorial representation of using a single ion to characterize the image plane field of a high numerical aperture (NA) optical system. The trapped ion's position can be changed by varying the voltages on the trap electrodes, which is used to scan the ion position in the image plane of the lens. At each position of the ion, the ion is prepared

¹At the time of writing this thesis. These detectors are available from several vendors and are based on the IMX250MZR CMOS sensor from Sony.

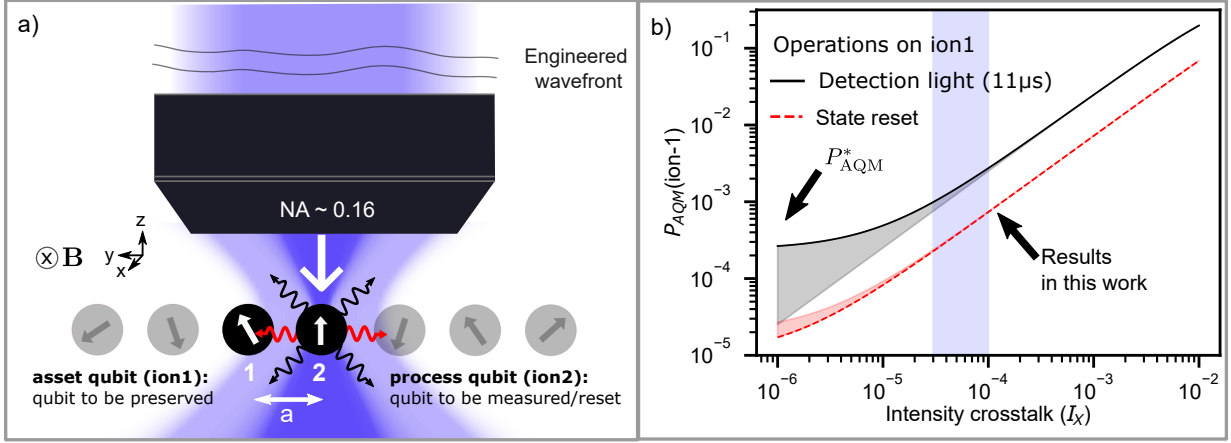


Figure 4.1: Accidental quantum measurement (AQM) of neighboring qubits.

a) While addressing a ‘process’ qubit (ion2) in a trapped ion chain, an ‘asset’ qubit (ion1) at a distance a away may be accidentally measured by photons that are either scattered from ion2 (red wavy lines) or from intensity crosstalk due to imperfect optical addressing (lightly shaded violet). AQM from imperfect optical addressing can be minimized by engineering the wavefronts incident on the microscope objective [136]. **b)** Calculated probability of AQM (P_{AQM}) of the asset qubit (ion1) as a function of intensity crosstalk (I_X). Here, P_{AQM} is estimated from the asset qubit’s infidelity after a state detection or reset on the process qubit. The fidelity is estimated with respect to $|\uparrow\rangle$ to represent the worst-case scenario. For this figure, we choose $a = 6 \mu\text{m}$, and $I_2 = I_{\text{sat}}$ (the saturation intensity of the transition $^2S_{1/2} \rightarrow ^2P_{1/2}$). For low crosstalk regime ($I_X < 1 \times 10^{-5}$), inter-ion scattering sets a fundamental limit, P_{AQM}^* , which can vary (shaded region) depending on the geometric properties of the system, such as the orientation of the magnetic field ($\vec{B}$) defining the quantization axis. The results presented in this manuscript are in the regime with $I_X \lesssim 8 \times 10^{-5}$, leading to $P_{\text{AQM}} < 4 \times 10^{-3}$ for state reset, and $P_{\text{AQM}} < 1 \times 10^{-3}$ with a detection beam applied for 11 μs [137].

in a known initial state, and the light to be detected is incident on the ion. Then, the light is shut off, and any property of the ion that is sensitive to the intensity and polarization of light is measured. The image plane field at the ion position is then calculated on the basis of the result of this measurement. Repeating this procedure for different positions of the ion in the image plane of the optical instrument allows for the reconstruction of the intensity and polarization of light in the entire image plane of the optical instrument.

Hence, the three requirements for this protocol are

- A measurement that is sensitive to the intensity and polarization of light
- A model for the ion-light interactions
- An efficient algorithm to extract light parameters from the measurement

In $^{171}\text{Yb}^+$ ions, the optical pumping operation (state reset) discussed in Section (2.5.3) is sensitive to both the intensity and the polarization of the optical pumping light. Therefore, the ion's optical pumping response can serve as a means to extract the intensity and polarization of the light. The modeling of this interaction using two distinct methods is discussed in the next two sections. Both methods are semi-classical, i.e., the light is treated classically, and the ion is treated quantum mechanically; however, the difference is in the approximations applied. In the first method, we consider all eight energy levels in the $^2\text{S}_{1/2}$ and $^2\text{P}_{1/2}$ manifold and solve for the quantum master equation resulting from the simplified Hamiltonian of the ion-light interactions. In the second method, we solve for the incoherent population dynamics in the four levels of the $^2\text{S}_{1/2}$ manifold in the presence of optical pumping light by generalizing the quantum mechanical solution for a two-level atom interacting with light. The dynamics generated by the two methods match well for the parameter ranges when their respective approximations overlap, giving confidence in the ability of these models to capture the physics of the ion-light interactions. Further, the experimental data fit very well, and the light intensity and polarization can be extracted by fitting the data to the models. Once the light parameters are extracted, the ion's dynamics can also be faithfully predicted for known changes to the light intensity and polarization. However, accurate estimation of the light intensity and polarization from fitting the experimental data comes at a high computational cost. Scaling up the technique to characterize optical fields in the image plane of a high-numerical-aperture optical setup requires a more efficient parameter estimation algorithm. For this, a deep neural network is used to learn the inverse of the model, i.e., a function that maps optical pumping curves to the respective intensity and polarization values. In the following sections, we discuss these results in detail.

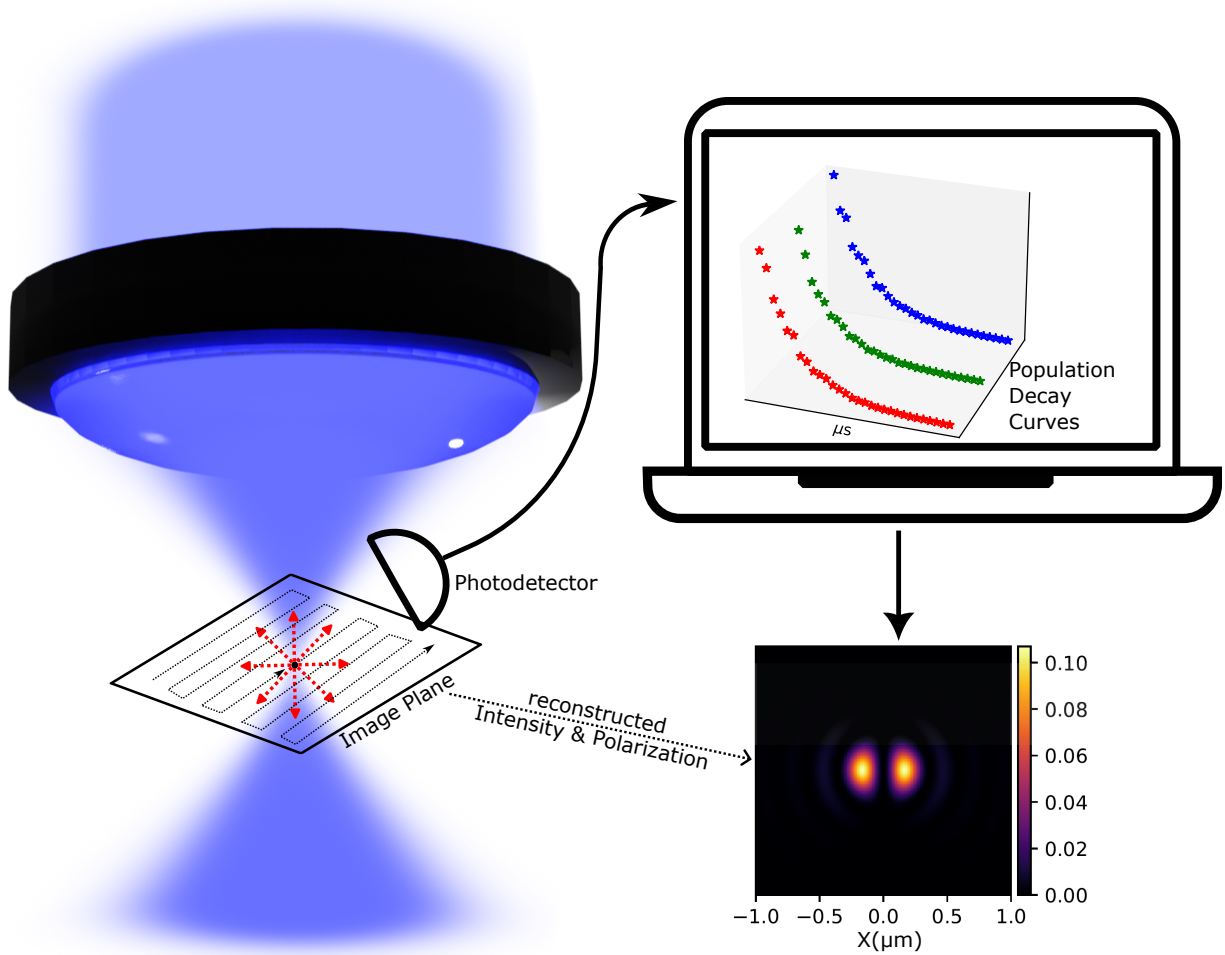


Figure 4.2: Single Ion Light Sensor Schematic

A single ion is trapped in an ion trap (not shown here), and the trapping region coincides with the image plane of the optical instrument to be characterized. The position of the ion is scanned along the entire image plane, and at each position, the ion is initialized in a known state and allowed to interact with the light. After the interaction, a convenient measurement is performed on the ion chosen to allow for the light intensity and polarization to be extracted. The measurement is compared with the model of the ion-light interaction, and the intensity and polarization at each ion position are characterized.

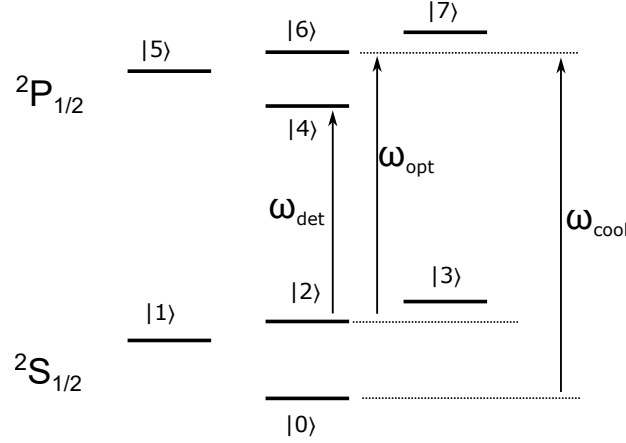


Figure 4.3: Labeling Scheme for energy levels in $^2S_{1/2}$ and $^2P_{1/2}$

With the above labeling convention, ω_{hf}^S is the frequency difference between $|0\rangle$ and $|2\rangle$, ω_{hf}^P is the frequency difference between $|4\rangle$ and $|6\rangle$, ω_{zm}^S is the frequency difference between $|1\rangle$ and $|2\rangle$, and ω_{zm}^P is the frequency difference between $|6\rangle$ and $|7\rangle$.

4.3 Modelling ion-light interactions: Full density matrix evolution

To model the dynamics in the 8-level subspace of $^2S_{1/2}$ and $^2P_{1/2}$, we can start by labeling the energy levels as shown in Fig. 4.3. With $|i\rangle$ as the basis ket for level i , we can define the atomic Hamiltonian as follows

$$\begin{aligned}
H_{\text{atom}} = & |1\rangle \langle 1| \omega_{\text{hf}}^S - \omega_{\text{zm}}^S + |2\rangle \langle 2| \omega_{\text{hf}}^S + |3\rangle \langle 3| \omega_{\text{hf}}^S + \omega_{\text{zm}}^S \\
& + |4\rangle \langle 4| \omega_{\text{SP}} + \omega_{\text{hf}}^S + |5\rangle \langle 5| \omega_{\text{SP}} + \omega_{\text{hf}}^P + \omega_{\text{hf}}^S - \omega_{\text{zm}}^P \\
& + |6\rangle \langle 6| \omega_{\text{SP}} + \omega_{\text{hf}}^P + \omega_{\text{hf}}^S + |7\rangle \langle 7| \omega_{\text{SP}} + \omega_{\text{hf}}^P + \omega_{\text{hf}}^S + \omega_{\text{zm}}^P
\end{aligned} \tag{4.1}$$

Here, ω_{SP} is the frequency difference between the $^2S_{1/2}$ and $^2P_{1/2}$ levels, ω_{hf}^S is the hyperfine splitting in the $^2S_{1/2}$, ω_{hf}^P is the hyperfine splitting in $^2P_{1/2}$, ω_{zm}^S is the Zeeman splitting in $^2S_{1/2}$, and ω_{zm}^P is the Zeeman splitting in $^2P_{1/2}$.

We now model the interactions with light and microwave radiation at various frequencies. If we ignore the Zeeman splitting in $^2S_{1/2}$ and $^2P_{1/2}$, there are three optical transitions possible, i.e. $^2S_{1/2} F = 0 \rightarrow ^2P_{1/2} F' = 1$, $^2S_{1/2} F = 1 \rightarrow ^2P_{1/2} F' = 0$, $^2S_{1/2} F = 1 \rightarrow ^2P_{1/2} F' = 1$. Since the Zeeman splitting in our experiment is smaller than the linewidth of the

$^2S_{1/2}$ to $^2P_{1/2}$ transition, only one frequency is considered for each of these transitions, and the allowed transitions between the Zeeman levels are induced by the same. The Hamiltonian for the light-ion interaction is a straightforward dipole interaction Hamiltonian of the form.

$$H_{light} = -\vec{d} \cdot \vec{E}(t) \quad (4.2)$$

Where $\vec{E}(t) = \vec{E}_{\text{opt}} \cos(\omega_{\text{opt}}t) + \vec{E}_{\text{det}} \cos(\omega_{\text{det}}t) + \vec{E}_{\text{cool}} \cos(\omega_{\text{cool}}t)$. Here, the three frequencies ω_{opt} , ω_{det} , and ω_{cool} correspond to the transitions $F=1 \rightarrow F' = 1$, $F=1 \rightarrow F' = 0$, and $F=0 \rightarrow F' = 1$ respectively.

$$H_{\text{opt}} = \frac{1}{2} \left(\Omega_{15} |1\rangle \langle 5| + \Omega_{16} |1\rangle \langle 6| + \Omega_{25} |2\rangle \langle 5| \dots \right. \\ \left. + \Omega_{27} |2\rangle \langle 7| + \Omega_{36} |3\rangle \langle 6| + |3\rangle \langle 7| \right) e^{i\omega_{\text{opt}}t} + h.c. \quad (4.3)$$

$$H_{\text{det}} = \frac{1}{2} \left(\Omega_{14} |1\rangle \langle 4| + \Omega_{24} |2\rangle \langle 4| + \Omega_{34} |3\rangle \langle 4| \right) e^{i\omega_{\text{det}}t} + h.c. \quad (4.4)$$

$$H_{\text{cool}} = \frac{1}{2} \left(\Omega_{05} |0\rangle \langle 5| + \Omega_{06} |0\rangle \langle 6| + \Omega_{07} |0\rangle \langle 7| \right) e^{i\omega_{\text{cool}}t} + h.c. \quad (4.5)$$

The Rabi frequencies are defined as follows.

$$\Omega_{ij} = \begin{cases} \langle i | \vec{d} \cdot \vec{E}_{\text{opt}} | j \rangle / \hbar & \text{if } F = 1 \rightarrow F' = 1 \\ \langle i | \vec{d} \cdot \vec{E}_{\text{det}} | j \rangle / \hbar & \text{if } F = 1 \rightarrow F' = 0 \\ \langle i | \vec{d} \cdot \vec{E}_{\text{cool}} | j \rangle / \hbar & \text{if } F = 0 \rightarrow F' = 1 \end{cases} \quad (4.6)$$

In this way, we are only considering the resonant couplings.

The only other applied field to consider is the microwave field applied to couple the clock states.

$$H_{\text{micro}} = \frac{1}{2} \left(\Omega_{02} |0\rangle \langle 2| \right) e^{-i\omega_{\text{micro}}t} + h.c. \quad (4.7)$$

The total Hamiltonian of the atom is then given as

$$H_{\text{tot}} = H_{\text{atom}} + H_{\text{opt}} + H_{\text{det}} + H_{\text{cool}} + H_{\text{micro}} \quad (4.8)$$

To consider off-resonant interactions, we can define the detunings as follows.

$$\begin{aligned} \Delta_{\text{mic}} &= \omega_{\text{micro}} - \omega_{\text{hf}}^{\text{S}} \\ \Delta_{\text{opt}} &= \omega_{\text{opt}} - \omega_{\text{SP}} - \omega_{\text{hf}}^{\text{P}} \\ \Delta_{\text{det}} &= \omega_{\text{det}} - \omega_{\text{SP}} \\ \Delta_{\text{cool}} &= \omega_{\text{cool}} - \omega_{\text{hf}}^{\text{S}} - \omega_{\text{SP}} - \omega_{\text{hf}}^{\text{P}} \end{aligned} \quad (4.9)$$

With the above definitions, the total Hamiltonian in the interaction frame of the atom is given as²

$$\begin{aligned} H_{\text{rot}} = \frac{1}{2} \bigg(& |0\rangle \langle 2| \Omega_{02} e^{i\Delta_{\text{mic}} t} + |0\rangle \langle 5| \Omega_{05} e^{it(\Delta_{\text{cool}} + \omega_{\text{zm}}^{\text{P}})} + |0\rangle \langle 6| \Omega_{06} e^{i\Delta_{\text{cool}} t} \\ & + |0\rangle \langle 7| \Omega_{07} e^{it(\Delta_{\text{cool}} - \omega_{\text{zm}}^{\text{P}})} + |1\rangle \langle 4| \Omega_{14} e^{it(\Delta_{\text{det}} - \omega_{\text{zm}}^{\text{S}})} + |1\rangle \langle 5| \Omega_{15} e^{it(\Delta_{\text{opt}} + \omega_{\text{zm}}^{\text{P}} - \omega_{\text{zm}}^{\text{S}})} \\ & + |1\rangle \langle 6| \Omega_{16} e^{it(\Delta_{\text{opt}} - \omega_{\text{zm}}^{\text{S}})} + |2\rangle \langle 4| \Omega_{24} e^{i\Delta_{\text{det}} t} + |2\rangle \langle 5| \Omega_{25} e^{it(\Delta_{\text{opt}} + \omega_{\text{zm}}^{\text{P}})} \\ & + |2\rangle \langle 7| \Omega_{27} e^{it(\Delta_{\text{opt}} - \omega_{\text{zm}}^{\text{P}})} + |3\rangle \langle 4| \Omega_{34} e^{it(\Delta_{\text{det}} + \omega_{\text{zm}}^{\text{S}})} + |3\rangle \langle 6| \Omega_{36} e^{it(\Delta_{\text{opt}} + \omega_{\text{zm}}^{\text{S}})} \\ & + |3\rangle \langle 7| \Omega_{37} e^{it(\Delta_{\text{opt}} - \omega_{\text{zm}}^{\text{P}} + \omega_{\text{zm}}^{\text{S}})} \bigg) + h.c. \end{aligned} \quad (4.10)$$

The above Hamiltonian has time dependence at several frequencies, and since the goal of the modeling is to have an efficient numerical simulation of the ion-light dynamics, removing the time dependence of the Hamiltonian is essential. In order to remove the time dependence, we need to switch into an interaction frame that removes the time dependence. We can proceed with first defining a unitary transformation.

$$U = \sum_i e^{i\omega_i t} |i\rangle \langle i|, \quad (4.11)$$

And demand that the interaction Hamiltonian, H_U in the interaction frame of U , be time-independent.

² $H_{\text{rot}} = U H U^\dagger + i\hbar \dot{U} U^\dagger$ with $U = e^{iH_{\text{atom}} t}$.

$$\begin{aligned}
H_U = & - \sum_i |i\rangle \langle i| \omega_i + \\
& \frac{1}{2} \left(|0\rangle \langle 2| \Omega_{02} e^{it(\Delta_{\text{mic}} + \omega_0 - \omega_2)} + |0\rangle \langle 5| \Omega_{05} e^{it(\Delta_{\text{cool}} + \omega_0 - \omega_5 + \omega_{\text{zm}}^{\text{P}})} \right. \\
& + |0\rangle \langle 6| \Omega_{06} e^{it(\Delta_{\text{cool}} + \omega_0 - \omega_6)} + |0\rangle \langle 7| \Omega_{07} e^{it(\Delta_{\text{cool}} + \omega_0 - \omega_7 - \omega_{\text{zm}}^{\text{P}})} \\
& + |1\rangle \langle 4| \Omega_{14} e^{it(\Delta_{\text{det}} + \omega_1 - \omega_4 - \omega_{\text{zm}}^{\text{S}})} + |1\rangle \langle 5| \Omega_{15} e^{it(\Delta_{\text{opt}} + \omega_1 - \omega_5 + \omega_{\text{zm}}^{\text{P}} - \omega_{\text{zm}}^{\text{S}})} \\
& + |1\rangle \langle 6| \Omega_{16} e^{it(\Delta_{\text{opt}} + \omega_1 - \omega_6 - \omega_{\text{zm}}^{\text{S}})} + |2\rangle \langle 4| \Omega_{24} e^{it(\Delta_{\text{det}} + \omega_2 - \omega_4)} \\
& + |2\rangle \langle 5| \Omega_{25} e^{it(\Delta_{\text{opt}} + \omega_2 - \omega_5 + \omega_{\text{zm}}^{\text{P}})} + |2\rangle \langle 7| \Omega_{27} e^{it(\Delta_{\text{opt}} + \omega_2 - \omega_7 - \omega_{\text{zm}}^{\text{P}})} \\
& + |3\rangle \langle 4| \Omega_{34} e^{it(\Delta_{\text{det}} + \omega_3 - \omega_4 + \omega_{\text{zm}}^{\text{S}})} + |3\rangle \langle 6| \Omega_{36} e^{it(\Delta_{\text{opt}} + \omega_3 - \omega_6 + \omega_{\text{zm}}^{\text{S}})} \\
& + |3\rangle \langle 7| \Omega_{37} e^{it(\Delta_{\text{opt}} + \omega_3 - \omega_7 - \omega_{\text{zm}}^{\text{P}} + \omega_{\text{zm}}^{\text{S}})} + |4\rangle \langle 1| \Omega_{14} e^{it(-\Delta_{\text{det}} - \omega_1 + \omega_4 + \omega_{\text{zm}}^{\text{S}})} \\
& + |4\rangle \langle 2| \Omega_{24} e^{it(-\Delta_{\text{det}} - \omega_2 + \omega_4)} + |4\rangle \langle 3| \Omega_{34} e^{it(-\Delta_{\text{det}} - \omega_3 + \omega_4 - \omega_{\text{zm}}^{\text{S}})} \\
& + |5\rangle \langle 0| \Omega_{05} e^{it(-\Delta_{\text{cool}} - \omega_0 + \omega_5 - \omega_{\text{zm}}^{\text{P}})} + |5\rangle \langle 1| \Omega_{15} e^{it(-\Delta_{\text{opt}} - \omega_1 + \omega_5 - \omega_{\text{zm}}^{\text{P}} + \omega_{\text{zm}}^{\text{S}})} \\
& + |5\rangle \langle 2| \Omega_{25} e^{it(-\Delta_{\text{opt}} - \omega_2 + \omega_5 - \omega_{\text{zm}}^{\text{P}})} + |6\rangle \langle 0| \Omega_{06} e^{it(-\Delta_{\text{cool}} - \omega_0 + \omega_6)} \\
& + |6\rangle \langle 1| \Omega_{16} e^{it(-\Delta_{\text{opt}} - \omega_1 + \omega_6 + \omega_{\text{zm}}^{\text{S}})} + |6\rangle \langle 3| \Omega_{36} e^{it(-\Delta_{\text{opt}} - \omega_3 + \omega_6 - \omega_{\text{zm}}^{\text{S}})} \\
& + |7\rangle \langle 0| \Omega_{07} e^{it(-\Delta_{\text{cool}} - \omega_0 + \omega_7 + \omega_{\text{zm}}^{\text{P}})} + |7\rangle \langle 2| \Omega_{27} e^{it(-\Delta_{\text{opt}} - \omega_2 + \omega_7 + \omega_{\text{zm}}^{\text{P}})} \\
& \left. + |7\rangle \langle 3| \Omega_{37} e^{it(-\Delta_{\text{opt}} - \omega_3 + \omega_7 + \omega_{\text{zm}}^{\text{P}} - \omega_{\text{zm}}^{\text{S}})} + |2\rangle \langle 0| \Omega_{02} e^{it(-\Delta_{\text{mic}} - \omega_0 + \omega_2)} \right). \tag{4.12}
\end{aligned}$$

It can be seen that the problem has now been reduced to finding the values of ω_i such that each of the following equations is satisfied.

$$\begin{aligned}
\Delta_{\text{mic}} + \omega_0 - \omega_2 &= 0 \\
\Delta_{\text{cool}} + \omega_0 - \omega_5 + \omega_{\text{zm}}^{\text{P}} &= 0 \\
\Delta_{\text{cool}} + \omega_0 - \omega_6 &= 0 \\
\Delta_{\text{cool}} + \omega_0 - \omega_7 - \omega_{\text{zm}}^{\text{P}} &= 0 \\
\Delta_{\text{det}} + \omega_1 - \omega_4 - \omega_{\text{zm}}^{\text{S}} &= 0 \\
\Delta_{\text{opt}} + \omega_1 - \omega_5 + \omega_{\text{zm}}^{\text{P}} - \omega_{\text{zm}}^{\text{S}} &= 0 \\
\Delta_{\text{opt}} + \omega_1 - \omega_6 - \omega_{\text{zm}}^{\text{S}} &= 0 \\
\Delta_{\text{det}} + \omega_2 - \omega_4 &= 0 \\
\Delta_{\text{opt}} + \omega_2 - \omega_5 + \omega_{\text{zm}}^{\text{P}} &= 0 \\
\Delta_{\text{opt}} + \omega_2 - \omega_7 - \omega_{\text{zm}}^{\text{P}} &= 0 \\
\Delta_{\text{det}} + \omega_3 - \omega_4 + \omega_{\text{zm}}^{\text{S}} &= 0 \\
\Delta_{\text{opt}} + \omega_3 - \omega_6 + \omega_{\text{zm}}^{\text{S}} &= 0 \\
\Delta_{\text{opt}} + \omega_3 - \omega_7 - \omega_{\text{zm}}^{\text{P}} + \omega_{\text{zm}}^{\text{S}} &= 0
\end{aligned} \tag{4.13}$$

These equations are not always solvable; however, it turns out that there is an elegant graph theory approach to treating such multi-level problems [138] that gives conditions for the existence of the solution and also how to assign values to each ω_i .

We first start by drawing graphs that describe the system and the couplings as shown in Fig. 4.4 a) and b). In Fig. 4.4 a), we consider all the couplings defined in Eq. (4.8) and in Fig. 4.4 b) where we have left out the couplings of $F = 0 \rightarrow F' = 1$ or levels coupled through light at frequency ω_{cool} . Here, the vertices of the graph are the energy levels, and only the energy levels coupled by light are connected through the edges. Once the edges are drawn, we assign weights to the edges connecting the i^{th} and j^{th} vertices such that the weight of each edge is the ‘effective detuning’, i.e., the coefficient in the exponential in the $(i, j)^{\text{th}}$ term³ in the matrix representation of H_{rot} from Eq. (4.10). Now we identify all the closed loops in the graph and if the sum of the ‘effective detunings’ in each closed loop is zero then the system is solvable, i.e. the time dependence of the Hamiltonian can be removed. Note that while summing the detunings in a given closed loop, the vertices need to be iterated in order, and the calculation of the effective detunings should take this order into account.

³The order of i and j matters, so this is not precisely the weight.

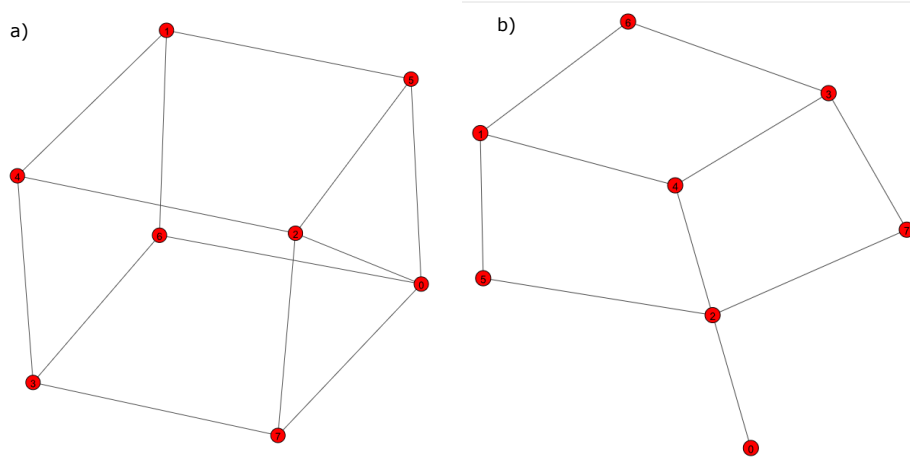


Figure 4.4: Coupling graphs for $^{171}\text{Yb}^+$ ion interacting with light and microwave radiation

a) All allowed $^2\text{S}_{1/2}$ to $^2\text{P}_{1/2}$ transitions and microwave coupling of the clock states. We shall define this as the system A.

b) All couplings in **a)** except $^2\text{S}_{1/2} F=0$ to $^2\text{P}_{1/2} F'=1$. We shall define this as the system B.

For the graph in Fig. 4.4 b) (system B), the effective detunings on all closed loops add up to zero; however, for the graph in Fig. 4.4 a) (system A) the effective detunings do not add up to zero for all closed loops. This means that for all values of Δ_{micro} , Δ_{opt} , Δ_{det} , the time dependence in system B can be removed; however, this is not true for the case of system A where the time dependence can be removed only for specific values of ω_{cool} . To assign values to all ω_i s, we proceed by solving Equations (4.13) following the graph for system B in the following order.

- set $\omega_0 = 0$
- solve for ω_2
- solve for ω_4 , ω_5 and ω_7
- solve for ω_1 and ω_3
- solve for ω_6

Plugging the values of ω_i from above into Eq. (4.12) and defining $\delta := \Delta_{\text{cool}} - \Delta_{\text{micro}} - \Delta_{\text{opt}}$, we get the following simplified form of H_U .

$$H_U = \begin{bmatrix} 0 & 0 & \frac{\Omega_{02}}{2} & 0 & 0 & \frac{\Omega_{05}}{2}e^{i\delta t} & \frac{\Omega_{06}}{2}e^{i\delta t} & \frac{\Omega_{07}}{2}e^{i\delta t} \\ 0 & \Delta_1 & 0 & 0 & \frac{\Omega_{14}}{2} & \frac{\Omega_{15}}{2} & \frac{\Omega_{16}}{2} & 0 \\ \frac{\Omega_{02}}{2} & 0 & \Delta_2 & 0 & \frac{\Omega_{24}}{2} & \frac{\Omega_{25}}{2} & 0 & \frac{\Omega_{27}}{2} \\ 0 & 0 & 0 & \Delta_3 & \frac{\Omega_{34}}{2} & 0 & \frac{\Omega_{36}}{2} & \frac{\Omega_{37}}{2} \\ 0 & \frac{\Omega_{14}}{2} & \frac{\Omega_{24}}{2} & \frac{\Omega_{34}}{2} & \Delta_4 & 0 & 0 & 0 \\ \frac{\Omega_{05}}{2}e^{-i\delta t} & \frac{\Omega_{15}}{2} & \frac{\Omega_{25}}{2} & 0 & 0 & \Delta_5 & 0 & 0 \\ \frac{\Omega_{06}}{2}e^{-i\delta t} & \frac{\Omega_{16}}{2} & 0 & \frac{\Omega_{36}}{2} & 0 & 0 & \Delta_6 & 0 \\ \frac{\Omega_{07}}{2}e^{-i\delta t} & 0 & \frac{\Omega_{27}}{2} & \frac{\Omega_{37}}{2} & 0 & 0 & 0 & \Delta_7 \end{bmatrix}, \quad (4.14)$$

with

$$\begin{aligned} \Delta_1 &= -\Delta_{\text{mic}} - \omega_{\text{zm}}^{\text{S}} \\ \Delta_2 &= -\Delta_{\text{mic}} \\ \Delta_3 &= -\Delta_{\text{mic}} + \omega_{\text{zm}}^{\text{S}} \\ \Delta_4 &= -\Delta_{\text{det}} - \Delta_{\text{mic}} \\ \Delta_5 &= -\Delta_{\text{mic}} - \Delta_{\text{opt}} - \omega_{\text{zm}}^{\text{P}} \\ \Delta_6 &= -\Delta_{\text{mic}} - \Delta_{\text{opt}} \\ \Delta_7 &= -\Delta_{\text{mic}} - \Delta_{\text{opt}} + \omega_{\text{zm}}^{\text{P}}. \end{aligned} \quad (4.15)$$

Note the presence of $e^{\pm i\delta t}$ in some of the off-diagonal elements of H_U . Since we concluded from the graph approach that the complete system was not solvable, we do not expect the complete time dependence of the problem to be removed; however, when $\delta = 0$, the system becomes solvable.

In our experimental setup, the frequency ω_{cool} comes from the same beam as ω_{opt} with EOM modulation at frequency $\omega_{\text{hf}}^{\text{S}}$, and hence the condition $\delta = 0$ is satisfied. With this, we get the fully time-independent Hamiltonian.

$$H_U = \begin{bmatrix} 0 & 0 & \frac{\Omega_{02}}{2} & 0 & 0 & \frac{\Omega_{05}}{2} & \frac{\Omega_{06}}{2} & \frac{\Omega_{07}}{2} \\ 0 & \Delta_1 & 0 & 0 & \frac{\Omega_{14}}{2} & \frac{\Omega_{15}}{2} & \frac{\Omega_{16}}{2} & 0 \\ \frac{\Omega_{02}}{2} & 0 & \Delta_2 & 0 & \frac{\Omega_{24}}{2} & \frac{\Omega_{25}}{2} & 0 & \frac{\Omega_{27}}{2} \\ 0 & 0 & 0 & \Delta_3 & \frac{\Omega_{34}}{2} & 0 & \frac{\Omega_{36}}{2} & \frac{\Omega_{37}}{2} \\ 0 & \frac{\Omega_{14}}{2} & \frac{\Omega_{24}}{2} & \frac{\Omega_{34}}{2} & \Delta_4 & 0 & 0 & 0 \\ \frac{\Omega_{05}}{2} & \frac{\Omega_{15}}{2} & \frac{\Omega_{25}}{2} & 0 & 0 & \Delta_5 & 0 & 0 \\ \frac{\Omega_{06}}{2} & \frac{\Omega_{16}}{2} & 0 & \frac{\Omega_{36}}{2} & 0 & 0 & \Delta_6 & 0 \\ \frac{\Omega_{07}}{2} & 0 & \frac{\Omega_{27}}{2} & \frac{\Omega_{37}}{2} & 0 & 0 & 0 & \Delta_7 \end{bmatrix}, \quad (4.16)$$

With the diagonal elements given in Eq. (4.15).

Since $^2S_{1/2}$ to $^2P_{1/2}$ is a dipole transition, $^2P_{1/2}$ can decay back to $^2S_{1/2}$ through spontaneous emission. The spontaneous emission results from the coupling of the atom (ion) to the vacuum modes of radiation and can be accounted for through a master equation approach as shown in [139]. Instead of solving the Schrodinger's equation for the system, we now have to solve for the Lindblad (or Gorini-Kossakowski-Sudarshan-Lindblad) master equation.

$$\dot{\rho}(t) = -\frac{i}{\hbar}[H(t), \rho(t)] + \sum_n \frac{1}{2} [2C_n \rho(t) C_n^\dagger - \rho(t) C_n^\dagger C_n - C_n^\dagger C_n \rho(t)]. \quad (4.17)$$

Where ρ is the density matrix, and $C_n = \sqrt{\Gamma_n} A_n$ are the collapse operators, with A_n being the operators that describe the action the environment induces on the system. The collapse operators that account for the spontaneous emission of the population in $^2P_{1/2}$ into $^2S_{1/2}$ are

$$\begin{aligned}
C_{14} &= \sqrt{\frac{\Gamma_P}{3}} |1\rangle \langle 4|, C_{24} = \sqrt{\frac{\Gamma_P}{3}} |2\rangle \langle 4|, C_{34} = \sqrt{\frac{\Gamma_P}{3}} |3\rangle \langle 4|, \\
C_{05} &= \sqrt{\frac{\Gamma_P}{3}} |0\rangle \langle 5|, C_{15} = \sqrt{\frac{\Gamma_P}{3}} |1\rangle \langle 5|, C_{25} = \sqrt{\frac{\Gamma_P}{3}} |2\rangle \langle 5|, \\
C_{06} &= \sqrt{\frac{\Gamma_P}{3}} |0\rangle \langle 6|, C_{16} = \sqrt{\frac{\Gamma_P}{3}} |1\rangle \langle 6|, C_{36} = \sqrt{\frac{\Gamma_P}{3}} |3\rangle \langle 6|, \\
C_{07} &= \sqrt{\frac{\Gamma_P}{3}} |0\rangle \langle 7|, C_{27} = \sqrt{\frac{\Gamma_P}{3}} |2\rangle \langle 7|, C_{37} = \sqrt{\frac{\Gamma_P}{3}} |3\rangle \langle 7|.
\end{aligned} \tag{4.18}$$

To get the time evolution under the applied optical and microwave frequencies, we numerically solve for the master equation with the Hamiltonian H_U in Eq. (4.16), and the collapse operators above using the quip package in Python [124].

4.3.1 Rabi Frequencies and Polarization

The above analysis is presented in terms of the Rabi frequencies; however, in the lab, the laser power is usually measured as an intensity, and hence, conversion between these two is required. The Rabi frequencies for a simple 2-level system are set according to the formula:

$$\frac{I}{I_{\text{sat}}} = \frac{2\Omega^2}{\Gamma^2},$$

where I is the intensity of the laser, I_{sat} is the saturation intensity [21], and Γ is the spontaneous emission rate of the transition. In our case, we are interested in finding the Rabi frequency pertaining to a specific transition, i.e

$$\Omega_{F,m_F,F',m_{F'}} = \frac{\langle F, m_F | \vec{d} \cdot \vec{E} | F', m_{F'} \rangle}{\hbar}$$

To calculate the above expression, we will follow the approach in [140]. We begin by writing the dot product in the above equation in the spherical basis since it is more convenient when dealing with angular momentum. The unit vectors in the spherical basis are given as

$$\begin{aligned}
\hat{e}_{\pm 1} &:= \mp \frac{1}{\sqrt{2}} (\hat{x} \pm i\hat{y}) = -(\hat{e}_{\mp 1})^*, \\
\hat{e}_0 &:= \hat{z} = (\hat{e}_0)^*.
\end{aligned} \tag{4.19}$$

So, in the spherical basis, any vector $V = V_x\hat{x} + V_y\hat{y} + V_z\hat{z}$ has the following components.

$$V_{\pm 1} = \mp \frac{1}{\sqrt{2}} (V_x \pm iV_y),$$

$$V_0 = V_z.$$

The above also applies to the complex phasor $E = E_x\hat{x} + E_y\hat{y} + E_z\hat{z}$ and hence the dot product $\vec{d} \cdot \vec{E}$ can be written as

$$\vec{d} \cdot \vec{E} = \sum_q = (-1)^q E_q d_{-q}.$$

Since E_q is a complex number, we need to evaluate $\langle F, m_F | d_q | F', m_{F'} \rangle$ and applying the Wigner-Eckart theorem, we get

$$\langle F, m_F | d_q | F', m_{F'} \rangle = \langle F, m_F | F', m_{F'}, 1, q \rangle \langle F || d_q || F' \rangle.$$

Now, the reduced matrix element can be further broken down as

$$\begin{aligned} \langle F || d || F' \rangle &= \langle JIF || d || J'IF' \rangle \\ &= \langle J || d || J' \rangle (-1)^{F'+J+1+I} \\ &\quad \sqrt{(2F'+1)(2J+1)} \begin{Bmatrix} J & J' & 1 \\ F' & F & I \end{Bmatrix}. \end{aligned}$$

The reduced matrix element between the J levels can simply be calculated from the decay rate of the excited state using Fermi's golden rule as follows:

$$\Gamma_{J_g J_e} = \frac{\omega_0^3}{3\pi\epsilon_0 \hbar c^3} \frac{2J_g + 1}{2J_e + 1} |\langle J_g || d || J_e \rangle|^2$$

Where J_g and J_e correspond to the ground and the excited states. Since it is commonly used in $^{171}\text{Yb}^+$ literature, we introduce the saturation intensity as defined for the $^2\text{S}_{1/2}$ to $^2\text{P}_{1/2}$ ignoring the hyperfine structure:

$$I_{\text{sat}} = \frac{\pi \Gamma c \hbar}{3\lambda^3}. \quad (4.20)$$

Combining these equations along with $|E_q| = \sqrt{I_q/2c\epsilon_0}$, we get

$$\Omega_{F,m_F,F',m_{F'}}^2 = \frac{I_q}{I_{\text{sat}}} \frac{\Gamma_{J_g J_e}^2}{2} |\langle F, m_F | F', m_{F',1,q} \rangle|^2 \times \\ (2F' + 1)(2J + 1) \left\{ \begin{matrix} J & J' & 1 \\ F' & F & I \end{matrix} \right\}^2 \times \frac{2J_e + 1}{2J_g + 1}. \quad (4.21)$$

In the case of $^{171}\text{Yb}^+$, for all transitions between $^2\text{S}_{1/2}$ and $^2\text{P}_{1/2}$, the first line of the expression in Eq. (4.21) gives the selection rules. The $E_{\pm}$ components of the electric field induce the transitions $m_F = m_{F'} \pm 1$ and the E_{π} component induces the transition $m_F = m_{F'}$, $F \neq F'$. The second line of the above expression evaluates to $1/3$, leaving us with a particularly simple expression for the Rabi frequency

$$\Omega^2 = \frac{I_q}{I_{\text{sat}}} \frac{\Gamma^2}{6} \quad (4.22)$$

For simulations, we set the Rabi frequencies according to a total s parameter $s = I/I_{\text{sat}}$, and the intensity ratios, c_+ , c_- , c_{π} . Where $c_q = I_q/I$ are the intensity ratios corresponding to the respective polarization components and the expression in Eq. (4.22) can be used to set the Rabi frequency whenever I_q leads to a transition satisfying the selection rules.

4.4 Modelling ion-light interactions: Reduced ground state evolution

In the previous section, we discussed the modeling of ion-light interactions by simulating the complete atomic density matrix for the eight levels in $^2\text{S}_{1/2}$ and $^2\text{P}_{1/2}$ under the effective Hamiltonian for the interaction. It turns out that if coherent effects are discarded, simulating the population dynamics in the $^2\text{S}_{1/2}$ manifold under the influence of optical pumping light can be drastically simplified [141]. We first start by noting that the optical pumping light connects different magnetic sublevels in $^2\text{S}_{1/2}$ to $^2\text{P}_{1/2}$ $F'=1$, and each pair of connected levels can be treated as a separate two-level system. Since the lifetime of the $^2\text{P}_{1/2}$ is very small, the population mainly stays in the $^2\text{S}_{1/2}$ manifold, and redistribution of the population within the $^2\text{S}_{1/2}$ manifold occurs due to the applied light. This redistribution can be modeled as a system of differential equations that govern the population

of each sublevel depending on its absorption rate and collection rate (due to decay from $^2P_{1/2}$). It should be noted that this technique is only valid for modeling incoherent population transfer within the $^2S_{1/2}$ manifold, and all information about the induced coherences and light shifts is lost. However, compared to the previous section where a (8×8) density matrix was being evolved, this technique is computationally less expensive because the dynamics are modelled as the evolution of a (4×1) population vector.

We now discuss the general theoretical framework to model the optical pumping rate equations in $^{171}\text{Yb}^+$. The general formalism will be as follows: g_n represents the ground state levels, and the set e_n represents the excited state levels. If the radiative lifetime of any of the excited states e_k is τ_k , then the natural linewidth of any transition to the excited state will be

$$\Gamma_k = \frac{1}{\tau_k} = \sum_{j=1}^{N_g} A_{jk} = \Gamma_k \sum_{j=1}^{N_g} \beta_{jk}. \quad (4.23)$$

Here, β_{jk} is the branching ratio of the radiative decay from state e_k to g_j and we have that $\sum_{j=1}^{N_g} \beta_{jk} = 1$. The notation here is such that the first index denotes the levels in the ground manifold, and the second index denotes the levels in the excited manifold. Since the idea here is to treat each 2-level system of coupled ground and excited states separately, we only require an expression for the rate of excitation from the i^{th} ground state to the j^{th} excited state R_{jk}^l . From standard textbook calculation for two-level systems [21] we have that

$$R_{jk}^l(s, \Delta) = \frac{\Gamma_k}{2} \frac{s}{1 + s + (2\Delta_{jk}^l/\Gamma_k)^2}, \quad (4.24)$$

where $s = I/I_{\text{sat}}$, I_{sat} is the saturation intensity as defined in Eq. (4.20) and the third index l accounts for the different frequencies of light.

4.4.1 Time evolution

For calculating the time evolution of the ground state populations, we now have to account for two factors

- rate of excitation from g_j to e_k for all j, k
- rate of decay of e_k through all possible dipole allowed paths

This means that if we have two ground state levels g_1 and g_2 , the population transfer from g_1 to g_2 can happen through excitation from g_1 to any/all excited states e_k such that e_k can decay into g_2 . We assume that the spontaneous decay is instantaneous compared to the timescales in the problem. In the limit that the intensity is much below the saturation intensity, this is a valid assumption. In general, we can show that the differential equation governing the populations in the ground-state manifold will be [141]

$$\frac{d}{dt}G_n(t) = \sum_{j \neq n} G_j(t) \left[\sum_k R_{jk}^l \beta_{jk} \beta_{nk} \right] - G_n(t) \left[\sum_k R_{nk}^l \beta_{nk} (1 - \beta_{nk}) \right]. \quad (4.25)$$

The index l above denotes each of the different beams used to couple the ground and excited state manifolds. For example, in our model, this denotes each polarization component, hence $l \in \{\sigma_+, \sigma_-, \pi\}$. We can now write the differential equations governing the time evolution of the ground state population vector, $G = (g_0, g_1, g_2, g_3)$, in terms of two matrices; matrix R accounts for the absorption rates and matrix B that accounts for the branching ratios.

$$\dot{G}(t) = MG = \sum_l (\mathbf{R}^l \odot \mathbf{B}^l)G \quad (4.26)$$

Where $\odot$ represents element-wise multiplication. For $^{171}\text{Yb}^+$, each component of light (σ_+, σ_-, π) connects each ground level only to a single excited state, and also each of the β 's is $1/3$ yielding

$$\mathbf{B}_{mn}^l = \beta_{mk} \beta_{nk} + \delta_{mn} \beta_{nk} (1 - \beta_{nk}) \quad (4.27)$$

Where $k = m + 1, m - 1, m$ for $l = \sigma_+, \sigma_-, \pi$. Written out explicitly, the $\mathbf{B}$ matrices are

$$\mathbf{B}^\pi = \frac{1}{9} \begin{bmatrix} 0 & 1 & 0 & 1 \\ 0 & -2 & 0 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & -2 \end{bmatrix},$$

$$\mathbf{B}^{\sigma_+} = \frac{1}{9} \begin{bmatrix} 0 & 1 & 1 & 0 \\ 0 & -2 & 0 & 0 \\ 0 & 0 & -2 & 0 \\ 0 & 1 & 1 & 0 \end{bmatrix},$$

$$\mathbf{B}^{\sigma_-} = \frac{1}{9} \begin{bmatrix} 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & -2 \end{bmatrix}. \quad (4.28)$$

Similarly, the $\mathbf{R}$ matrices for each of the polarization are given as

$$\begin{aligned} \mathbf{R}^\pi &= \begin{bmatrix} 0 & R(s, \Delta - (\omega_{\text{zm}}^{\text{S}} - \omega_{\text{zm}}^{\text{P}})) & 0 & R(s, \Delta - (\omega_{\text{zm}}^{\text{P}} - \omega_{\text{zm}}^{\text{S}})) \\ 0 & R(s, \Delta - (\omega_{\text{zm}}^{\text{S}} - \omega_{\text{zm}}^{\text{P}})) & 0 & 0 \\ 0 & R(s, \Delta - (\omega_{\text{zm}}^{\text{S}} - \omega_{\text{zm}}^{\text{P}})) & 0 & R(s, \Delta - (\omega_{\text{zm}}^{\text{P}} - \omega_{\text{zm}}^{\text{S}})) \\ 0 & 0 & 0 & R(s, \Delta - (\omega_{\text{zm}}^{\text{P}} - \omega_{\text{zm}}^{\text{S}})) \end{bmatrix}, \\ \mathbf{R}^{\sigma_+} &= \begin{bmatrix} 0 & R(s, \Delta - \omega_{\text{zm}}^{\text{S}}) & R(s, \Delta - \omega_{\text{zm}}^{\text{P}}) & 0 \\ 0 & R(s, \Delta - \omega_{\text{zm}}^{\text{S}}) & 0 & 0 \\ 0 & 0 & R(s, \Delta - \omega_{\text{zm}}^{\text{P}}) & 0 \\ 0 & R(s, \Delta - \omega_{\text{zm}}^{\text{S}}) & R(s, \Delta - \omega_{\text{zm}}^{\text{P}}) & 0 \end{bmatrix}, \\ \mathbf{R}^{\sigma_-} &= \begin{bmatrix} 0 & 0 & R(s, \Delta + \omega_{\text{zm}}^{\text{P}}) & R(s, \Delta + \omega_{\text{zm}}^{\text{S}}) \\ 0 & 0 & R(s, \Delta + \omega_{\text{zm}}^{\text{P}}) & R(s, \Delta + \omega_{\text{zm}}^{\text{S}}) \\ 0 & 0 & R(s, \Delta + \omega_{\text{zm}}^{\text{P}}) & 0 \\ 0 & 0 & 0 & R(s, \Delta + \omega_{\text{zm}}^{\text{S}}) \end{bmatrix}. \end{aligned} \quad (4.29)$$

Here, the function R is defined in Eq. (4.24), and since the decay rate of all excited states is the same, the functional form is the same. The other symbols are the same as defined in the last section, and the detuning Δ is defined as $\Delta := (\omega_{\text{opt}} - \omega_{\text{SP}})$. Note that typically in an experiment, the three polarizations come from the same beam. However, the above $\mathbf{R}$ matrices can also account for different detunings for each beam by simply replacing the Δ in each expression with the specific detuning Δ^l . With the $\mathbf{R}$ and $\mathbf{B}$ matrices, the redistribution of the populations in the ground state can be found by simply evolving the initial population vector in $^2\text{S}_{1/2}$, $G(t = t_0)$, according to Eq. (4.25).

4.5 Model Verification

The first step towards verification of the two models above is the comparison between their results. Since the full-density matrix approach automatically accounts for the Stark shifts induced as a result of the interacting light, we expect the results to be more accurate. Fig. 4.5 shows the optical pumping curves generated for ions initialized in $^2S_{1/2} F=1$ in a mixed state with the same probability of being in $m_F = \pm 1, 0$ and the light intensity varied from $s = 0.2$ to $s = 1$ where $s = I/I_{\text{sat}}$ and arbitrarily chosen polarization. For low values of s , the curves mostly overlap; however, for higher values of s , slight deviations occur in the curves. The same trend can be observed in Fig. 4.6, where the results are plotted for the light intensity from $s = 1$ to $s = 10$.

The two models produce dynamics consistent with each other, but the real test would be fitting the experimental data. Fig. 4.7 shows a schematic of the setup used for data acquisition to validate the models. The optical pumping light is incident on the ion through an acousto-optic modulator (AOM) and a half-wave plate. The AOM allows us to change the beam power and, hence, the intensity of the optical pumping beam at the ion location by changing the RF power sent to the AOM. The AOM response, i.e., optical beam power vs. RF power, is calibrated before the data is taken so that the precise scaling in the optical power with respect to the RF power is known. The half-wave plate allows us to rotate the polarization of the beam incident on the ion by a known amount. With these two variables that allow us to change the intensity and polarization of light with known amounts, we took multiple optical pumping curves for the ions initialized in $^2S_{1/2} F = 1$ $m_F = 0$, that is, the clock state $|\uparrow\rangle$. Some of these curves are shown in Fig. 4.7. To experimentally acquire the optical pumping curves, we measured the population of in the $^2S_{1/2} F=1$ manifold at different interaction times τ between the optical pumping light and the ion. The pumping curves were acquired for eight different values of s corresponding to AOM powers P_{AOM} from -3 dBm to 4 dBm and eleven different values of the wave plate angle θ from $\theta = 0$ to $\theta = 45$ degrees.

To fit the experimental data to the model, we assumed an arbitrary initial guess of the intensity s^0 at the lowest AOM power and an arbitrary initial guess of the light polarization Jones vector (c_x^0, c_y^0) at the waveplate angle $\theta = 0$ with c_z being complex. Note that since the AOM and wave plate transfer functions are known, these values can be used to generate intensity and polarization values for all the curves. To fit the data to the model, we minimize the mean squared error between the predicted and experimental curves in the entire dataset by varying $s, (c_x, c_y)$. The values $s^{\text{fit}}, (c_x^{\text{fit}}, c_y^{\text{fit}})$ that minimize the error are the intensity and polarization of the beam extracted at $P_{\text{AOM}} = -3$ dBm and $\theta = 0$ and the beam parameters at different values of P_{AOM} and θ can be extracted simply by applying

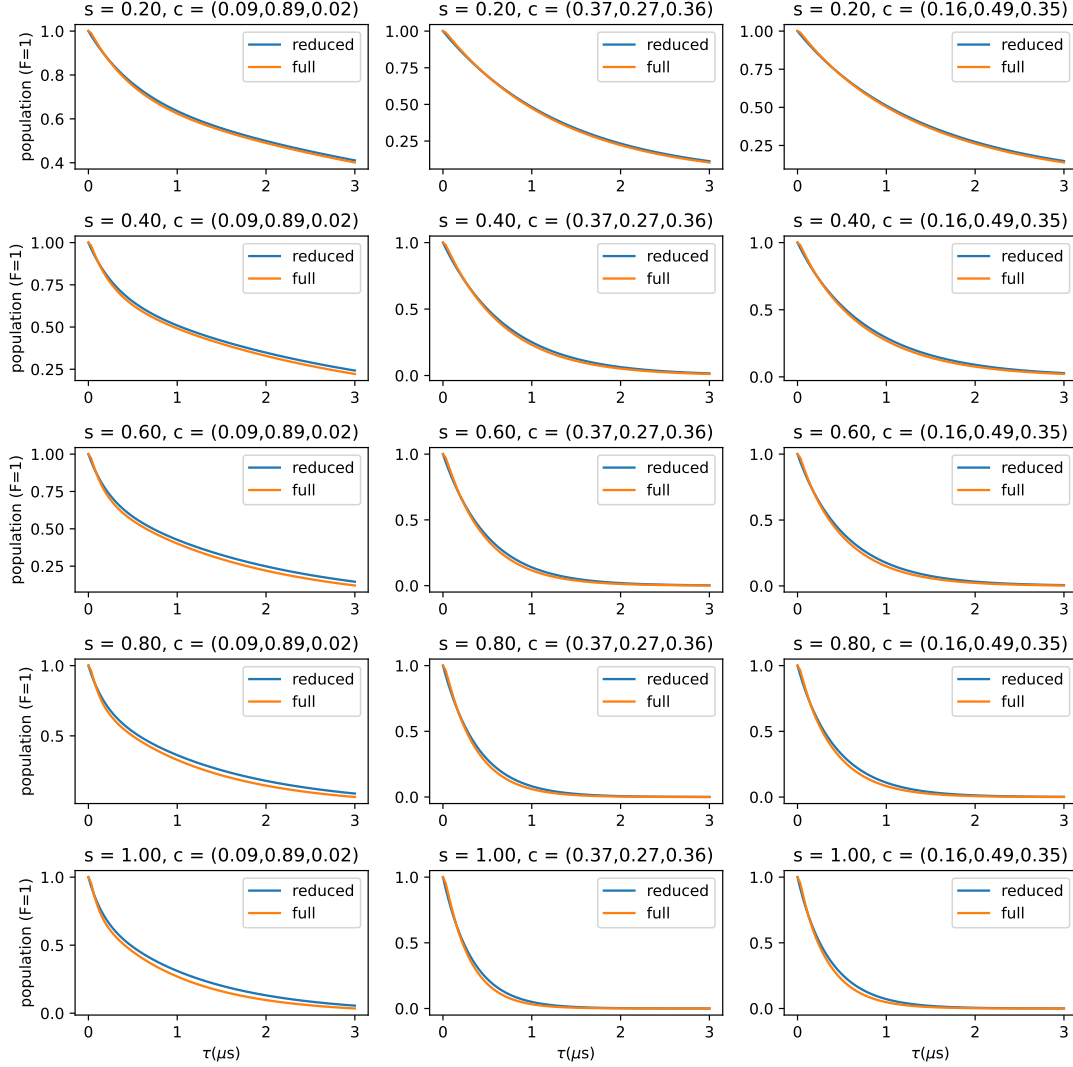


Figure 4.5: Comparison between full and reduced solver: I

The initial state for all simulations is a mixed state with an equal mixture of $^2S_{1/2} F=1$ $m_F = \pm 1, 0$. All rows have the same polarization, and all columns have the same intensity. light intensity is varied from $s = 0.2$ to $s = 1$ where $s = I/I_{\text{sat}}$ and arbitrarily chosen values of polarization. The deviations between the two models increase as the light intensity increases.

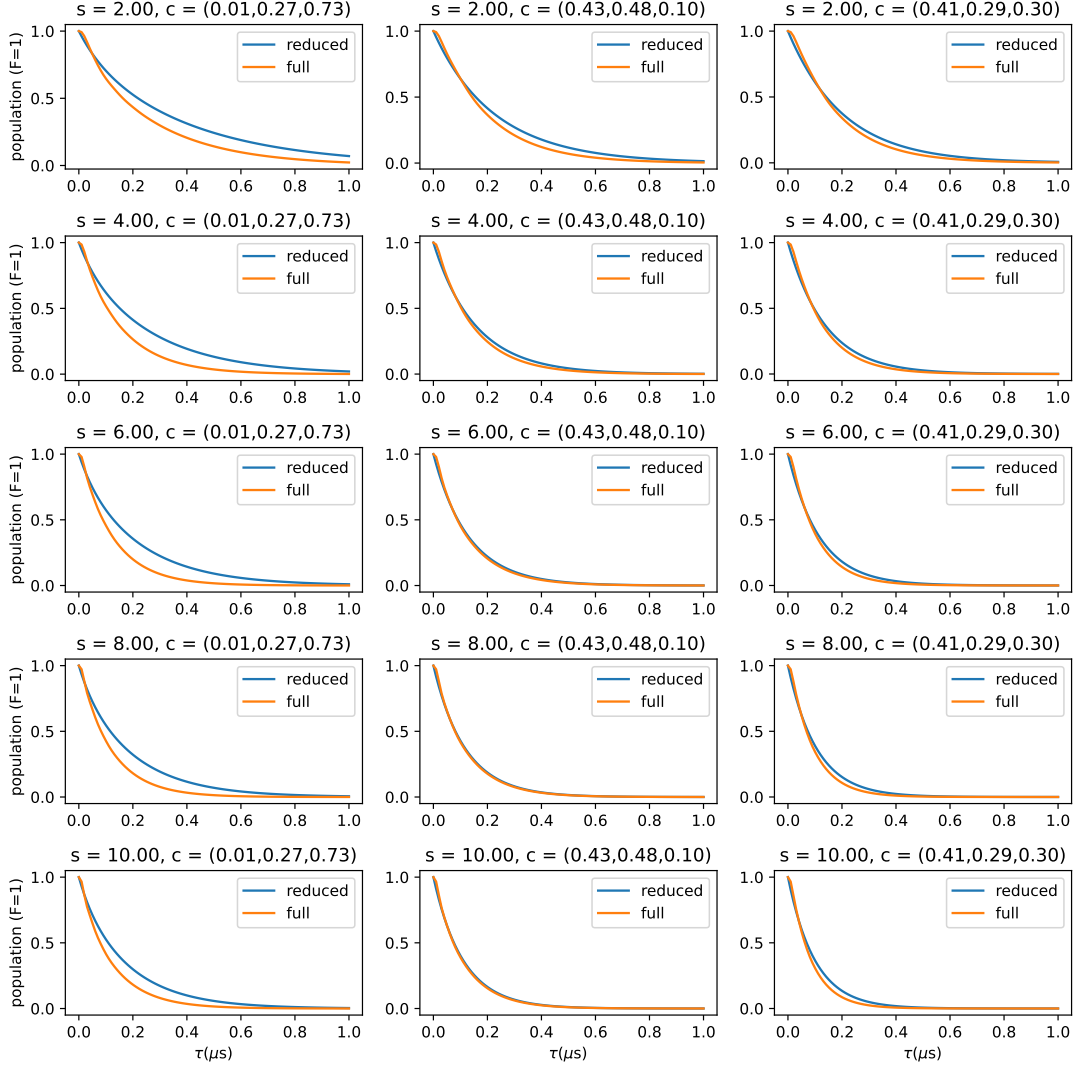


Figure 4.6: Comparison between full and reduced solver: II

The initial state for all simulations is a mixed state with an equal mixture of $^2S_{1/2} F=1$ $m_F = \pm 1, 0$. All rows have the same polarization, and all columns have the same intensity. light intensity is varied from $s = 2$ to $s = 10$ where $s = I/I_{\text{sat}}$ and arbitrarily chosen values of polarization. The deviations between the two models increase as the light intensity increases.

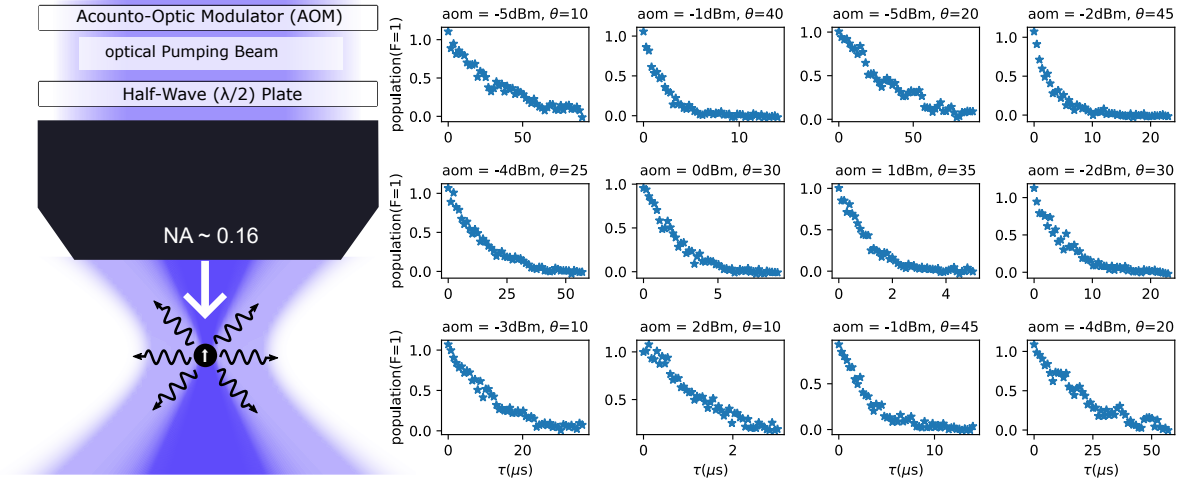


Figure 4.7: Data Acquisition for Model Validation

To validate the models developed earlier, several optical pumping curves of the ions were recorded. The power in the optical pumping beam was changed using the RF power sent to the AOM, and the polarization was changed by rotating the $\lambda/2$ plate. The transfer function of the AOM, i.e., RF power vs Optical power, was characterized before recording the curves, and the wave-plate transfer function is known trivially. A total of 88 optical pumping curves were recorded, twelve of which are shown on the right with the AOM power and waveplate angle θ labeled on each plot.

the known AOM and waveplate transfer functions. Before fitting, twelve randomly chosen pumping curves were excluded from the fitting as a test set to check if the pumping curves predicted by the simulation model for values of $s, (c_x, c_y)$ corresponding to the respective P_{AOM} and θ for these curves match the experimental curves. Fig. 4.8 shows these twelve predicted curves together with the experimental data; the predictions match well with the experimental curves.

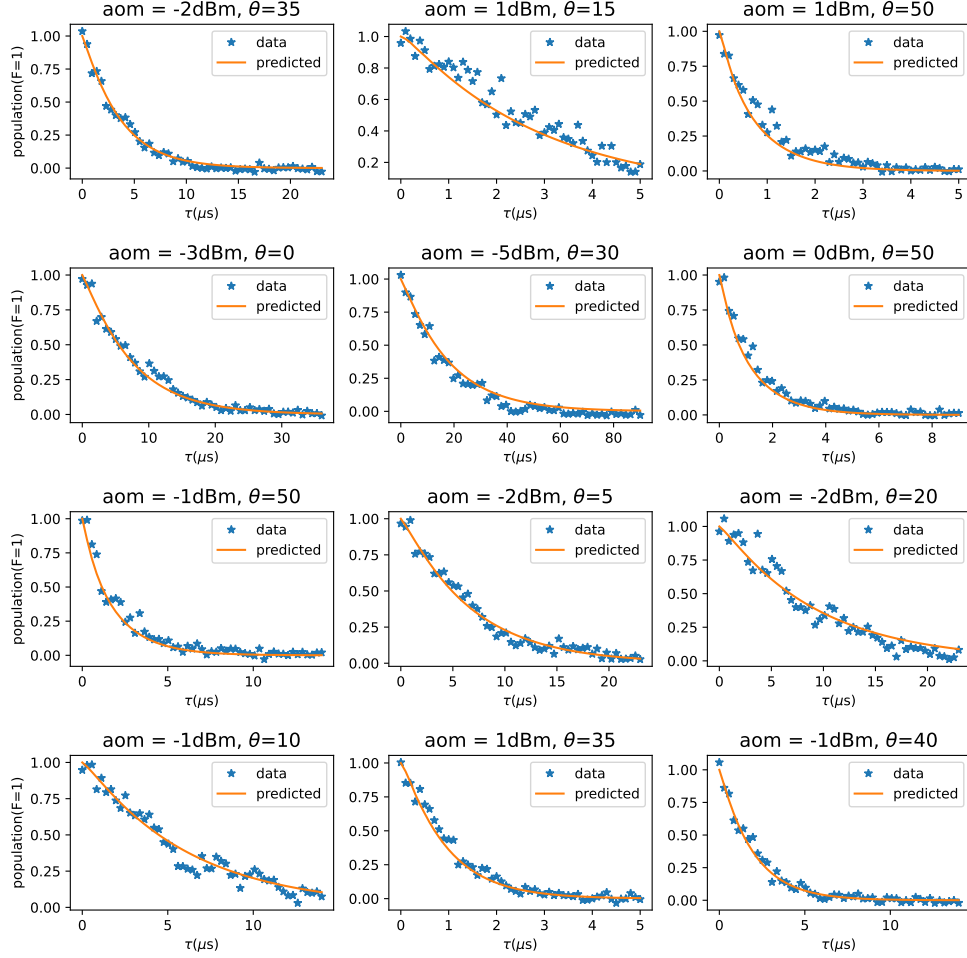


Figure 4.8: Model Validation using test set

Out of the 88 recorded optical pumping curves (see text), some shown in Fig. 4.7, twelve were excluded from fitting as a test set for validating the model accuracy. The above plots show the experimental along with the predicted curves. The predictions match well with the experimental curves, validating the accuracy of the modeling technique.

4.6 Intelligent Sensing

The function, F_{fwd} , that maps the intensity and polarization values of light to the optical pumping decay curves, i.e., our simulation model, is not a one-to-one function, and in general, several different values of beam parameters can lead to similar population decay curves. The previous method of fitting the experimental data set to F_{fwd} works well because we fit several optical pumping curves generated from different beam parameters constrained by a known functional dependence, i.e., we know precisely the AOM and the wave plate transformations. For the discussion from now on, we will use F_{fwd} to denote the full density matrix evolution model in Sec. 4.3. The procedure of fitting the data set shown in Fig. 4.7 to F_{fwd} took more than an hour on an advanced desktop computer with an AMD Ryzen 7 2700x 8 core CPU. In fact, the motivation behind developing the second simulation method discussed in Sec. 4.4 was to reduce the computational cost of parameter extraction and generate efficient guesses for parameter estimation using the full-density matrix solver.

Through experimentation, we found that the least number of decay curves to extract the beam intensity and polarization is three: one decay curve for the ion initialized in each of the magnetic sublevels in $^2\text{S}_{1/2} F = 1$. This also makes intuitive sense because the population in $m_F = 1, 0, -1$ is more sensitive to $\sigma_+, \sigma_\pi, \sigma_-$ polarized light. However, from a computational point of view, fitting is an inherently sequential operation with minimal parallelization possible. While minimizing the least-square error between the experimental and predicted decay curves, new decay curves need to be simulated at each update of the laser parameters. This computational bottleneck severely limits the applicability of this technique to characterize optical setups in which light parameters at several points in the image plane have to be reconstructed. To scale up this technique, a different method for parameter extraction is required that can overcome the computational overhead of fitting.

The task of estimating the beam parameters from the optical pumping curves falls under the category of inverse problems [142], where the goal is to calculate the causal factors that produced a set of observations. Inverse problems have wide applicability in signal processing, computer vision [143], machine learning [144], and physics [145], as they allow the estimation of parameters that may not be observed directly. Finding F_{back} , which is the inverse function corresponding to F_{fwd} , is, in general, a difficult task and may not be useful for the extraction of beam parameters since F_{fwd} is not a one-to-one function. For beam parameter extraction, the inverse function F'_{back} for the modified function F'_{fwd} , which gives the three optical pumping curves corresponding to the ion initialized in the three magnetic sublevels in $^2\text{S}_{1/2} F = 1$, is useful.

The problem of finding F'_{back} can be addressed by using machine learning algorithms [146] where F'_{back} is approximated by a deep neural network (See Fig. 4.9). The approach is

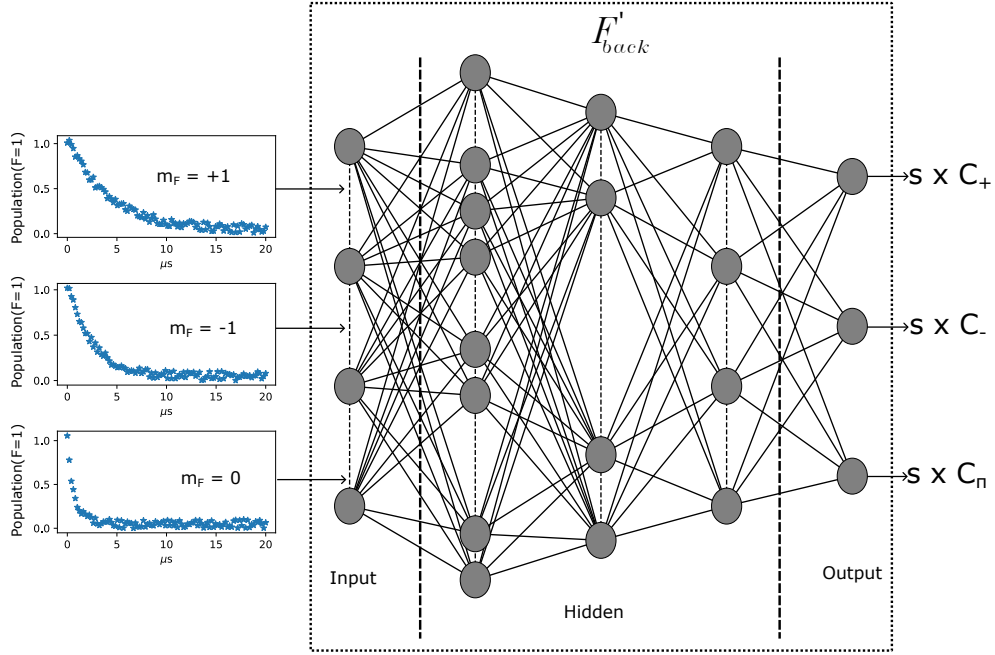


Figure 4.9: Deep Neural Network for approximating F'_{back}

The circles and dashed lines represent neurons, and only the number of neurons shown in the output layer corresponds to the actual value. The input of the neural is three optical pumping curves, one each for the ion initialized in $^2S_{1/2} F = 1$ $m_F = 1, -1, 0$. The number of hidden layers shown is only for representation purposes and may not correspond to the actual number of hidden layers used. The output of the network is three numbers corresponding to the s parameter for light in each component of polarization in the ion frame.

to generate a large number of solutions of F'_{fwd} with known input values to create a training dataset. This data set is then used to train the network, i.e. optimize the parameters of the deep neural network such that it matches the functional form of the training dataset. The hope is that a large enough but tractable training dataset allows the neural network to approximate the functional form well enough to perform well on data not contained in the training data set. To generate training data to find F'_{back} , approximately a million optical pumping curves ($N = 101^3 = 1030301$) were stimulated using F'_{fwd} . The parameter values for these simulations were chosen such that for a given value of s , the s parameter for each component of optical pumping light,

$$s_i = s \times C_i \text{ for } i \in \{+, -, \pi\}, \quad (4.30)$$

contained 101 evenly spaced values in log scale from 10^{-4} to 1. The simulation time for each simulation was chosen to be 20 microseconds and a total of 100 time steps to allow faithful learning of low-intensity pumping curves. Note that each of these simulations is independent of each other and hence can be parallelized, leading to large savings in simulation time, and in this case, this was approximately a 16X speedup due to the 16-core CPU used. The entire training set took ≈ 6 hours to simulate.

The structure of the general network is an input layer, followed by four hidden layers and an output layer. The input of the neural network is three optical pumping curves with 100 points each stacked to form a single vector, leading to an input layer size of 300 neurons. The number of neurons in the four hidden layers is 2400, 600, 120, and 20, respectively, and the output layer has three neurons. The activation function for all neurons in the hidden layers is a rectified linear unit (ReLU), and all layers, including the input, have full connectivity, i.e., each neuron in a given layer is connected to all the neurons in the next layer. For training the network, the initial data set with 101^3 samples was divided into *training*, *validation* and *test* datasets with 90% 9% and 1% of the samples in each data set, respectively. To optimize the parameters of the neural network, the ADAM algorithm [147] was used to minimize, over all samples in the training set, the following mean absolute error loss function.

$$L = \sum_n^{N'} \sqrt{(s_+^n - S_+^n)^2 + (s_-^n - S_-^n)^2 + (s_\pi^n - S_\pi^n)^2}, \quad (4.31)$$

where N' is the number of samples in the data set, (s_+^n, s_-^n, s_π^n) are the s parameters for the three polarization components of the optical pumping light and (S_+^n, S_-^n, S_π^n) are the values predicted by the neural network.

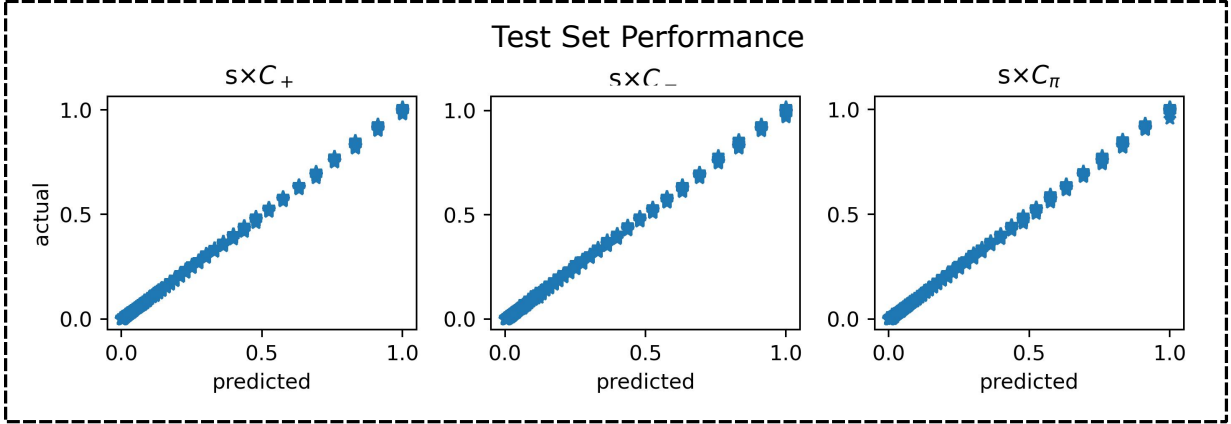


Figure 4.10: Test set performance of the neural net used to approximate F'_{back}

For the total dataset with $N = 101^3$ samples, the train, validation, and test split was 81%, 9%, and 10%, respectively. The validation data set was used to optimize the hyperparameters, which included the learning rate and the neural network configuration. The above plots show that the predicted values of s parameters for each light polarization match well with the actual values. It took 6 hours to generate the dataset and 2 hours for training on a modest CPU 8-core CPU (AMD Ryzen 7 2700x). After the one-time data generation and training, the 103031 test set predictions took less than a second, i.e., $\approx 10 \mu\text{s}$ per sample compared to ≈ 30 seconds per sample for the fitting approach. This demonstrates the efficacy of the *intelligent* approach in reducing the computational overhead for image field reconstruction.

The learning rate was chosen to have an initial value of 10^{-3} with a decay of 50% after every three epochs of training. Here, epoch refers to one cycle of neural network parameter update going over the training set once. The training was programmed to continue to a maximum of 50 epochs or until the loss only decreased by less than 10^{-5} . The validation loss L_{val} , that is, the loss calculated from the samples in the validation set, was used to tune the *hyperparameters* of the neural network, which in this case was the number of neurons in the hidden layers. It should be noted that the architecture of the neural network, i.e., four hidden layers with a gradual decrease in the number of neurons, was chosen rather arbitrarily and may not be the optimal choice. However, since the current architecture approximated the functional form of the data well ($L_{\text{val}} < 10^{-3}$), no further optimizations were done. Fig. 4.10 shows the performance of the neural network using samples in the test data set that were not used for training or validation.

4.7 Reconstructing Sub Wavelength Optical fields using Intelligent Sensing

Sub-wavelength optical features are highly sought after for various applications in research and industry, including, but not limited to, nanofabrication [148, 149, 150], high-resolution imaging [151], optical trapping [152], high-capacity optical data storage [153], etc. Characterizing the size, shape, and polarization of the focused spot is essential for applications involving submicrometer focal spots and nanostructures. Using a high numerical aperture objective lens, a tightly focused spot with sub-wavelength dimensions approaching the diffraction limit can be achieved. The sub-wavelength optical features created by such devices have not only intensity variation at the sub-wavelength scale but also polarization variation, and hence, the detectors used to characterize such features should be sensitive to both.

The focal spots or point spread functions of high NA optical objective lenses have been theoretically studied in detail in the literature [154, 155, 156], and much of the modeling follows the approach of the vector Debye model proposed by Richards and Wolf [157]. The counterintuitive insight is that increasing the NA of the objective lens does not always lead to a strong confinement of the optical field within the diffraction-limited spot size given the Rayleigh criterion ($1.22 \lambda/\text{NA}$). Rather, the spot size has a strong dependence on the input polarization on the objective lens. Fig. 4.11 shows the point spread function of an objective lens with $\text{NA} = 0.8$ and linearly polarized input light, simulated using the vector Debye model. Even though the input light is polarized in the x-direction, the image plane field contains a polarization component along the z-direction. The off-axis lobes in the z-polarized component of the image plane field lead to a spot size larger than expected from the Rayleigh criterion.

The point spread function shown in Fig. 4.11 corresponds to an ideal objective lens. Most commercial objective lenses have imperfections, and characterizing these is of paramount importance for characterization of real optical systems. Direct observation of the focal field on a camera is not useful for the characterization of sub-wavelength optical features, especially when polarization characterization is required. Similarly, the use of near-field optical microscopy (NSOM) fiber probes for field reconstruction [158] allows for a resolution ≈ 100 nm; however, the probes have a polarization-dependent absorption which is difficult to characterize, impeding faithful characterization of field polarization [159]. Finally, the knife edge-based beam tomography techniques [160] used in most commercial beam profilers do not allow characterization of beam polarization.

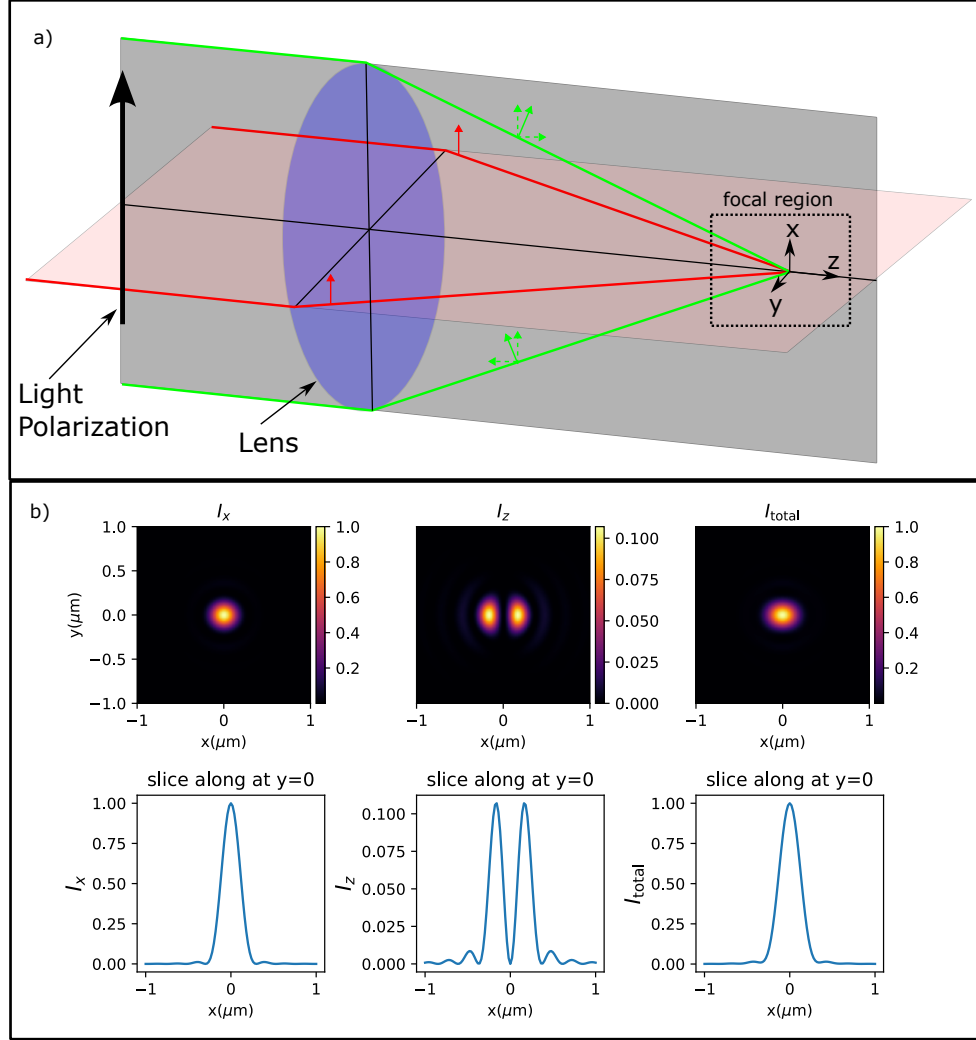


Figure 4.11: Vector-Debye Model simulation of a NA=0.8 focusing lens

a) Figure, adapted from [156], gives an intuitive picture for understanding the behavior of a high numerical aperture (NA) objective lens. Note the direction of polarization shown for the green and the red rays. The green rays lead to polarization components along the z-direction in the focal plane, even with input light polarized along the x-direction.

b) x and z components of the normalized intensity (I/I_{max}) in the focal plane of the objective lens with linearly polarized light ($\lambda = 369.5 \text{ nm}$)

The existing techniques for optical field characterization do not allow for the reconstruction of the image plane intensity and polarization in high-NA optical setups. As discussed in the previous sections, a single trapped ion is an excellent point probe for sensing light. We now study the use of $^{171}\text{Yb}^+$ ions to detect the image plane field of an ideal $\text{NA}=0.8$ objective lens using the technique discussed in Section (4.6). We currently do not have a high NA objective lens in our experimental apparatus; however, the ion response (optical pumping curves) at each point in the image plane of such a lens is easily simulated using the modeling techniques discussed in Sections 4.3 and 4.4. Since the response generated from the model agrees excellently with the experimental results, this provides a faithful representation of an actual experiment. We generate three optical pumping curves at each point in the image plane of the lens, one each for the ion initialized in $^2\text{S}_{1/2} \text{F} = 1$ $m_F = 1, -1, 0$ and input them into the inverse function F'_{back} discussed in Sec. 4.6 to get the values for the predicted intensity and polarization. During the generation of the simulated experimental curves, we assume that the quantization axis (B-field) points along the z -axis of the optical system (see Fig. 4.11) and the polarization components C_x and C_y are appropriately converted to the ion frame polarization components C_+ , C_- , and C_π . For visualization of the reconstructed field components C'_+ , C'_- , and C'_π , these polarization components are converted back to the regular lab frame components C'_x and C'_y .

Fig. 4.12 shows the results of reconstruction of the image plane field on a rectangular grid of size $1\ \mu\text{m} \times 1\ \mu\text{m}$ and 101×101 points, i.e., a step size of $\approx 20\ \mu\text{m}$. The reconstructed field matches the input field almost exactly. Note that the state preparation and measurement fidelity of state-of-the-art ion trap quantum devices are above 99.9% and the results in Fig. 4.12 are quite representative of the performance in real systems. However, we wish to simulate the reconstruction performance in a highly noisy measurement apparatus, and hence, we try to reconstruct the field by adding noise to the simulated optical pumping curves. Figures (4.13) and (4.14) show the reconstruction performance with the added noise of 5% and 10%, respectively. Adding noise here refers to errors in the estimation of the population at each point in an optical pumping curve. For example, an error of 10% means that at each point in an optical pumping curve, the population measured in the $\text{F} = 1$ manifold can be wrong by $\pm$ five %. Even with such a high error, the reconstruction performance is excellent and points towards low experimental requirements of this method.

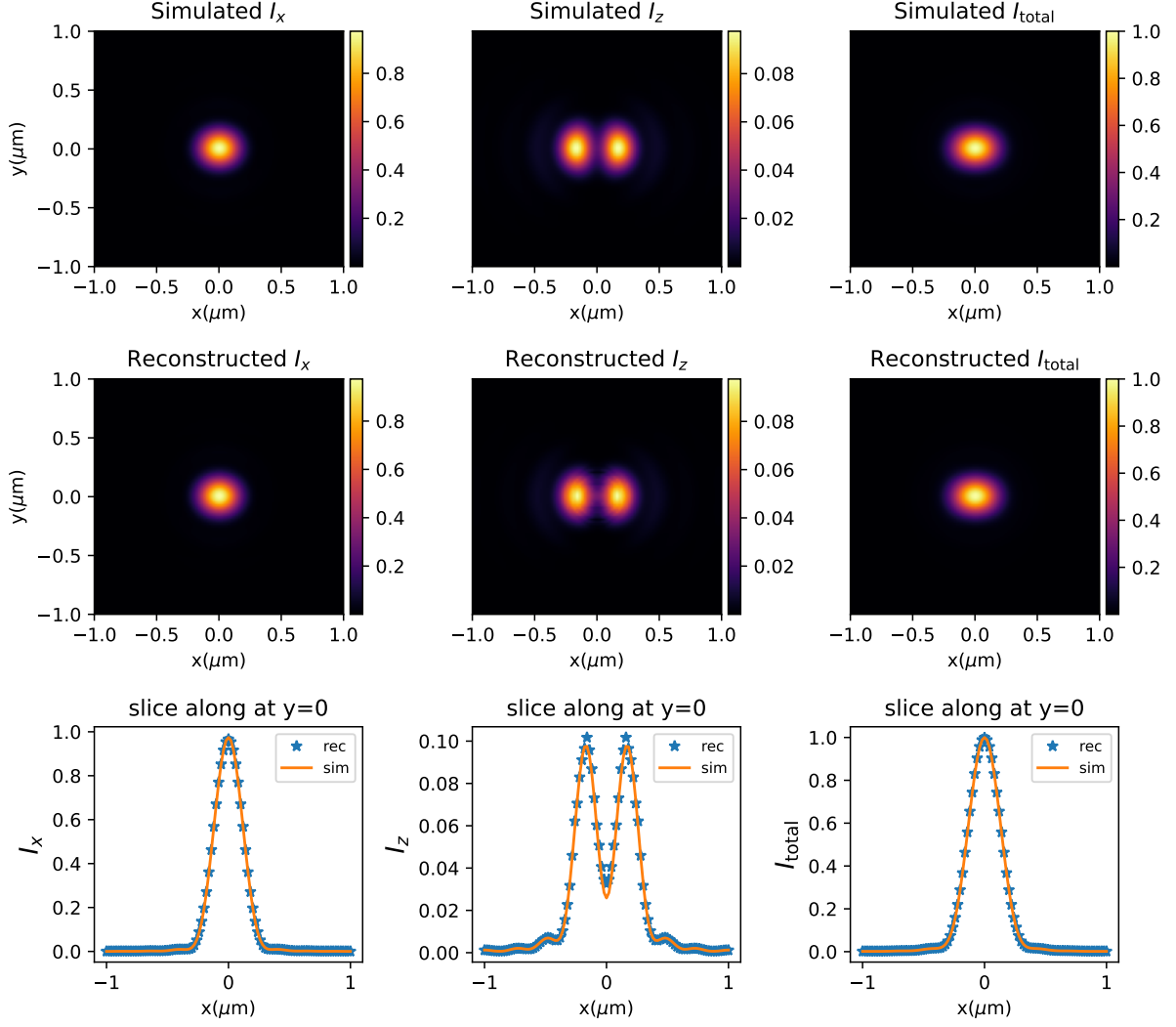


Figure 4.12: Intelligent Reconstruction

Top: Reconstructed image plane field 0.8 NA objective lens assuming perfect reconstruction with a detector of cross-section $\lambda^2/2\pi$. Here, the z-axis is the direction of propagation of the beam at the input of the objective lens. **Middle:** Reconstructed image plane field using intelligent reconstruction. **Bottom:** Reconstructed image plane field using intelligent reconstruction: Slice along $y=0$.

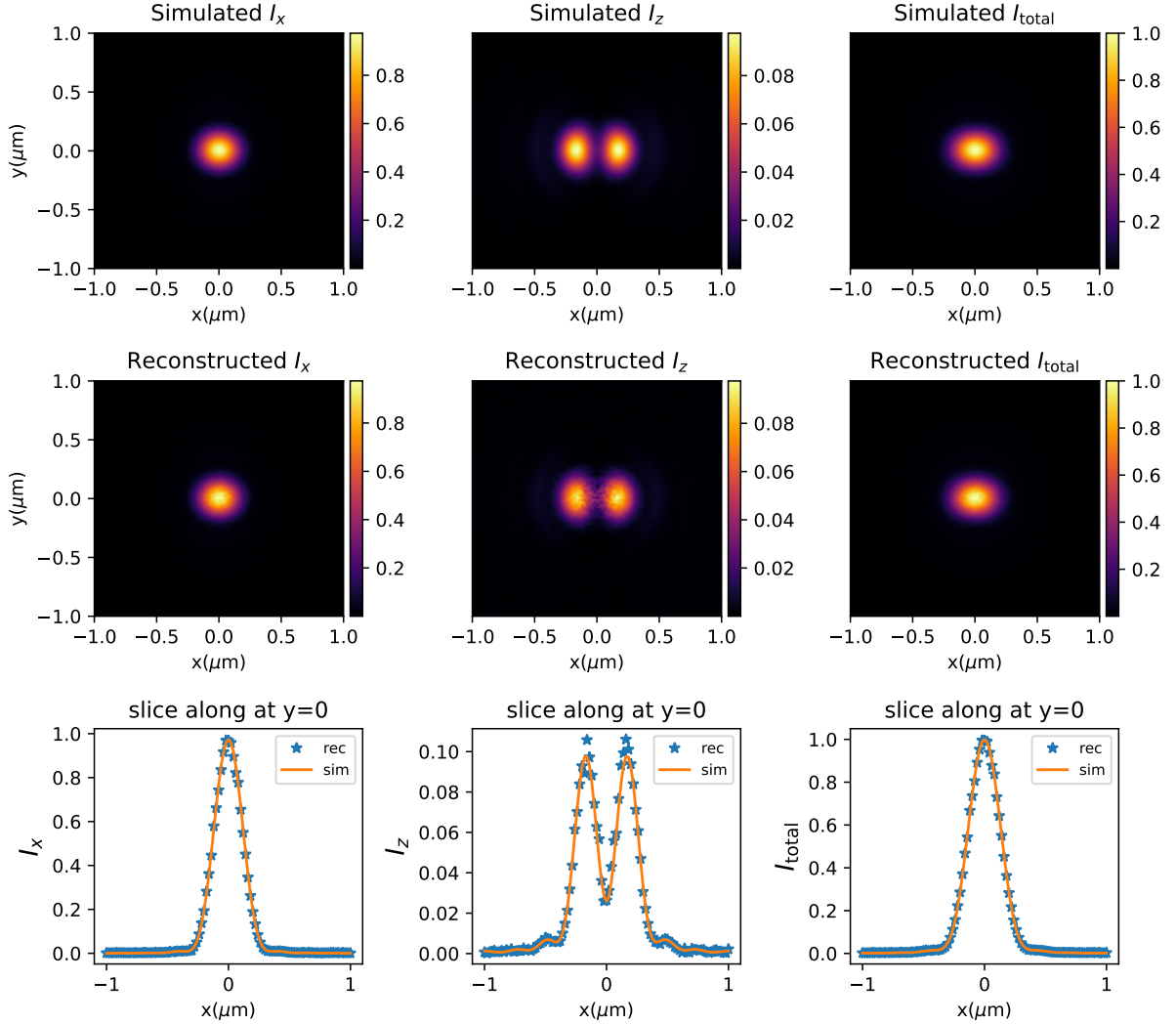


Figure 4.13: Intelligent Reconstruction with $\pm 2.5\%$ error

TOP: Reconstructed image plane field 0.8 NA objective lens assuming perfect reconstruction with a detector of cross-section $\lambda^2/2\pi$. Here, the z-axis is the direction of propagation of the beam at the input of the objective lens. **Middle:** Reconstructed image plane field using intelligent reconstruction. **Bottom:** Reconstructed image plane field using intelligent reconstruction: Slice along $y=0$.

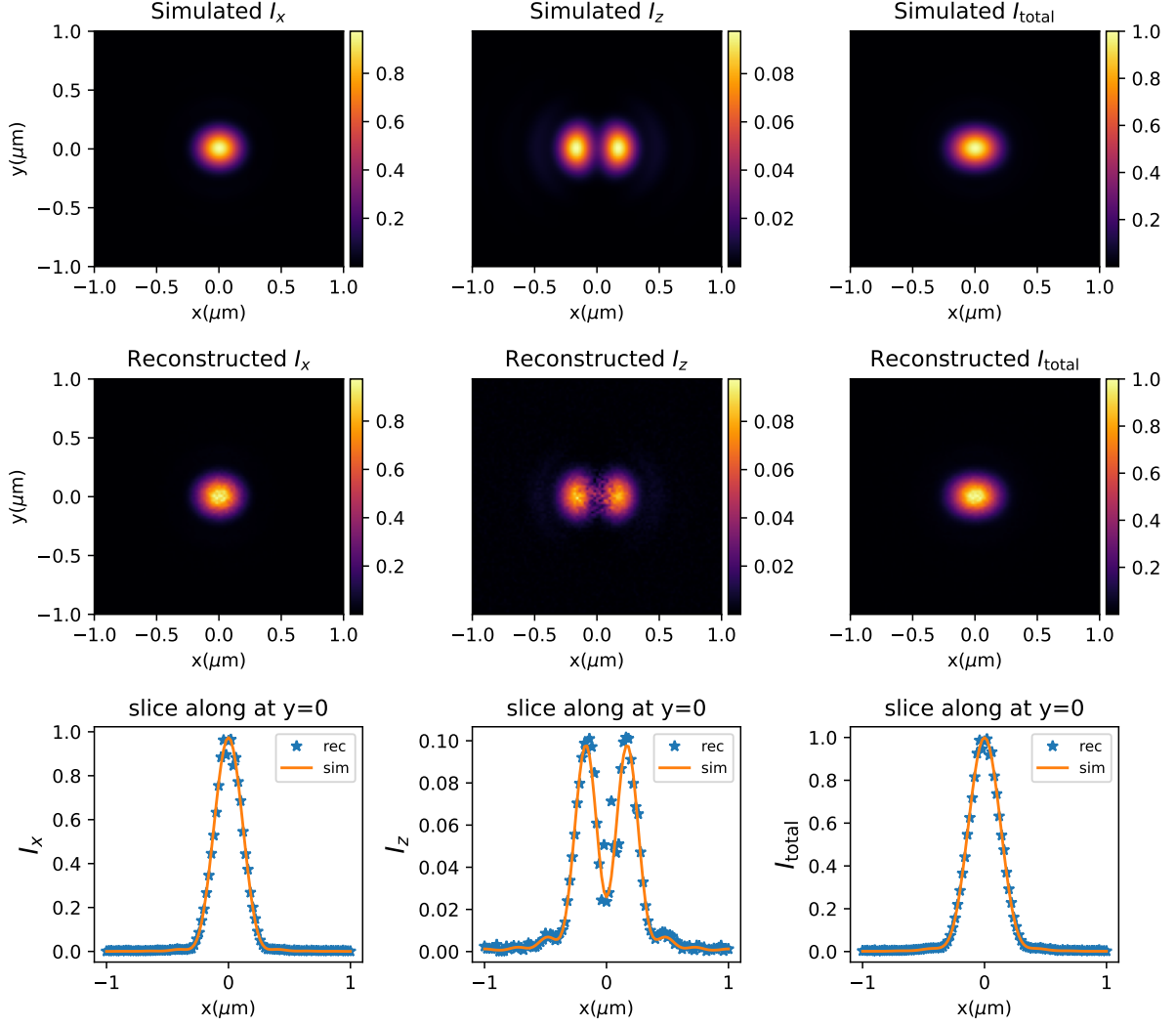


Figure 4.14: Intelligent Reconstruction with $\pm 5\%$ error

Top: Reconstructed image plane field 0.8 NA objective lens assuming perfect reconstruction with a detector of cross-section $\lambda^2/2\pi$. Here, the z-axis is the direction of propagation of the beam at the input of the objective lens. **Middle:** Reconstructed image plane field using intelligent reconstruction. **Bottom:** Reconstructed image plane field using intelligent reconstruction: Slice along $y=0$.

4.8 Conclusion and Outlook

In summary, we have demonstrated the sub-wavelength characterization of optical fields using a single ion as a light sensor. The technique utilizes the intensity and polarization-dependent optical pumping of $^{171}\text{Yb}^+$ ions as a signature to extract the light parameters. The spatial extent of the ion is much smaller than the absorption cross-section of a point-like resonant detector ($\lambda^2/2\pi$), and hence the resolution is only limited by the fundamental limit imposed by the absorption cross-section. The resolution can be further improved by making use of off-resonant detection since the cross section is the highest for the resonant case. For example, in $^{171}\text{Yb}^+$ ions, instead of using optical pumping as a signature, an intensity, and polarization-dependent Stark shift could be used to extract light parameters. This can be easily implemented by an off-resonant beam on the $^2\text{S}_{1/2}$ to $^2\text{P}_{1/2}$ transition, like the 355 nm laser already being used in the experiments, and measure the Stark shifts on the $^2\text{S}_{1/2}$, $m_f = 1, 0, -1$ levels. The spatial extent of the ions would then be the only limiting factor for the resolution, and, as discussed earlier, this can easily be in the order of 5 nm.

The wide adoption of this technique for characterizing optical systems would require overcoming of two main challenges. The first challenge is that the trapped ions are inside a vacuum system and that the optical field that needs to be characterized should pass through a vacuum window (effectively a thin slab of glass) before reaching the ions. This causes distortions to the optical field while it passes through the vacuum window and also limits the minimum working distance. For the special case of ion-based quantum computers, the optics in these systems are designed to function with the vacuum windows, producing miniature (sub-micron) optical features at the ions/atoms. Therefore, this technique can be directly applied to characterize optical addressing light in these systems using ions as sensors. However, to effectively characterize other optical systems, special vacuum systems need to be designed to allow the objective to be installed inside the vacuum. That way, the light could pass the vacuum viewport when it is a collimated beam, leading to minimal distortion of the field, and the in-vacuum objective brings the light to a sharp focal spot that can be characterized with the ion. This is not difficult and most systems in nanofabrication labs/cleanrooms, for example, sputtering and thermal deposition chambers, have vacuum systems that enable installation of samples and pumping to ultrahigh vacuum.

The second challenge stems from the requirement that the light must be resonant with certain transitions of the ions and this seems to limit the applicability of this technique for characterization of optical systems for use with multiple wavelengths or white light. Each ion species has several transitions that can be used for sensing; for example, the $^{171}\text{Yb}^+$ ion has transitions at 369 nm, 411 nm, 435 nm, and 935 nm that could be used for sensing.

Moreover, multispecies ion traps, i.e. traps that can confine different species of ions at the same time, are very common and this can further increase the optical bandwidth of the system. Since only a few wavelengths are required to characterize an imaging system, the resonance requirement of this technique does not pose any fundamental limitation in the characterization of multiwavelength optical systems. Similarly, the Stark shift-based approach does not require resonant detection and, hence, does not suffer from this limitation.

The light field characterization technique presented in this work opens new avenues for the characterization of complex optical systems capable of producing subwavelength optical features with unprecedented resolution. This is especially useful in characterizing light sources in optical lithography systems and atom-/ion-based quantum computers. The intelligent characterization technique will also drastically speed up the calibration of atom-/ion-based quantum computers.

Chapter 5

Construction of a blade style ion-trap with extreme high vacuum

Author Contributions:

During the early stages of the project (and my PhD), the blade trap project was divided into two major branches: Optical design, not discussed here, and Vacuum system + trap design. The author worked on the vacuum system and trap design. The author had a preliminary but complete design including trapping potential simulations, a science chamber internal design (except for the ablation target), and the vacuum system. Later, when simulation software (MolFlow) was used to optimize the performance of the vacuum system, the project grew in scale. Dr. Sainath Motlakunta took over the computer aided design (CAD) of the chamber internals, including the trap electrode holder design, and the author worked on the vacuum system design and simulation, atomic oven fabrication, ion trap electrode fabrication and testing, and developing of the prebaking technique for degassing the stainless steel components.

Unlike the design process, the construction process was not divided for practical considerations and efficiency. The author worked together with Dr. Sainath Motlakunta on the construction of the vacuum system, prebaking of the stainless steel components, alignment of blade electrodes on the trap, and assembly of the chamber internals. Toward the end of the project, Lewis Hahn also joined the blade trap construction and, among several other things, performed the high-temperature prebake of the ion trap electrode holder structure and also helped with testing the atomic ovens. Dr. Rajibul Islam supervised the entire project during both the design and construction phases.

5.1 Overview

The results discussed in the previous chapters play an important role in advancing quantum simulations with trapped ions. Programmable XY interactions will allow the exploration of a new class of Hamiltonians, and the low-light sensing technique will help to characterize crosstalk errors while performing local resets and readouts. However, these advances would only make an impact when the size of the Hilbert space explored in a quantum simulation is increased. The most straightforward way to achieve this is to increase the number of ion qubits in the simulator and allow for the exploration of quantum dynamics with system sizes where classical simulation becomes intractable. For about 30 qubits, classical simulations become difficult or, in some cases, intractable, and one of the major experimental projects in the group has been the building of a large-scale programmable quantum simulator with more than 50 ions. This system is based on a linear Paul trap with segmented blade-style electrodes, and we refer to it as the blade trap.

Increasing the number of qubits comes with a lot of challenges. One of the challenges is that the fidelity requirement for all operations is higher. Suppose, for example, that we have a state preparation and measurement (SPAM) fidelity, F , for a single qubit state $|\psi\rangle$, then the SPAM fidelity for the N -qubit state, $|\psi\rangle^{\otimes N}$ is F^N . With a single-qubit fidelity, $F = 0.99$, the SPAM fidelity for a 50-ion chain is $(0.99)^{50} \approx 60\%$. This exponential scaling puts stringent requirements on the operational fidelities, and the only way to ameliorate this (in the absence of error correction) is to increase the fidelity of single-qubit operations. For trapped ions, this translates into the requirement of high optical access (HOA). For measurement, HOA allows for the collection of a large fraction of the emitted fluorescence during state readout operations. For state preparation, HOA allows to create tightly focused beams to address individual ions for local coherent and incoherent operations, thereby allowing complicated state initialization (states other than $|\downarrow\rangle^{\otimes N}$ and $|\uparrow\rangle^{\otimes N}$) with high fidelity [101].

For a system capable of large-scale quantum simulations, there are added complications that arise from having a high number of ions. Generally, a low axial trapping frequency (ω_z) results in diminished operational fidelities, as elaborated in Refs. [161, 162]. Consequently, maintaining high axial trapping frequencies is important. The extent to which the axial trapping frequency can be increased is a function of the number of ions in the trap and the radial trapping frequencies (ω_x and ω_y). This is because for $\omega_z < 1.3 \times \omega_{x/y} \sqrt{\log N/N}$ [163], the ion crystal ceases to be a 1D chain due to a linear to zig-zag structural phase transition [163, 164]. Because of the above, as the number of ions in a trap increases, the trapping frequencies in all directions need to be increased.

However, there is a limit to how much trapping frequencies can be increased, primarily

due to technical challenges, particularly when it comes to increasing the radial trapping frequencies. In Section 2.1, we showed that the trap stability parameter $q_{x/y} \propto V_0/\Omega_T^2$ and the radial trapping frequencies $\omega_{x/y} \propto q_{x/y} \times \Omega_T$, where $\omega_{x/y}$ is the trapping frequency in the x/y direction, V_0 is the amplitude of the radiofrequency voltage applied to the trap electrodes at an angular frequency Ω_T . To operate the trap deep within the stability region and minimize susceptibility to micromotion induced ion heating, typical designs operate at $q_{x/y} < 0.4$ (see Fig. 2.2 for the stability diagram). For a given value of $q_{x/y}$, a higher Ω_T leads to higher $\omega_{x/y}$ and, in principle, it is possible to achieve an arbitrarily high $\omega_{x/y}$ by increasing Ω_T and commensurately increasing V_0 (to satisfy $q_{x/y} < 0.4$). However, both V_0 and Ω_T cannot be made arbitrarily high. In the case of V_0 , the limitation comes from the maximum allowable voltage on different elements of the system, for example, the trap electrodes and the feedthroughs in the vacuum system. Moreover, increasing Ω_T beyond a point is difficult because it becomes challenging to design a helical resonator to drive a trap¹. In the four-rod trap apparatus discussed in Ch 2 $\omega_x \approx 2\pi \times 1.1$ MHz, but several state-of-the-art large chain simulators operate at $\omega_{x/y} > 2\pi \times 4$ MHz. Higher trap frequencies generally also benefit from a lower ion heating rate [165], which is especially beneficial when considering axial-mode heating rates.

The requirement of high optical access and high trapping frequencies dictated the choice of the ion trap in the current design. The two broad categories of traps that are prevalent today are surface electrode traps [166, 167] and macroscopic 3D traps (like the four rod trap discussed in Chapter 2). More recently 3D printed ion traps [168] are being explored that combine the benefits of surface traps and macro traps; however, this architecture needs further research before being used for a full-scale quantum simulation apparatus. Macroscopic 3D traps generally offer high trapping frequencies, deep trapping potentials, while the surface traps tend to have lower trap depths and trapping frequencies. As per our previous discussion, high trapping frequencies were crucial to our design due to the intended purpose of performing large-scale ($N > 50$) quantum simulations, and hence we chose to use a macroscopic 3D trap in our design. The blade trap is functionally similar to the four-rod trap in the sense that the four rods have been replaced with segmented blade-like electrodes with sharp tips primarily to increase the optical access (See Fig. 5.2 for the electrode geometry). The electrodes are segmented in the direction of the ion chain, allowing higher control over the axial trapping potential to create ion chains that are more

¹The resonator and the trap can be thought as an RLC circuit where the inductance, L comes from the resonator coil and the capacitance, C , primarily comes from the trap. The resonant frequency, and hence the trap drive frequency, $\Omega_T = 1/\sqrt{LC}$. For a given trap (fixed C), increasing Ω_T requires reducing L , which is not possible indefinitely. In addition, the resonator quality factor $Q \propto \sqrt{L}$ and reducing L also has the effect of reducing the resonator quality factor which adds additional complexity for increasing V_0 .

equispaced compared to a trap with harmonic potential along the ion chain direction [169]. The blade-like electrodes with a tip dimension of 50 μm allow high optical access in four directions, as seen in Fig. 5.1.

Finally, a major challenge while developing a large trapped ion system comes from the non-zero background pressure in the vacuum vessels that house the trap. Collisions with background gas molecules in a trap could cause ion chain reordering events [170, 171], occasional ion loss, and chemical reactions between the ion and the gas molecule [172], all of which cause quantum simulation to be paused, and in some cases, reloading the trap. For systems with large ion chains and high trap frequencies, reloading the trap could lead to a high downtime of the equipment. The reason is that the ion trap potentials have to be made shallower while trapping; this leads to local temperature changes at the trap and the relaxation times for such changes could be long.

The collisions between the ions and the background gas molecules are because of the electric field of the ions polarizing the gas molecule and leading to an induced dipole moment in the gas molecule. The dipole experiences a net attractive force, and a collision results when the gas molecule passes sufficiently close to the ion. The collision cross-section can be calculated from the Langevin model [173, 171], which leads to a collision rate γ proportional to the background pressure.

$$\gamma = \frac{PQ}{k_{\text{B}}T} \sqrt{\frac{\pi\alpha}{\mu\epsilon_0}}, \quad (5.1)$$

Where P is the background pressure, Q is the net charge on the ion, k_{B} is the Boltzmann constant, α is the polarizability of the gas molecule, μ is its reduced mass and ϵ_0 is the vacuum permittivity. For state-of-the-art room temperature vacuum chambers that house ion traps, the pressure is in the range of mid to low 10^{-11} mbar, and the dominant gas is hydrogen. $P \approx 2 \times 10^{-11}$ mbar leads to a collision rate, $\gamma \approx 5 \times 10^{-4}$ Hz, or one collision every 33 minutes.

At first glance, 33 minutes seems like a long time given the quantum simulation times of 10 to 100 ms; however, with a large number of ions, this is not the case. In Fig. 3.6, we observed the dynamics of two ions under an XY Hamiltonian with $J_{12}^X = J_{12}^Y = 2\pi \times 80$ Hz, for the total duration $T = 30$ ms in steps of $\Delta T \approx 300 \mu\text{s}$. There, the fluorescence counts of the ions were plotted at each time step by repeating the experiment $N_{\text{shot}} = 200$ times. The energy scale in the simulation, i.e., $J \approx 2\pi \times 100$ Hz, is quite representative of typical experiments with a large number of ions ($N \approx 50$). Observing the dynamics under such a Hamiltonian for a total time $T \approx 10/J$ leads to $T = 100$ ms.

A back of the envelope estimate of the data taking time, T_{sim} , for running a quantum

simulation observing dynamics for a total time of T seconds, with dynamics observed, i.e., measurements, every δT seconds, and the overhead time of T_O per shot required for state preparation, reset, cooling, etc. , is the following,

$$T_{\text{sim}} = N_{\text{shots}} N_{\text{steps}} \left[\frac{T + \delta T}{2} + T_O \right], \quad (5.2)$$

where $N_{\text{steps}} = T/\delta T$. For $T = 100$ ms, $\delta T = 1$ ms, $T_O = 40$ ms² and $N_{\text{shots}} = 200$, the data taking time $T_{\text{sim}} = 1800$ s ≈ 30 minutes³.

For N ions in the trap, the collision rate for the entire chain is expected to scale linearly with the number of ions, $\gamma_N = N \times \gamma$. Hence, to observe the dynamics for 100 ms in a quantum simulation on a chain of N ions with a low probability of background collisions, the pressure should be at least $2/N \times 10^{-11}$ mbar. For a chain of 50 ions, this leads to a required pressure of 4×10^{-13} mbar. To the best of my knowledge, such background pressure has not been achieved in a room-temperature ion-trapping apparatus. Cryogenic systems allow such low pressures; however, cryogenic systems are large and expensive, and the closed-cycle cryostats generate vibrations in the system, and the mitigation of these vibrations is an active field research and development.

Figure 5.1 shows a picture of the CAD design of the blade trap apparatus. The design allows for high optical access from four directions; the trap is optimized to achieve radial trapping frequencies of $\approx 2\pi \times 5$ MHz while maintaining high optical access, and the base pressure of the constructed system is below 1.5×10^{-12} mbar (limited by the measurement capability of the gauge). The design and construction of the system took almost three years since we optimized every component to achieve its highest performance. The trap electrodes were fabricated in-house using the nanofabrication capabilities at QNFCF, the cleanroom facility at the University of Waterloo because we found it difficult to find vendors that could make them to our required specifications. Upon fabrication, thorough electrical testing was done to ensure compliance with requirements. Similarly, the vacuum system design has been thoroughly optimized, possibly to the limit of attainable pressures in room-temperature vacuum apparatuses using current pumping technology and commercially available vacuum chambers, using open-source Monte Carlo simulation software MolFlow from CERN. After construction, the vacuum system pressure was below the gauge

²The chosen value for T_O is an overestimate for a small number of ions $\mathcal{O}(1)$; however, it is representative of the overhead in a large system.

³Recent 53 ion experiments [75] reported a collision free lifetime of approximately 5 minutes for a 53-ion chain.

detection limit within a few days after baking⁴ was complete, suggesting that the actual pressure might be much lower. In this chapter, I will go over the design and construction process for the trap electrodes, vacuum internals, alignment of the trap, and the design and construction of the vacuum system. In the end, I will share the valuable insights that we have learned during this process.

⁴As we will discuss later, vacuum systems attaining low pressure need to go through high-temperature baking before they attain the desired pressure at room temperature.

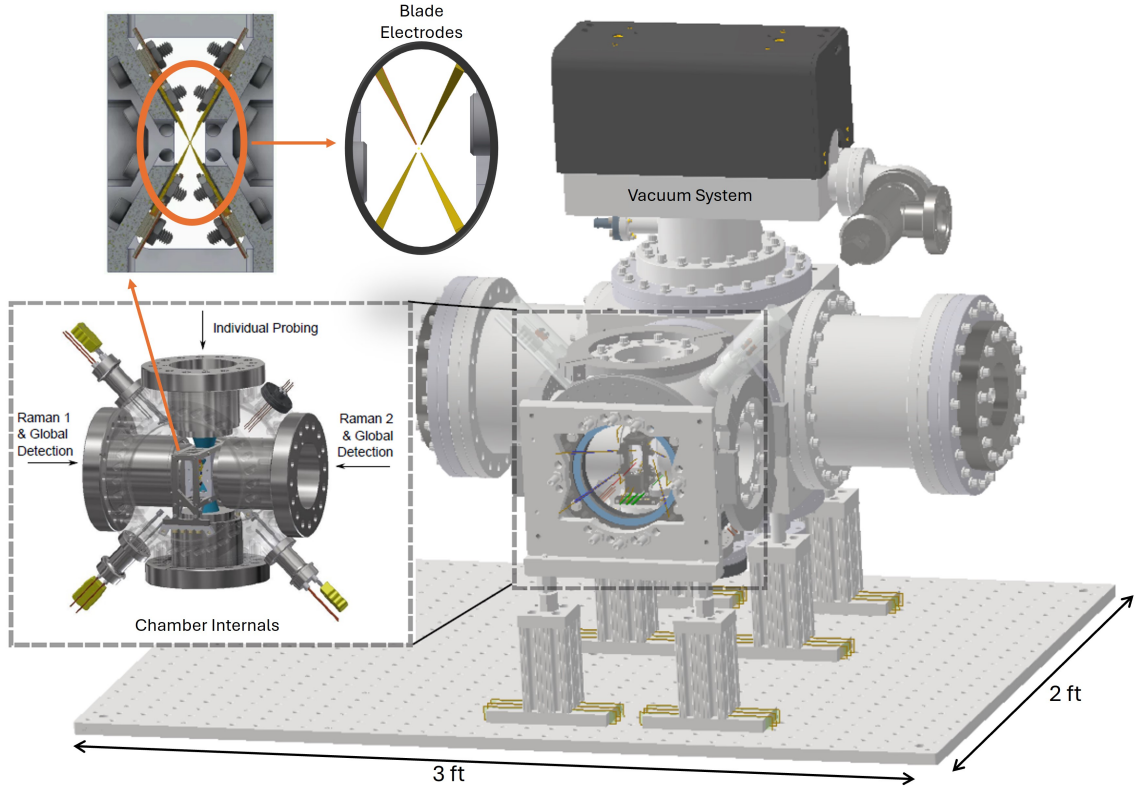


Figure 5.1: Blade Trap System Overview

The figure shows the CAD model of the vacuum system housing the blade trap. There are two nonevaporable getter (NEG) pumps and an ion pump for pumping and the science chamber has been chosen to provide high-efficiency pumping while also maintaining high optical access from four sides of the trap. As shown in the inset, the science chamber has re-entrant (recessed) vacuum windows to make use of the high optical access of the trap. The two side directions will be used for state detection and coherent operations using Raman beams. The vertical high optical access port will be used for high-fidelity individual addressing of the ions for site-selective state preparation and readout. The ion trap lies at the center of the science chamber.

5.2 Trap Design

As noted previously, the design requirement for the trap was to have radial trap frequencies $\omega_{x/y} \approx 2\pi \times 5$ MHz. In terms of optical access, we set separate requirements for numerical aperture (NA) required for fluorescence collection for state detection, coherent individual addressing, and incoherent individual probing light for state reset and detection. For fluorescence collection, we want $\text{NA} \geq 0.5$ to perform high-fidelity readout [137, 96]. Individual addressing of the ions using Raman beams can also be performed from the same directions as fluorescence collection because these operations do not occur at the same time. For individual addressing, the image-space NA determines the scale of the smallest optical feature in the focal region of an addressing lens. Using the Rayleigh criterion, the spot size (limited only by diffraction) is $\approx 0.61\lambda/\text{NA}$. For the Raman beams ($\lambda = 355$ nm), $\text{NA} \geq 0.5$ allows for a diffraction-limited spot size of < 0.5 μm , and comparing with the typical ion-ion separation of 4-6 μm the optical access was deemed sufficient. For individual addressing for state reset and detection, $\text{NA} = 0.3$ would allow us to achieve a diffraction-limited spot size of $\approx 2\lambda$. With $\lambda = 369$ nm this would allow us to create a beam waist of ≈ 0.8 μm which is five times lower than the typical ion-ion separation of 4-6 μm . In our earlier results, we have shown the diffraction-limited performance of the optical setup [136] and the preservation of the state of the neighboring ion (four beam waists away) with a fidelity of 0.999 [126]. Therefore, the NA requirement for the incoherent addressing was chosen to be $\text{NA} \geq 0.3$.

These requirements determined the dimensions of the trap electrodes and their proximity to the ions. Fig. 5.2 a) shows a CAD model of a blade electrode, and Fig. 5.2 b) shows the relative positions of the four blades with respect to each other for trapping ions. The ends of the blade that face the ions are tapered to a size of 50 μm . Note that the angles between the blade surfaces are unequal. This was done to achieve high optical access in two directions with minimal compromise on the radial trapping frequencies by keeping the ion-electrode distance small. In the two directions where the angle is 120° , the NA limited only by the electrodes is greater than 0.55. In the other two directions, the NA limited by the blades themselves is ≈ 0.35 . The ion-electrode distance to all four blades, as shown in Fig. 5.2 b), is $R_0 = 200$ μm .

Similarly to the four-rod trap discussed in Section 2.1, trapping in the radial direction (XY plane) is achieved using out-of-phase radio frequency (RF) voltages on the two diagonally opposite pairs. However, unlike the four-rod trap, the axial trapping potential is not created using separate DC electrodes; it is achieved by segmenting each blade electrode into five segments, as shown in Fig. 5.2 a). Since each of the blades has five electrodes, there are effectively 20 electrodes, all of which serve as RF and DC electrodes. As shown

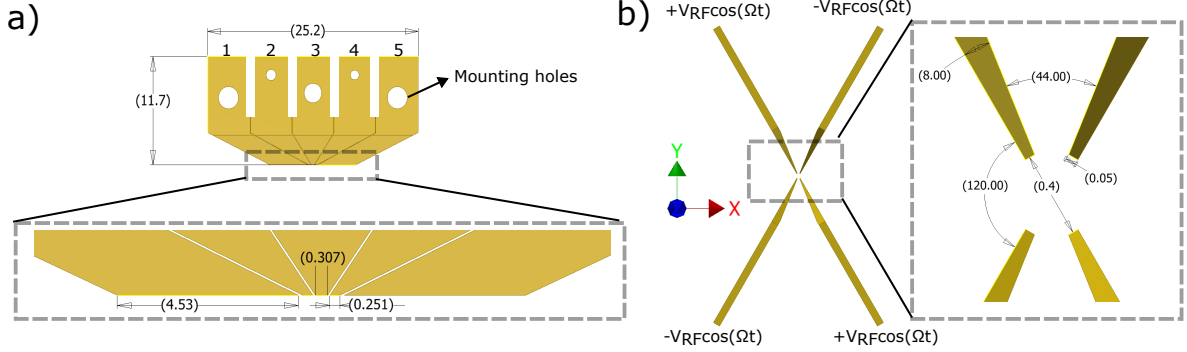


Figure 5.2: Blade Trap Electrode Geometry

All dimensions in mm. **a)** Segmented blade electrode with five segments acting as separate electrodes. Each electrode serves as a DC as well as an RF electrode. The electrodes number 1,5 on each blade are referred to as end cap electrodes, 2,4 are referred to as mid-cap electrodes, and three are referred to as central electrodes.

b) Relative orientation of four blade electrodes in the trap. The thickness of the electrode substrate is $500 \mu\text{m}$, and the ion-facing end of the electrode is tapered to a width of $50 \mu\text{m}$. The distance between the electrode and the ion electrode $R_0 = 200 \mu\text{m}$.

in Fig. 5.2 b), the ten electrodes in a diagonal pair are applied with RF voltage, and the other ten electrodes on the opposite diagonal are applied the same voltage out of phase. All 20 electrodes will also be applied an added DC voltage, which is primarily used to create confinement in the axial direction and compensate for stray fields that create excess micromotion in a real setup.

We will now discuss the radial potentials created in this trap. To avoid confusion the symbol $\mathcal{V}$ will be used to denote a potential and the symbol V will be used to denote an applied voltage. The quantities denoted by the symbols $\mathcal{V}$ and V both have units of volts. Occasionally, if we need to use a mechanical potential, with units in Joules, the symbol ϕ will be used. The geometry and blade labeling convention is shown in Fig. 5.3 a). From the discussion in Section 2.1, we expect the potential in the radial plane of the trap, $\mathcal{V}_{\text{rad}}^{\text{exp}}$ to be a quadrupole potential scaled by the characteristic distance R_0 hence,

$$\mathcal{V}_{\text{rad}}^{\text{exp}} = \kappa V_0 \left(\frac{x'^2 - y'^2}{R_0^2} \right), \quad (5.3)$$

Here, x' and y' are the coordinates of ions' positions with respect to some chosen unit vectors $\hat{x}'$ and $\hat{y}'$ that define the “principal axes” of the trap, and $\pm V_0$ is applied to the two

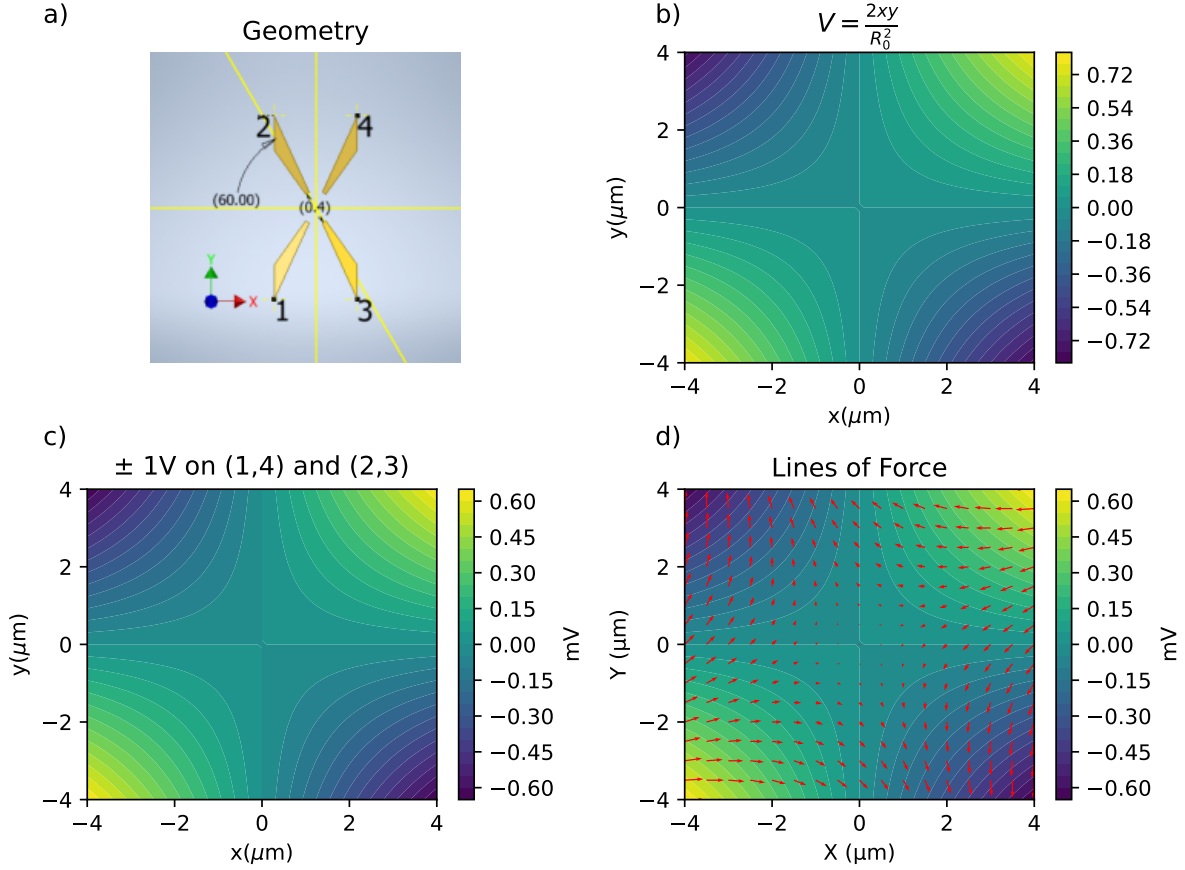


Figure 5.3: Blade trap Radial Potential

a) Picture describing the geometry and electrode labeling convention. b) Shaded contour plot of $\mathcal{V}_{rad}^{exp}$ with $\kappa = 1$. c) Shaded contour plot of the simulated potential in the trapping region. d) Plot in b) superimposed with arrows showing lines of force.

diagonal pairs of blades. As we shall see later, the principal axes are rotated 45 degrees from the axes drawn in Fig. 5.3 a). Hence, we have $x = (x' + y')/\sqrt{2}$ and $y = (x' - y')/\sqrt{2}$ and in the coordinate frame defined in Fig. 5.3 a) the radial potential is expected to be of the form.

$$\mathcal{V}_{\text{rad}}^{\text{exp}} = \kappa V_0 \left(\frac{2xy}{R_0^2} \right), \quad (5.4)$$

A shaded contour plot of $\mathcal{V}_{\text{rad}}^{\text{exp}}$ is shown in Fig. 5.3 b).

To assess the performance of the trap in generating the required trapping potentials, I numerically simulated the trap potentials using COMSOL and using these potentials I calculated the effective trapping potential ‘felt’ by the ion, i.e. the pseudopotential created from the radio frequency drive and the DC potential. Fig. 5.3 c) shows the potentials in the XY plane at $z=0$ when applying $\pm 1\text{V}$ DC on diagonally opposite blades. On cursory inspection, the potential looks very similar to the one generated from $\mathcal{V}_{\text{rad}}^{\text{exp}}$ with $\kappa = 1$. Upon fitting to a polynomial in x and y and restricting to only second-order terms, we find that $\kappa \approx 0.8$,

$$\mathcal{V}_{\text{rad}}^{\text{fit}} \approx 0.8V \left(\frac{2xy}{R_0^2} \right). \quad (5.5)$$

Fig. 5.3 d) shows the lines of force felt by a positively charged ion in such a potential. As expected from a quadrupole potential, it is attractive in one direction and repulsive in the perpendicular direction.

The principal axes of the configuration can be found by calculating the Hessian matrix of the potential defined as

$$H(\phi) = \begin{bmatrix} \frac{\partial^2 \phi}{\partial x^2} & \frac{\partial^2 \phi}{\partial x \partial y} & \frac{\partial^2 \phi}{\partial x \partial z} \\ \frac{\partial^2 \phi}{\partial y \partial x} & \frac{\partial^2 \phi}{\partial y^2} & \frac{\partial^2 \phi}{\partial y \partial z} \\ \frac{\partial^2 \phi}{\partial z \partial x} & \frac{\partial^2 \phi}{\partial z \partial y} & \frac{\partial^2 \phi}{\partial z^2} \end{bmatrix}. \quad (5.6)$$

Intuitively, the Hessian of a function calculated at a point describes how a function curves in different directions around the point. The diagonal elements pick out the curvature along a direction, and the off-diagonal elements pick out the change in curvature

in one direction with respect to translation in the other direction. The principal axes are the directions along which the Hessian becomes diagonal, i.e., the curvature along one direction is independent of the other directions. The Hessian for $\mathcal{V}_{\text{rad}}^{\text{fit}}$, extracted from the polynomial fit, is

$$H(\mathcal{V}_{\text{rad}}^{\text{fit}}) = \frac{V}{R_0^2} \begin{bmatrix} 0 & 1.6072303 & 0 \\ 1.6072303 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad (5.7)$$

To diagonalize the Hessian, we need to make the coordinate transformation using a transformation matrix P such that $H_D = P^{-1}HP$ where H_D is diagonal. It is straightforward to calculate

$$P = \begin{bmatrix} -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 1.0 \end{bmatrix}, \quad (5.8)$$

and

$$H_D = \frac{V}{R_0^2} \begin{bmatrix} -1.6072303 & 0 & 0 \\ 0 & 1.6072303 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \quad (5.9)$$

The columns/rows of P determine the directions of the principal axes, and the three diagonal elements of H_D determine the coefficients of x^2, y^2 , and z^2 terms in the new basis defined by P . Note that the trace of the hessian is zero, which is a direct consequence of the fact that the potential is the solution of the Laplace equation. The form of P corroborates our earlier assumption that the principal axes are 45 degrees from the axes drawn in Fig. 5.3 a).

The potential created by applying DC and RF voltages on the blades can, therefore, be written as

$$\begin{aligned}
\mathcal{V}_{\text{rad}} &= \mathcal{V}_{\text{rf}} + \mathcal{V}_{\text{skew}} \\
&= 0.8(V_{\text{rf}} \cos(\Omega_{\text{T}}t) + V_{\text{skew}}) \left(\frac{x'^2 - y'^2}{R_0^2} \right) \\
&= 1.6(V_{\text{rf}} \cos(\Omega_{\text{T}}t) + V_{\text{skew}}) \left(\frac{xy}{R_0^2} \right).
\end{aligned} \tag{5.10}$$

Here, 0.8 is the proportionality factor calculated in Eq. (5.5), V_{rf} and Ω_{T} are the amplitude and angular frequency of the RF voltage applied to the electrodes according to Fig. 5.2 b, and the DC voltage $\pm V_{\text{skew}}$ applied to diagonal pairs of electrodes. Similarly to the analysis in Section 2.1, the potentials in Eq. (5.10) can be used to write the parameters a and q for the blade trap.

$$a_x = -a_y = \frac{8q}{m\Omega_{\text{T}}^2 R_0^2} V_{\text{skew}}; \quad q_x = -q_y = \frac{4q}{m\Omega_{\text{T}}^2 R_0^2} V_{\text{rf}} \tag{5.11}$$

The effective radial potential (see Section 2.1) felt by the ions with the applied voltages in Eq. (5.10) is

$$\Phi_{\text{rad}} = \frac{1}{2}m\omega_x^2 x'^2 + \frac{1}{2}m\omega_y^2 y'^2, \tag{5.12}$$

The trapping frequencies are then given using the following expression.

$$\omega_i = \frac{\Omega}{2} \sqrt{q_i^2/2 + a_i} \quad \text{where } i = x, y \tag{5.13}$$

The reason for using the variable name V_{skew} should now be clear: V_{skew} changes the trapping strength along the two principal axes. With the formula in Eq. (5.13), the analysis of the radial effective potential is complete. However, we can further build intuition by calculating pseudopotentials. The pseudopotential or the potential felt by an ion, arising from the application of an oscillating potential $\mathcal{V}(\vec{r}, t) = \mathcal{V}(\vec{r}) \cos(\Omega t)$ [88, 86] can be calculated as

$$\mathcal{V}_{\text{ps}} = \frac{q(\vec{E}_0(\vec{r}))^2}{4m\Omega^2}, \tag{5.14}$$

where q is the charge of the ion, $\vec{E}_0(\vec{r}) = \nabla \mathcal{V}(\vec{r})$, m is the mass of the ion and Ω is the angular frequency of the oscillating potential. Using Eq. 5.10, the pseudopotential corresponding to $\mathcal{V}_{\text{rf}}$ is

$$\mathcal{V}_{\text{ps}} = 0.64 \frac{qV_{\text{rf}}^2}{m\Omega_{\text{T}}^2 R_0^4} (x^2 + y^2). \quad (5.15)$$

Fig. 5.4 shows the shaded contour plot of the effective trapping potential with $V_{\text{rf}} = 300$ Volts and various values of V_{skew} . Note that the contours are now circles and ellipses instead of hyperbolae in Fig. 5.3. This indicates that the coefficients of the terms x^2 and y^2 both have the same sign, and inspecting the values of the contours, we can see that the potentials are increasing away from the center, and hence the potentials are confining in the radial direction. In Fig. 5.4 a), the contours are circles, indicating the same trapping strength in all radial directions. When $V_{\text{skew}} \neq 0$, the contours are ellipses, indicating that the confinement along the two radial principal axes varies in strength. Figs. 5.4 b) and c) show the effective potential corresponding to $V_{\text{skew}} = 5$ volts and 10 volts, respectively. Note that the ellipses in Figs. 5.4 c) are more skewed, and in general, higher values of V_{skew} can be used to skew the trapping potentials, i.e., create asymmetric trapping frequencies along the two radial principal axes. The principal axes for the potentials in Figs. 5.4 b) and c) are still given by Eq. (5.8) since the pseudopotential term is isotropic and the skew term that breaks the symmetry has the principal axes defined in Eq. (5.8). Note that the skew of the trap potentials using V_{skew} increases the trapping frequency along one principal axis and decreases proportionally along the other, and there is a limit to the asymmetry that can be created in the two trap frequencies. In general, $a_{x/y}$ cannot be increased all the way to $\omega_{x/y} = 0$ in Eq. (5.13), the limit is set by the stability regions of the Mathieu equations [89].

Fig. 5.4 d) shows the effective potential in the trap with 200 volts on the end-cap electrodes (see Fig. 5.2 a) description for the naming convention). This configuration represents full 3D confinement since the potential is also confining in the z direction. Notice the orientation of the ellipses in Fig. 5.4 d), the major(minor) axes are not oriented as in Fig. 5.4 b) and c) hinting toward a different set of radial principal axes. This is indeed the case since the end-cap electrodes provide axial confinement and radial anti-confinement, which is the result of the potentials created by the DC fields having to satisfy the Laplace equation. Restricting up to second-order terms in the fit, the potential generated by the central, mid-cap, and end-cap electrodes in the trapping region is given as

$$\mathcal{V}_{\text{cen}} = \frac{V_{\text{cen}}}{R_0^2} (0.019696x^2 + 0.301437y^2 - 0.324475z^2), \quad (5.16)$$

$$\mathcal{V}_{\text{mid}} = \frac{V_{\text{cen}}}{R_0^2} (-0.031441x^2 - 0.2735587y^2 + 0.307642z^2), \quad (5.17)$$

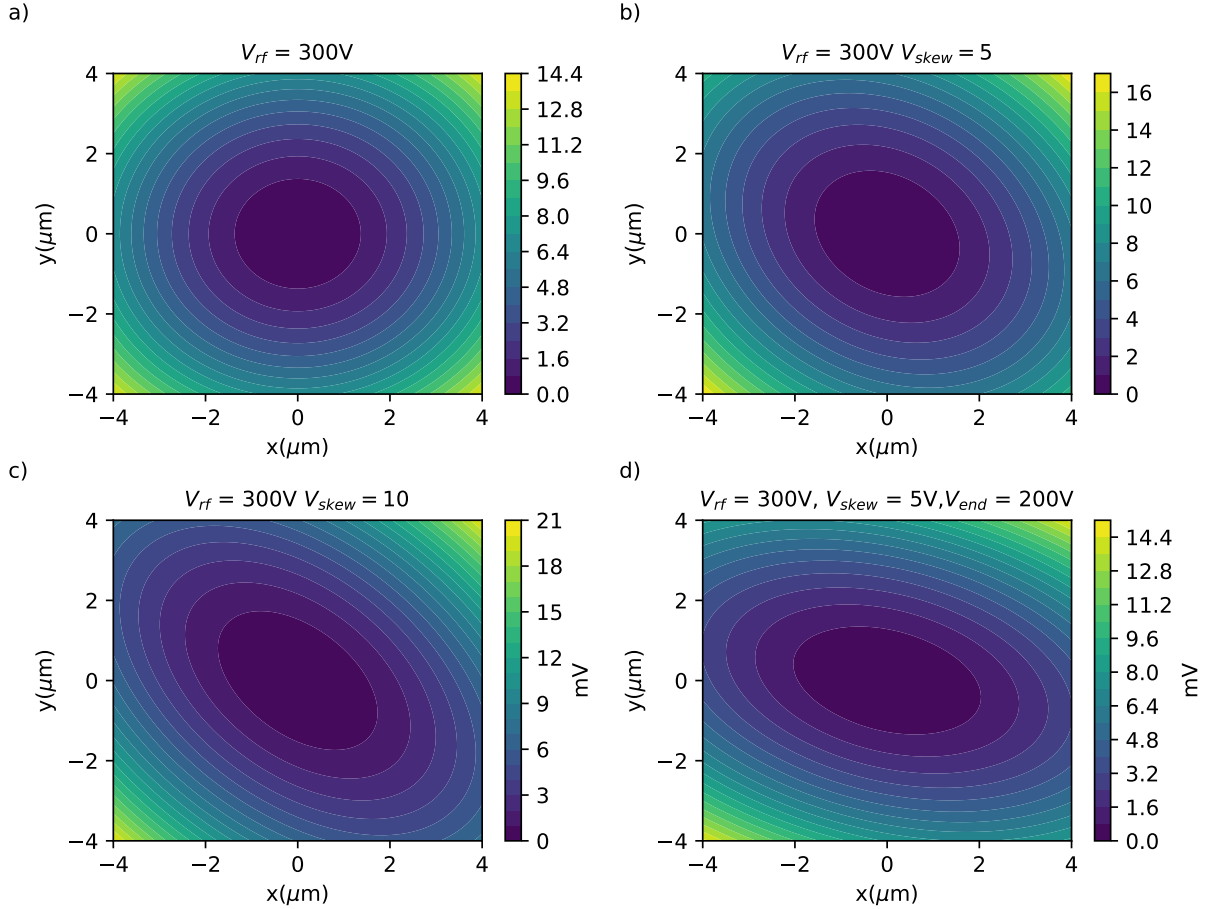


Figure 5.4: Effective Radial potential of Blade Trap

The effective potential is the sum of the pseudopotential and the potential created by the DC voltages on respective electrodes. **a)** $\pm V_{rf} \cos(\Omega_T t)$ applied to the diagonal pairs of blades. The trapping potential is isotropic in the XY plane when only RF voltages are applied. **b)** and **c)** $\pm V_{skew}$ DC voltages on the diagonal pairs adds asymmetry to the trap, i.e., the trapping frequency along the two principal axes is different. **d)** Adding DC voltages to end-caps adds not only axial confinement but also radial anti-confinement and, in general, reorients the radial principal axes.

$$\mathcal{V}_{\text{end}} = \frac{V_{\text{cen}}}{R_0^2} (0.008747x^2 - 0.028711y^2 + 0.019652z^2). \quad (5.18)$$

The total effective potential $\mathcal{V}_{\text{eff}}$ is the sum of $\mathcal{V}_{\text{ps}}$, $\mathcal{V}_{\text{skew}}$, $\mathcal{V}_{\text{cen}}$, $\mathcal{V}_{\text{mid}}$, and $\mathcal{V}_{\text{end}}$. To calculate the principal axes and corresponding trap frequencies, the same procedure of calculating the Hessian and diagonalizing it should be followed.

Below is an example with arbitrarily chosen values of $V_{\text{rf}} = 300$ V, $V_{\text{skew}} = 2$ V, $V_{\text{mid}} = 3$ V, and $V_{\text{end}} = 10$ V. Since I had the numerically simulated potentials, I used them directly to get the following effective potential; however, the equations for $\mathcal{V}_{\text{ps}}$, $\mathcal{V}_{\text{skew}}$, $\mathcal{V}_{\text{cen}}$, $\mathcal{V}_{\text{mid}}$, and $\mathcal{V}_{\text{end}}$ will give the same result.

$$\mathcal{V}_{\text{eff}} = 16.907892 \frac{x^2}{R_0^2} + 3.2144606 \frac{xy}{R_0^2} + 15.8147597 \frac{y^2}{R_0^2} + 1.11889712 \frac{z^2}{R_0^2} \quad (5.19)$$

Note that since we have substituted values for the different voltages, $\mathcal{V}_{\text{eff}}$ still has units of volts. This is also true for the Hessian,

$$H_{\text{eff}} = \frac{1}{R_0^2} \begin{bmatrix} 33.815784 & 3.214461 & 0 \\ 3.214461 & 31.629519 & 0 \\ 0 & 0 & 2.237794 \end{bmatrix}, \quad (5.20)$$

Which has the correct units (V/m^2) as well.

After diagonalization, we have $H_D = P^{-1}HP$ where columns of P give the directions of the trap principal axes,

$$P = \begin{bmatrix} 0.813007 & -0.582254 & 0 \\ 0.582254 & 0.813007 & 0 \\ 0 & 0 & 1.0 \end{bmatrix}, \quad (5.21)$$

$$H_D = \frac{1}{R_0^2} \begin{bmatrix} 36.117898 & 0 & 0 \\ 0 & 29.327406 & 0 \\ 0 & 0 & 2.237794 \end{bmatrix}. \quad (5.22)$$

The trap frequencies can be calculated from the diagonal elements of H_D , using $\omega_i = \sqrt{2qH_D(i, i)/m}$ to give $(\omega_1, \omega_2, \omega_z) = 2\pi \times (5.0804123, 4.57798696, 1.26458435)$ MHz. Note that the radial principal axes are no longer aligned 45 degrees from the x- and y-axes.

In the above discussion of the trapping potentials, the polynomial fit was restricted to the second order only, and the potential was simulated on a grid of size $4\mu m \times 4\mu m \times 40\mu m$ in the x, y, and z directions, respectively. For working with a small number of ions and performing preliminary calculations, the derived expressions will be useful; however, at least in the z direction, this is a drastic simplification. Fig. 5.5 shows the potentials generated along the z axis when 1 volt is applied to the end caps, mid-caps, and central segments separately while keeping all other electrodes at ground potential ($V = 0$). Comparing the form of the end-cap and the mid-cap potential, it is clear that the potentials generated by these have different shapes and, in general, at least fourth-order terms must be included in the polynomial fit. The primary use for these electrodes was to create ion chains with equally spaced ions, but we soon realized that the available controls were not enough. Fig. 5.6 a) and b) show the calculated equilibrium positions of 18 ions with and without optimization for equispaced chains. The ion positions in the intended equispaced chain are more equispaced than the ion positions generated from purely harmonic confinement; however, the spacings are not precisely equal. The high level of control afforded by having 20 DC electrodes will be useful for other purposes, such as orienting the trap principal axes and micromotion compensation. It is also possible to create double well potentials as shown in Fig. 5.6 c) which may be useful. As the experiment progresses towards large-scale quantum simulations, a careful analysis of the trap principal axes and the normal modes along the lines of the previous discussion and Section 2.1 will have to be performed.

5.3 Trap Fabrication

Fig. 5.2 a) shows a schematic of the blade electrodes with five segments on each electrode. The substrate of the blade is made out of Alumina, and the segments of the blade are defined with galvanically separated gold deposits. Fig. 5.7 shows a picture of a fabricated blade electrode with laser-cut segments and gold deposits on each segment.

For the fabrication of the blade electrodes, our first choice was to not fabricate the electrodes in-house in order to save time. I had contacted several micromachining companies for the fabrication of the electrodes; however, very few companies returned with a quote. In particular, Translume Inc was the only company that reverted back with a quote for a completely fabricated electrode. Because we were not the first research group to use blade electrodes in ion traps, we benefited from the experience of other groups using

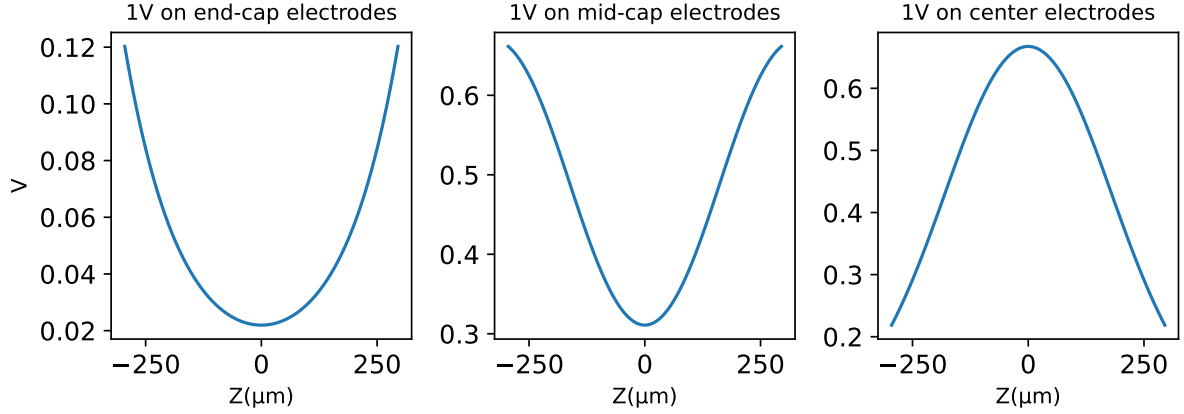


Figure 5.5: Potential along the z axis for different trap electrodes
All other electrodes other than the labeled electrodes are at $V = 0$.

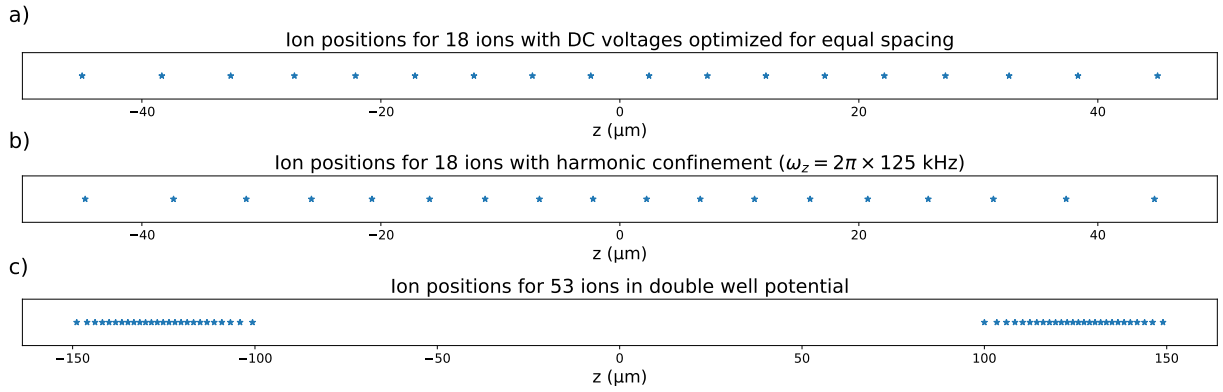


Figure 5.6: Calculated ion positions in blade trap

a) 18 ion chain optimized for equal spacing. Voltages on central, mid-cap, and end cap electrodes are 0.45, -0.95, and 16.5 V respectively. **b)** 18 ion chain in harmonic confinement. **c)** Double well potential. Voltages on central, mid-cap, and end cap electrodes are 1.4, 0.15, and 11 V respectively.

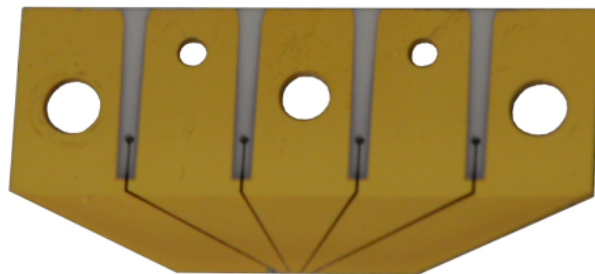


Figure 5.7: Fabricated Blade Electrode

Picture of actual blade electrode. Segmented electrodes are achieved by depositing galvanically isolated gold deposits on an alumina substrate (white)

electrodes fabricated at Translume. The main issues with these fabricated electrodes were their surface roughness, and some groups faced issues with the gold coating flaking off when applying high-voltage RF signals.

Of the companies contacted for the fabrication of the electrodes, several companies contacted back for partial fabrication of the electrodes. In particular, Centerline Technologies, USA, agreed to laser cut the segments in the electrodes, and Laser Micromachining Limited, UK, agreed to laser cut the segments and also to make the taper in the side of the electrode facing the ions (see Fig. 5.2 b)). An important requirement that we had for our electrodes was that the laser cut tips should also be polished to achieve a very smooth surface finish. This is especially important because the tip is the electrode's surface that is directly 'visible' from the trapping region. None of the companies agreed to this requirement.

Given the high technical requirements of the blade electrodes, we finally decided to fabricate the blades in-house. We decided that we will purchase $500\text{ }\mu\text{m}$ ⁵ thickness Alumina wafers with laser cut segments from Centerline Technologies, and I will perform the rest of the micromachining given my previous experience in microfabrication [174]. The fabrication procedure can be divided into the following broad steps:

- Chamfer: Taper the ion end of the blade to a thickness of $50\text{ }\mu\text{m}$
- Polish: the tip of the $50\text{ }\mu\text{m}$ end
- Gold Coat: Apply Gold coating on micromachined blades

⁵I also experimented with a $300\text{ }\mu\text{m}$ substrate and found that the $500\text{ }\mu\text{m}$ substrate is much easier to work with because it is stiff and does not break easily.

Fig. 5.8 gives an overview of the blade electrode microfabrication apparatus. We were fortunate to have a wafer polishing setup available to use at QNFCF, the cleanroom facility at the University of Waterloo. Fig. 5.8 a) shows a picture of the wafer polishing machine, MultiprepTM from Allied High Tech Products Inc., and a cartoon schematic of the polishing procedure. The general idea of polishing is to rub the substrate against a harder and smoother material to achieve a smooth mirror-like finish. This is usually achieved by bringing the substrate in contact with a rotating abrasive disk, and usually, the substrate itself is mounted on a mount rotating in opposite directions. In our case, for the Chamfering process, we are more interested in removing the material from the alumina substrate at an angle rather than polishing. For this, I designed an angle mount that holds the blade at an angle of 8 degrees with respect to the abrasive disk, as shown in the cartoon schematic in Fig. 5.8 a). The angle mount was machined by the personnel at the Science Technical Services (STS) machine shop at the University of Waterloo. Fig. 5.8 c) shows an alumina blade mounted on the angle mount. Once the chamfer process is complete, the polishing step involves mounting the vertical mount shown in Fig. 5.9 b) so that once mounted on the polishing apparatus, the 50 μm tip comes into contact with the rotating abrasive disk.

Fig. 5.9 shows images of the blade substrate tip in various stages of micromachining. Note that the segment tips of the laser-machined wafer are not flat surfaces but round edges, and I had a difficult time imaging the bare tips because of surface undulations. In addition, the end cap segment tips were at a different height compared to the electrode tips of the central segment, and this added further complication in characterizing the pre-machined blade tips. As a rule, I always started the fabrication of each blade with a first round of tip polishing and removed approximately 10 μm of material on a 15 μm diamond lapping paper⁶. We will call this the facing operation. Fig. 5.9 a) shows a pre-machined blade with a 10 μm facing operation performed. The flat edges can now be clearly seen on the end cap tips, although the central segments have not yet been polished and cannot be clearly resolved in the imaging setup. After performing a 20 μm facing operation, the blade tips, which are now approximately in the same plane, can be easily resolved as flat surfaces on a microscope, as seen in Fig. 5.9 b). The next step in the fabrication was the chamfer process, which involved mounting the blade on the angle mount discussed earlier in Fig. 5.8 c). The chamfer operation was performed in small increments, and the blade was imaged at each step to take measurements. Figs. 5.9 c) and d) show one such blade where the edge has been reduced to $\approx 120 \mu\text{m}$ and $\approx 50 \mu\text{m}$, respectively. After some iterations of the facing and chamfering, The final step of the microfabrication included polishing the 50 μm tips that will face the ions. This polishing was performed using an

⁶15 μm refers to the size of the ground diamond particles on the lapping paper.

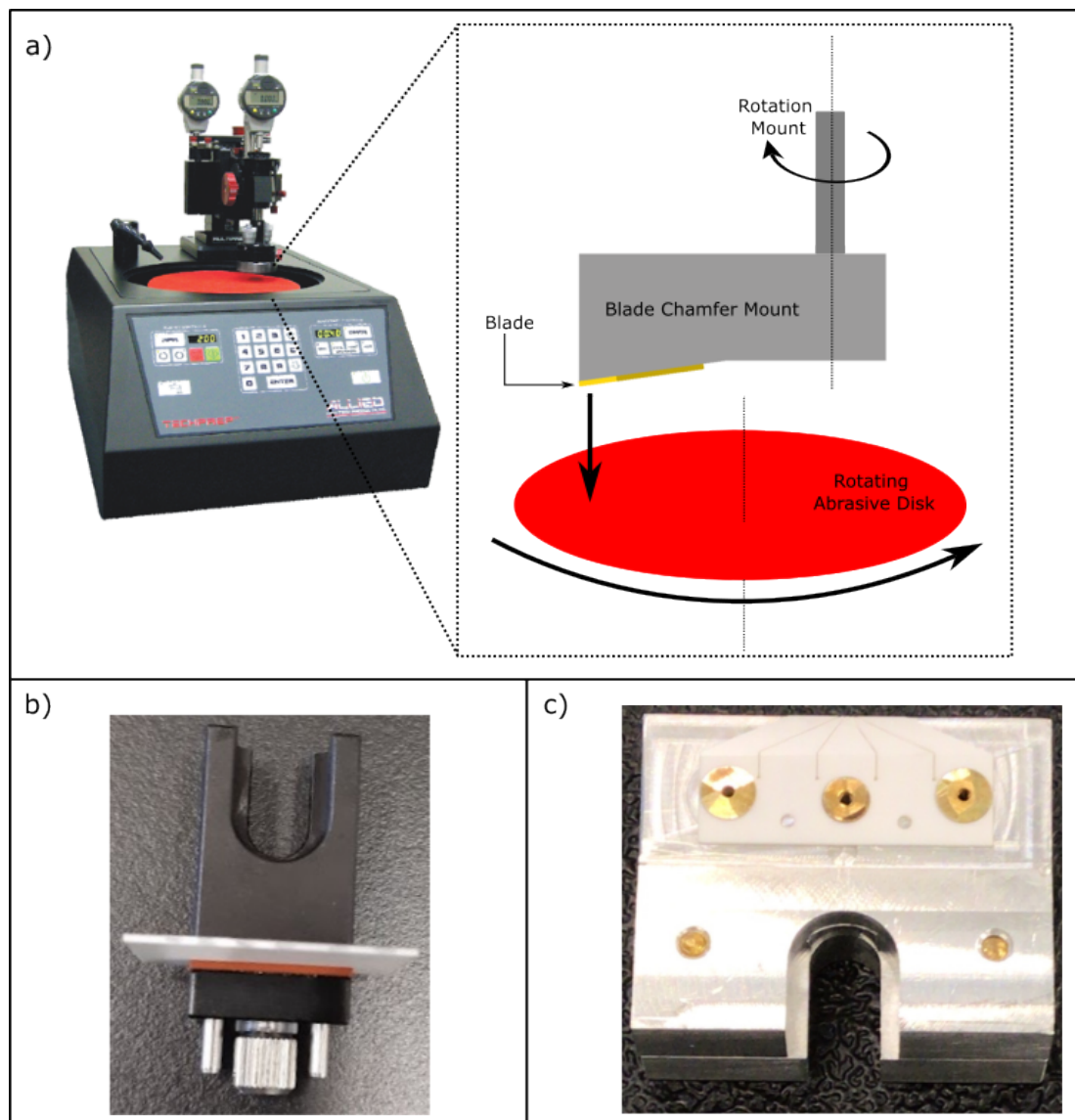


Figure 5.8: Blade Chamfer and Tip Polishing Technique

a) MultiprepTM from Allied High Tech Products Inc. for micromachining the taper on the alumina substrate of the blade electrode. b) Vertical holder mount to polish the edge of a wafer/substrate. c) Angle mount designed for holding the blade at 8 degrees with respect to the abrasive disk.

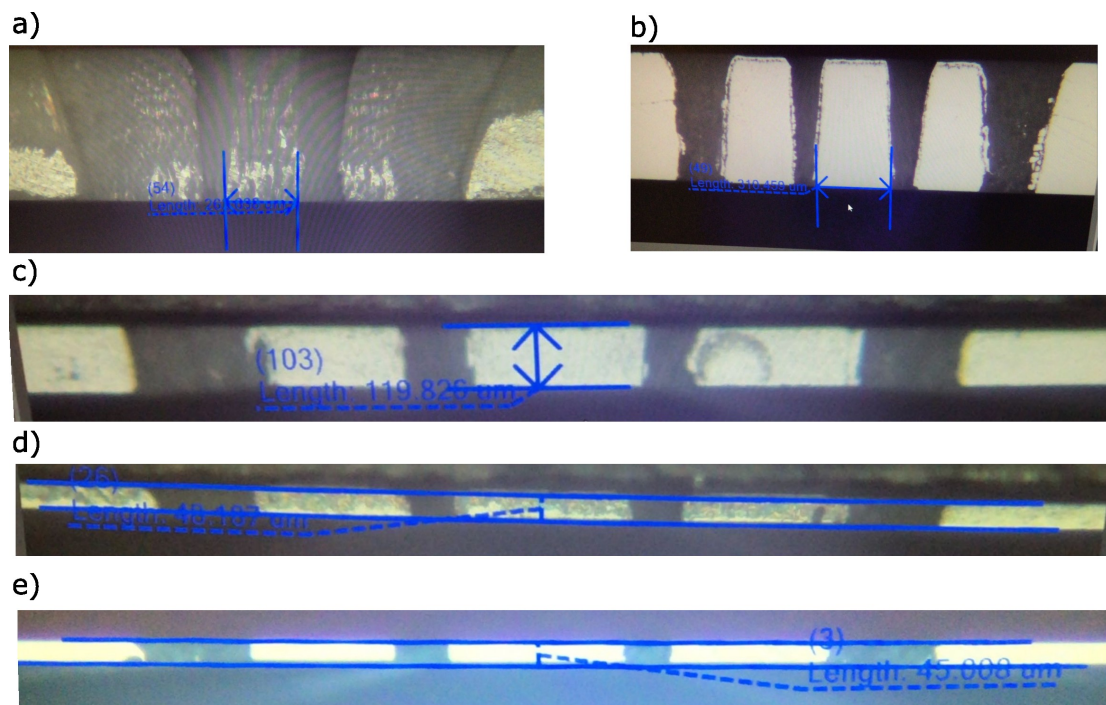


Figure 5.9: Blade Micromachining Results

a) and b) Tip images after 10μm and 20μm facing respectively. c) and d) Tip images after multiple iterations of chamfering e) Tip image after polishing tip to mirror-like finish.

ultrafine 0.1 μm diamond paper, and the end result was tips that had a mirror-like finish as shown in Fig. 5.9 e).

Micro-machining is quite difficult because of the several different parameters that have to be optimized in the machining. There is the rotation speed of the substrate holder and the abrasive disk, additional weights and spring tension settings to press the sample against the abrasive disk, the oscillation speed⁷ of the rotating mount, the grit of the diamond paper, and the process feed, that is, how much material to remove in each step. Because we had laser-cut tracks on our substrate, there was a high tendency of breakage at the point where the laser-cut track ended on the substrate. To minimize the breakage a diamond paper with a small particle size is required, but this comes at the cost of a long process time. The highest particle size that leads to minimal breakage should be used. Similarly, the substrate mount needs to be lowered very carefully onto the rotating abrasive disk to minimize the rather high chance of breaking at first contact. After optimizing the various settings, I fabricated the blades in batch style, i.e., I performed the same operation on different blades and moved on to the next operation. Table 5.1 documents the recipe steps and parameters used and could be used as is for blades with similar dimensions and substrate material or could serve as starting points for a new recipe.

Step name	Paper grit (μm)	Spring tension	Max feed(mm)	OSC/ROT
Rough facing	15	2.5	10	OFF/OFF
Rough facing 2	15	2.5	3	OFF/OFF
Rough chamfer	30	5	350	3/ON
Fine facing 1	6	2.5	3	OFF/OFF
Fine facing 2	3	2.5	3	OFF/OFF
Fine facing 3	1	2.5	3	OFF/OFF
Fine chamfer	30	5	5	3/ON
Final polish	0.1	1	10	1/OFF

Table 5.1: Process parameters for blade micromachining

Max feed refers to the amount of time the sample can be lowered onto the abrasive disk while polishing.

OSC/ROT refers to the substrate holder oscillation and rotation. Only steps Rough chamfer and fine chamfer use weights of 300 g and 150 g respectively.

Compared with the micro-machining step, the gold coating of the blades was quite straightforward. Before gold coating the blades, they were cleaned in two steps: low-power

⁷The mount that houses the substrate also oscillates perpendicular to the axis of rotation

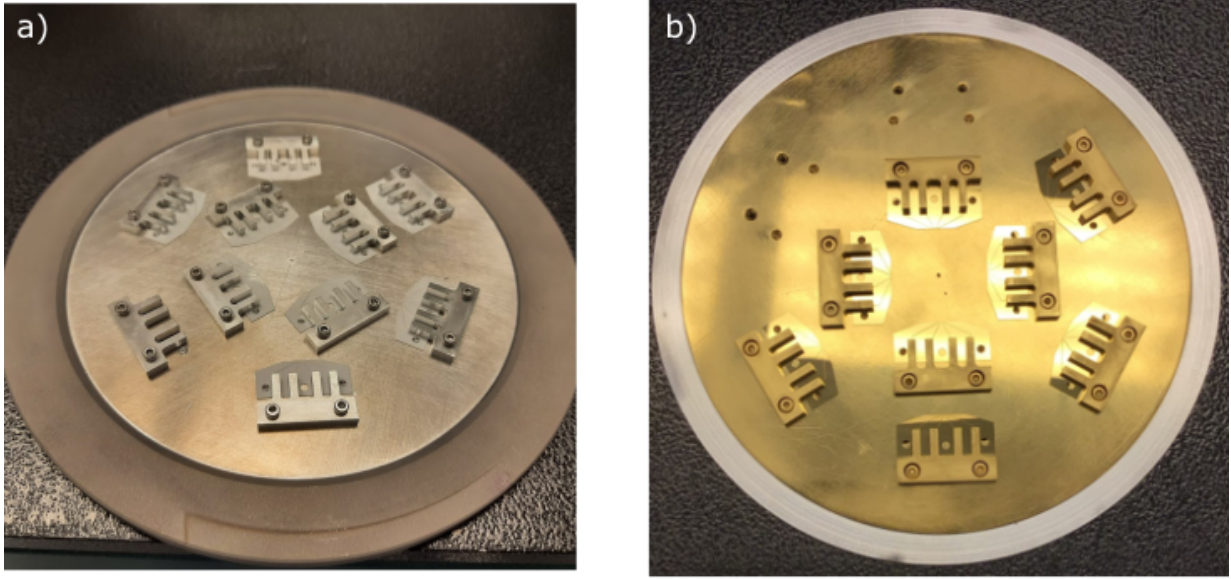


Figure 5.10: Sputtering Mount
a) Before gold coating **b)** After gold coating

sonication in DI water to remove debris from the micromachining followed by cleaning with piranha solution (3:1 H_2O_2 : H_2SO_4). The cleaning ensures that there are no debris or organic deposits on the substrate before gold deposition. This is very important because the adhesion of the deposited metals is also a function of the surface cleanliness. The next step was the gold coating, which was performed on the AJA sputter chamber at QNFCF, the cleanroom at the University of Waterloo. We decided to use RF sputtering because the deposition is isotropic and results in uniform deposition even inside the laser cut tracks, so that there is no exposed dielectric facing the ions. Care was taken to avoid deposition completely inside the laser cut tracks in order to avoid electrically shorting the electrodes. This is usually done using sputter masks that create shadow regions where the coating is not deposited.

Fig. 5.10 shows the sputtering mount that I designed to mount multiple blades for gold coating while creating shadow regions for the tracks. The fork-like holders create the appropriate shadow regions and also serve as clamps to hold the blades in place. This allows for processing multiple blades in a single batch. As discussed earlier, we had reports from other groups using similar blade-shaped electrodes for their traps that the gold coating was

a point of failure as a result of the flaking of the gold coating. Thin film deposition is a vast and complicated topic, and optimizing coatings can be very challenging, but thankfully, our task was simply to maximize the gold adhesion. Since thin film deposition is not an area of expertise in the group, I reached out to Nathan Nelson Fitzpatrick, now Director of the Quantum Nano Fabrication and Characterization Facility (QNFCF), who was in charge of the deposition processes at QNFCF. It turns out that one of the main factors that affect the adhesion of the coatings is the temperature of deposition [175, 176]. This is because temperature increases the mobility of the deposited atoms and increases their chance of finding energetically favorable deposition sites. In addition, the deposition at high temperatures leads to a more uniform coating, which further helps with the adhesion. The only drawback of high coating temperature is that the deposition rate is slower, and high temperatures also cause unequal expansion of the substrate and the structures that mount the substrate, leading to a possibility of cracking the ceramic substrate.

With all the above factors taken into account, the final goal coating recipe is as follows:

- Pump down to 1E-7 mbar
- Anneal at 200°C for 1 hour
- Ramp substrate temperature to 100°C
- Seed layer deposition: 150 nm Titanium
- Gold layer deposition: 1.1 μm

The annealing of the substrate ensures that the deposition surface has no water vapor deposits on it. The titanium seed layer was deposited because gold does not deposit directly on ceramic substrates. The thickness of the Ti seed layer was greater than the conventionally used value of 20-50 μm to ensure that the Ti layer is deposited evenly inside the laser cut tracks.

Before the final batch of electrodes was made for use in the trap, several electrodes were gold-coated using the technique explained above, for the purpose of high voltage testing. Since, at the time of the test, we did not have a trap for testing, I designed a test fixture to mount two blades with tips facing each other with a tip-to-tip distance of approximately $2R_0$. Fig. 5.11 shows the picture of the fixture mounted inside a vacuum chamber. The reason for using a vacuum chamber is so that the test conditions mimic well the use case. The pressure in the chamber at the time of the test was $\approx 10^{-7}$ mbar, mimicking the thermal dissipation to the surroundings in a UHV chamber. Similarly, the

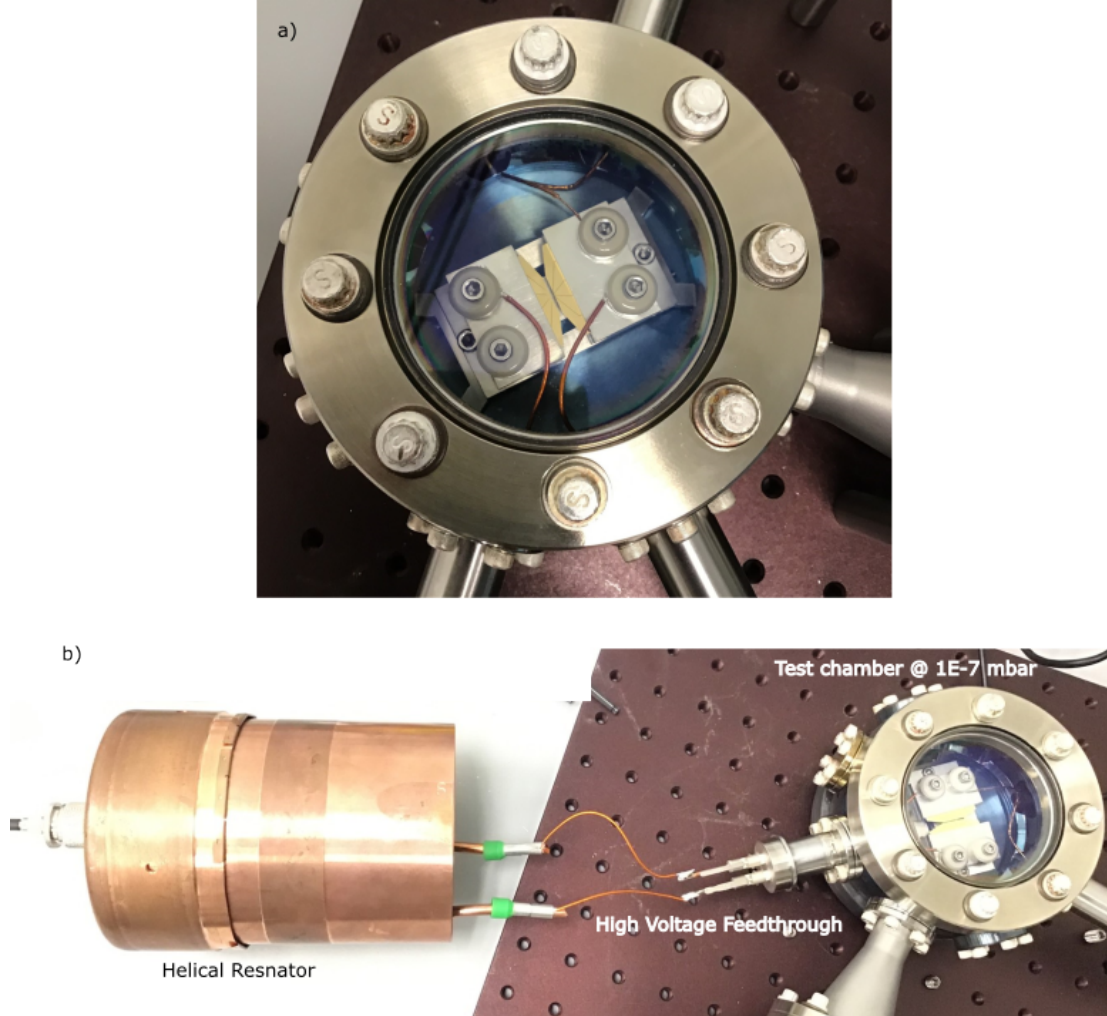


Figure 5.11: Blade Electrode Test Jig

Test apparatus for high voltage testing of the blade electrode gold coating.

- a)** Test fixture mounted inside a vacuum chamber. The blade tips are held at approximately a distance of $2 \times R_0$. There are three wires attached: two for applying high-voltage RF and one for attaching a thermocouple for measuring the temperature of the test fixture.
- b)** High voltage applied through a Helical resonator with unloaded resonant frequency $\approx 2\pi \times 89$ MHz and a loaded frequency of $\approx 2\pi \times 42$ MHz. The unloaded and loaded Q-factors were 780 and 240, respectively. A test voltage of 1 kV at 42 MHz was applied to the blades.

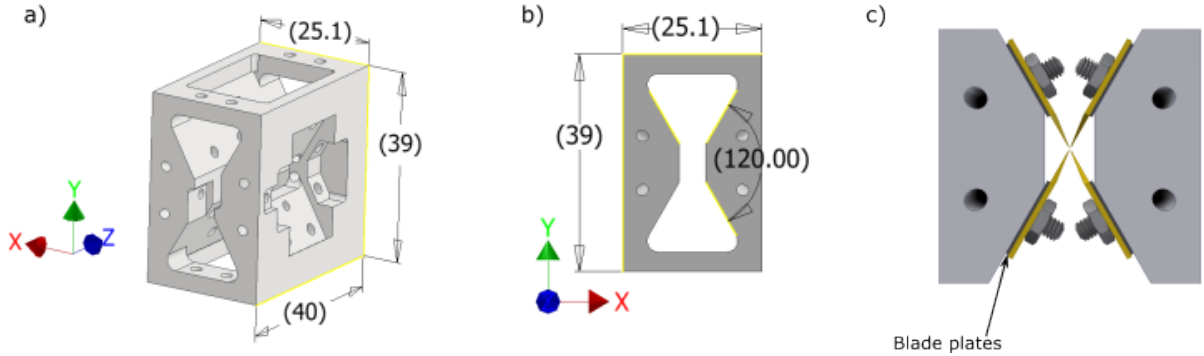


Figure 5.12: Blade Trap Mount

a) Isotropic view b) Side view showing asymmetric blade angle c) Zoomed side view showing blade plates. Blade plates are polished alumina wafers that allow for precision adjustment of blade position by using blade plates of different thickness.

breakdown voltage, given by the Paschen curves [177] for $P \approx 10^{-7}$ mbar, and the extreme high vacuum in the blade trap chamber are well above the test and operational voltages. Before testing, we took several pictures of the blade tips at a high zoom level on a soldering microscope. We first proceeded with the application of DC voltages of up to 1.8 kV to the blades in the test setup through a high-voltage vacuum feedthrough. Later, after imaging the tips of the blades, we found no observable change in the coating. The DC test was just a preliminary test, and the main objective of the tests was to apply high radio frequency voltages to the electrodes. To apply the radio frequency voltages, I constructed a helical resonator [178] to apply high voltage at 42 MHz and 1 kV to the electrodes. We left the setup with the high voltage applied for several hours. Within the first two hours, the temperature of the fixture, measured through a thermocouple attached to one of the blade mounts, reached approximately 130°C. This was expected because there was a large macor block underneath the blades to isolate them from the chamber that led to dielectric losses. After approximately 5 hours, we removed the blades from the test fixture and imaged them again on the same imaging setup. No observable signs of coating damage or flaking were found on the blades.

5.4 Trap Assembly

To achieve the expected performance of the trap, the alignment of the electrodes with respect to each other is as important as the fabrication quality of the electrodes themselves.

Table 5.2: Ceramic Material Properties

Holder Material	Thermal Conductivity (W/m·K)	Loss Tangent (10^{-4})	Thermal Expansion (10^{-6} /K)	Dielectric Strength (kV/mm)
Alumina	30	1	8.4	31.5
Sapphire	40	0.2	7.8	48
Macor	4.6	70	9	45
Aluminum Nitride	180	5	4.5	17
Shapal	92	10	4.3	65
Boron Nitride	80	12	2	79

Fig. 5.12 shows the holder, designed by Dr. Sainath Motlakunta, on which the trap electrodes are mounted. The material for the holder is a relatively new machinable ceramic called Shapal which is a hybrid composite material consisting of aluminium nitride and boron nitride. The appropriate material for use in this application is one that has low dielectric loss, high thermal conductivity, and low thermal expansion. This is because the application of high radio frequency voltages required in ion traps leads to losses in the dielectrics around them, causing the temperature to rise, which in turn causes a change in the dimensions of the structure. This is especially important in an ion trap where the trapping frequency has a squared dependence on the ion electrode distance, and structural deformations translate to trap frequency variations. The problem is compounded by the fact that the typical use of a trap requires the RF voltages to be changed during the ion loading operations, leading to changing temperature of the structure. A material with low dielectric loss, high thermal conductivity, and low thermal expansion produces less heat from RF losses, dissipates the heat better to the surrounding metallic structure, and expands less for a given temperature rise.

Table 5.2 shows the different ceramics used in vacuum applications and their respective material properties. Macor, which is among the most common dielectrics used in ultra-high-vacuum design, was discarded because of the high RF loss tangent. Alumina, aluminum nitride, and sapphire were discarded because of their lack of easy machinability. This left us with Shapal, which was the chosen ceramic.

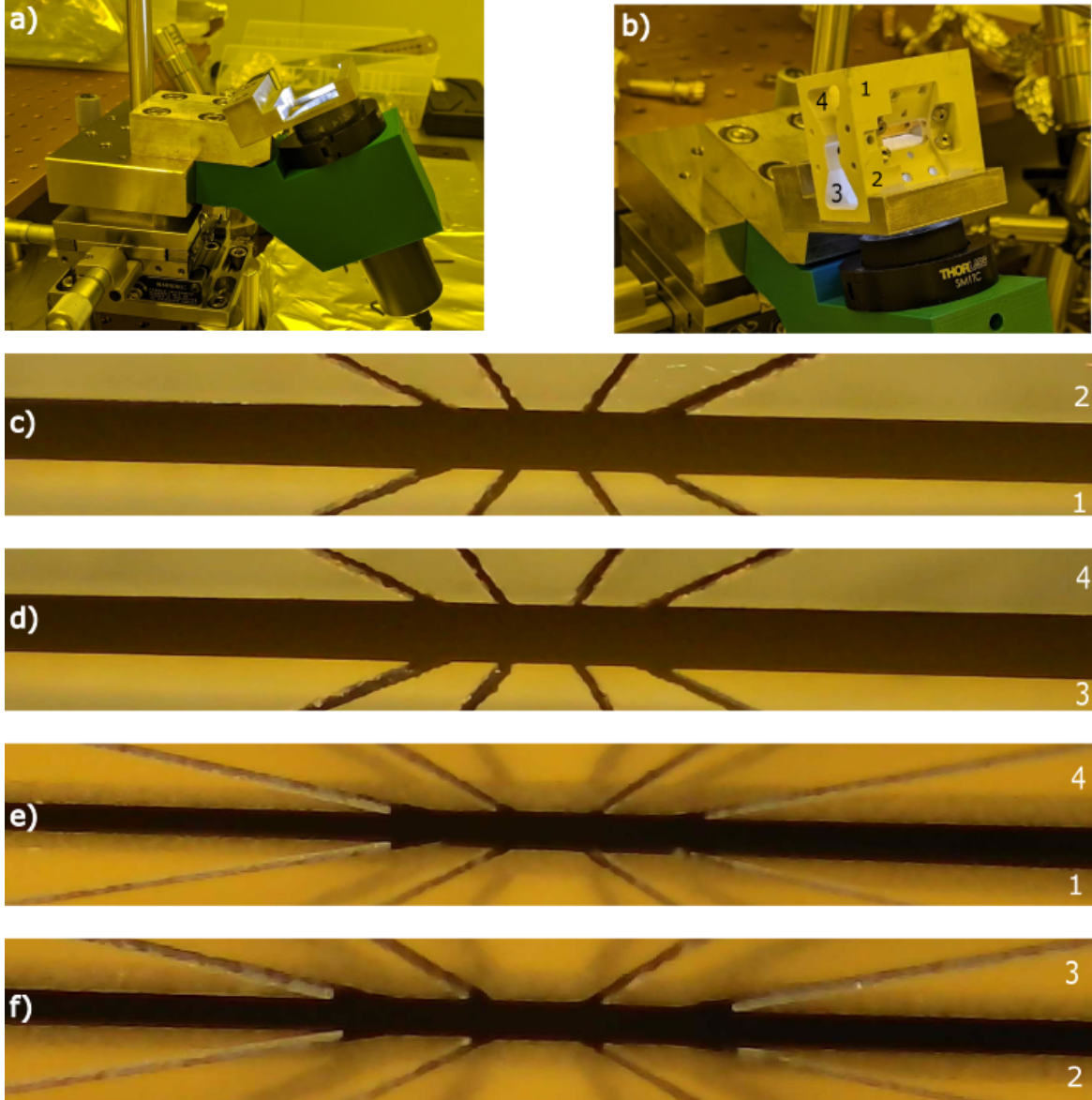


Figure 5.13: Blade Alignment

a) and b) pictures of the alignment jig used for mounting the trap and the soldering microscope for viewing blade tips. c), d), e), and f) Images captured on the microscope showing the final alignment of the blades. The distances between the blades are $316 \mu\text{m} \pm 2.5 \mu\text{m}$, $317 \mu\text{m} \pm 2.5 \mu\text{m}$, $165 \mu\text{m} \pm 2.5 \mu\text{m}$, $141 \mu\text{m} \pm 2.5 \mu\text{m}$ on blade pairs (2,1), (4,3), (4,1), (3,2) respectively.

One of the most time-consuming procedures in the assembly of the trap and vacuum internals was the alignment of the blades on the shapal holder. Fig. 5.12 c) shows a unique feature that we added to the blade holder design: blade plates. The blade plate is an alumina plate between the shapal holder and the blade electrode, which allows the manufacturing imperfections in the shapal holder to be compensated for by choosing among blade plates of multiple thicknesses. Even with the blade plates, finding an optimal alignment strategy was quite difficult, especially because the blades had to be aligned by hand. An optimal alignment strategy is one that is quick and repeatable. This is so that the blades do not rub excessively against the resting surface and cause the gold coating to be scratched excessively. The alignment apparatus should also allow for high-resolution viewing of the blade electrodes while the operator is aligning the blades. Fig. 5.13 a) shows the alignment jig, mounted on a translation stage to house the blade holder during alignment operations. The alignment jig was designed by Anthony Vogliano, and later, I added a 3D printed fixture to attach a 4K soldering microscope⁸ to the alignment jig. This ensured that the imaging assembly was mounted directly on the alignment jig, and there was less chance of the imaging setup getting misaligned. Fig. 5.13 b) shows the alignment jig along with the shapal holder on it and the various numbered blade attachment positions.

Trying different alignment strategies with test blades, we realized that the main failure point in any strategy is not the act of alignment itself but rather the tightening of the fasteners to hold the blade in place after completing the alignment. The main reason for this was that while trying to tighten the nut that held the blades in place (see Fig. 5.12), there was inevitably some force applied to the mating bolt perpendicular to the bolt axis, which moved the position of the blade. We quickly realized that the only way to tighten the blades in place without disturbing the alignment was to interchange the direction of the insertion of the bolt. If the bolt is at the top, the tightening could be performed using a ball driver, and since a ball driver can tighten bolts even at sharp angles the operator can tighten the blades in place without applying a force perpendicular to the bolt axis and this leads to minimal disturbance to the blade position. Inverting the bolt insertion direction seems straightforward; however, it was complicated by the fact that the dimensions of the holder could only allow the insertion of a very short (1.4 mm) bolt to be inserted from the top, and with this length, it would not be possible to attach a nut from the other side. To remedy this, I designed an internal thread bolt, as shown in Fig. 5.13 b), which looks like a regular bolt but has a hollow shaft with internal threads. The design is trivial; however, the machining is not, and the personnel at Science and Technical Services (STS), University of Waterloo, machined this bolt for us. With these changes to the fastening strategy, the alignment of the blade became very quick and repeatable. Sainath Motlakunta and

⁸These are readily available on online marketplaces like Amazon and are quite inexpensive (<\$50)

I performed the final alignment of the blades, with one person on the alignment jig and another on the computer taking microscope measurements. Figs. 5.13 c) to f) show the final alignment pictures of all the blade pairs.

The final step in the assembly of the trap was to attach the electrical connections. Fig. 5.14 shows the procedure for attaching electrical connections. There are two parts to the electrical connections: a vacuum-compatible PCB with Kapton-coated wires soldered on them and a fuzz button holder that creates robust electrical contact between the PCB and the blade electrodes. The PCB was designed by Dr. Sainath Motlakunta and fabricated in-house by Roberto Romero, Electronics and Instrumentation Technologist at the Institute for Quantum Computing. The PCB substrate was Rogers 4350, as is standard for UHV applications [179]. To solder the wires on the PCB we used ultrasonic soldering to avoid using solder flux, which is a known contaminant in vacuum systems. The solder alloy we used was cerasolzer, which is a flux-free solder alloy, and the specific part number of the solder alloy was GS220ME from MBR electronics.

5.5 Science Chamber Design and Construction

The next step after the assembly of the trap was the assembly of the internals of the science chamber. Fig. 5.15 shows the cross-sectional view of the science chamber with the trap mounted in the center. The high optical access provided by the trap (inset picture) is made usable by the reentrant windows on the vacuum chamber. The reentrant windows allow us to bring the optics as close to the trap as possible, and the minimum working distance from the ion plane is 15.7 mm and 35.7 mm in the side and vertical directions, respectively. The optical element in the reentrant is fused silica and has a thickness of 5 mm. The diameter of the tube on all the reentrants is ≈ 60 mm, allowing for easy mounting of 2-inch optics.

The windows were manufactured by MPF Products, and the anti-reflective coating on the optic was done by FiveNine Optics, Inc. The general procedure in reentrant fabrication is that the optic is first brazed onto a small cylindrical sleeve such that the dimension of the part is small enough to fit inside a physical vapor deposition (PVD) setup. The coating specific to the requirement is then deposited on the optic, and then the sleeve is welded onto a larger tube which is already welded to the vacuum flange. Although MPF has a manufacturing setup capable of performing all of these steps, their optical coating was not as per our specifications. Due to this, the sleeves with the optic brazed on them were sent to FiveNine Inc., where the coating was done, and then they were sent back to MPF for the rest of the procedure. The FiveNine coating specifications had reflectivity below 0.5%

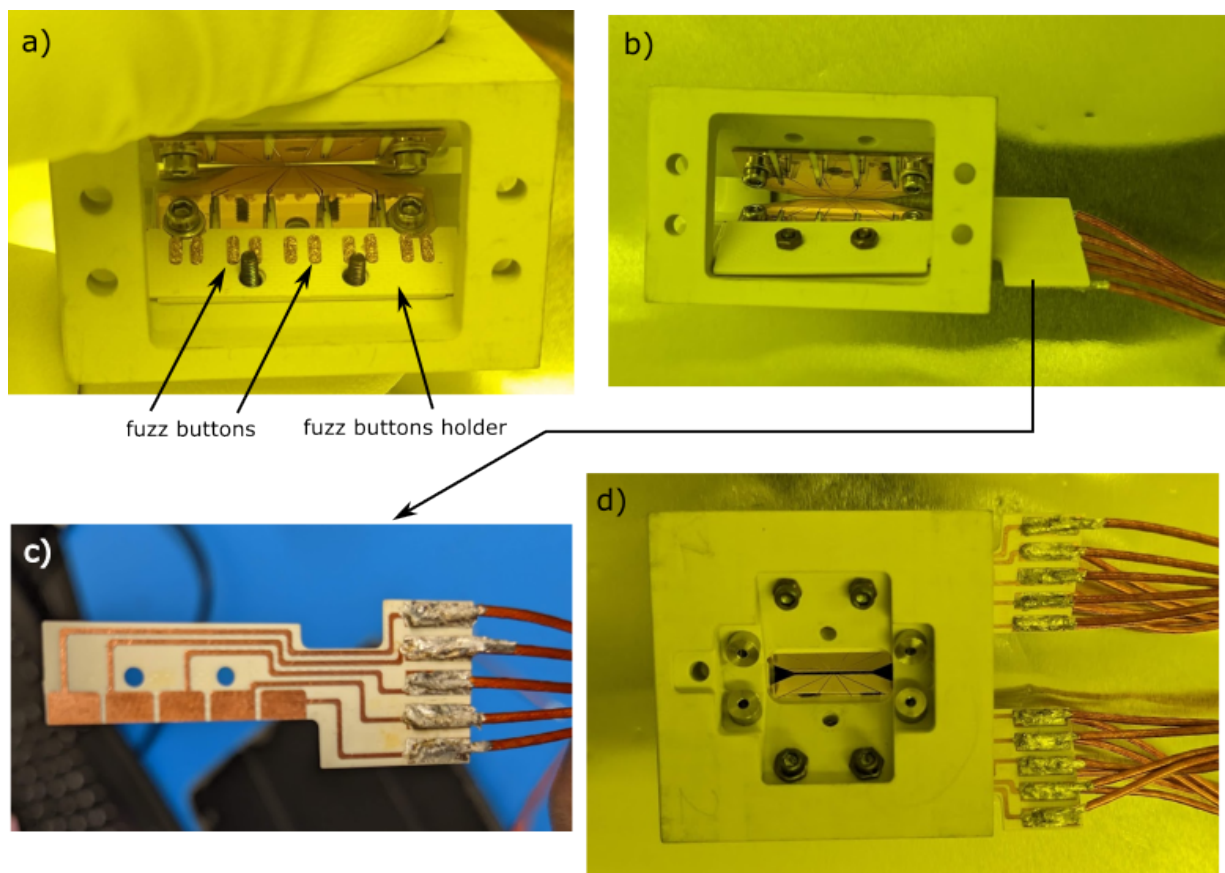


Figure 5.14: Blade trap assembly

Figures show various steps in the assembly of the trap **a)** Electrical connections made using gold fuzz buttons held in place by custom designed PCBs **b)** PCB attached **c)** Picture of PCB with ultrasonically soldered kapton-coated wires (20 AWG stranded wire from AccuGlass). Solder alloy: GS220ME from MBR electronics **d)** Fully assembled trap

at both 369 nm and 355 nm with a numerical aperture of 0.6. Additionally, the coating exhibited a reflectivity of less than 15% over a broad range of 400 to 1800 nm.

The cross-sectional view in the YZ plane is shown in Fig. 5.16. Here, the various beam delivery ports and the mounting structure for the trap can be seen. The beams labeled ‘111 beams’ have projections on all the three trap axes and hence allow for sending cooling beams. In-vacuum mirrors deflect the beams out of the vacuum chamber to minimize scattered light during experiments.

The mounting structure on which the trap is mounted is in the form of a bridge, also shown in Fig. 5.17. I designed the bridge structure as a multi-component assembly that has trusses for mechanical rigidity, and since the structure is made out of multiple components that are bolted to each other, it provides a natural damping of vibrations. The oven assembly and the ablation oven mount, designed by Dr. Sainath Motlakunta, ensure that their respective atomic flux is directed to the trap center within the tolerances of the machining. Dowel references were added to the entire assembly to ensure that the trap position is highly accurate and the trapping region overlaps the atomic flux from both sources. All of the above components, except the atomic oven tubes, were fabricated by personnel from the Science and Technical Services. The atomic oven is simply a stainless steel tube that houses a chunk of ytterbium, and upon heating the tube by passage of current, a plume of neutral ytterbium atoms is emitted from the tube. The oven tube was made very similarly to our previous experimental apparatus, and for details of the fabrication, the reader is referred to Ref. [88]. The only difference in the current design is that the tube is laser-welded to the current through it, ensuring a tight seal and only emitting atomic flux in the forward direction. I performed the welding on the ROFIN 7002 laser welding setup by Protec at QNFCF, the cleanroom at the Institute for Quantum Computing.

It may come to the reader’s attention that all the parts appear brownish/bronze-colored, and the color on the surface is nonuniform. This is because we prebaked all components at 400°C in vacuum for 3 days followed by a 400°C air bake. Fig. 5.19 shows details of the internals prebake. As we will see in the next section, the prebaking ensured low outgassing of components, essential for creating an extreme high-vacuum environment. The discoloration is due to the formation of an oxide layer in stainless steel.

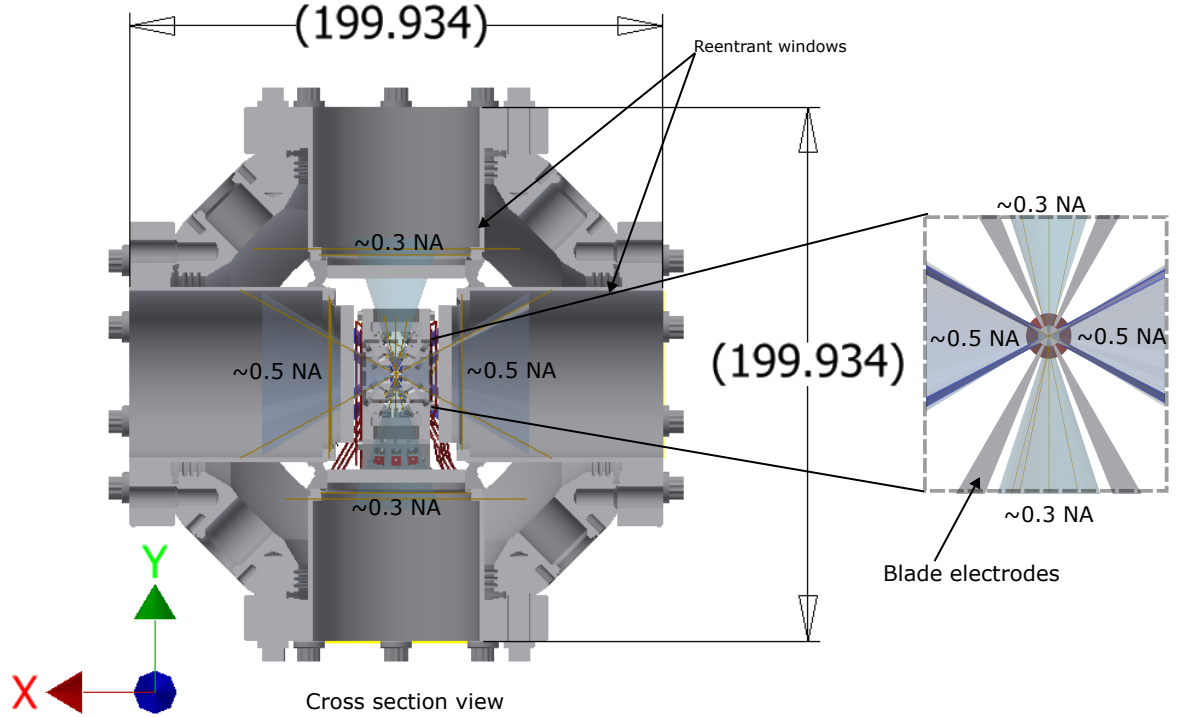


Figure 5.15: High Numerical Aperture Optical Access

Cross-sectional view of science chamber CAD model in the XY plane. All dimensions are in mm. The side directions ($NA \approx 0.5$) are for coherent individual addressing with Raman beams (355 nm) and for ion fluorescence collection during detection. Any beams from the side directions are also perpendicular to the atomic plume emitted from the oven, and hence, these directions will also be used for the first ionization beam (399 nm). The vertical directions ($NA \approx 0.3$) are for incoherent individual addressing of ions for state reset and readout and a lower NA imaging setup for addressing beam calibration.

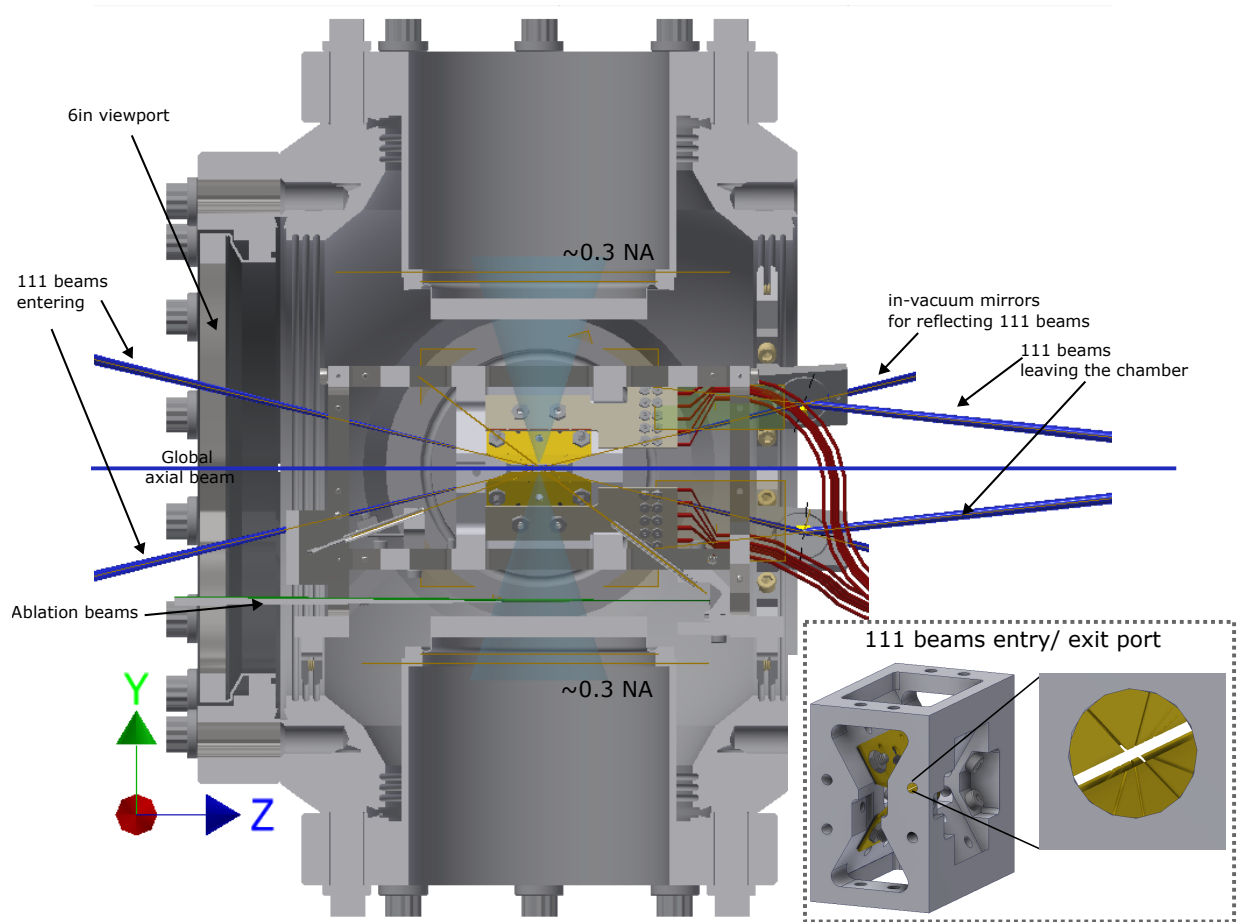


Figure 5.16: Low Numerical Aperture Optical Access

Cross-sectional view of science chamber CAD model in the YZ plane. The beam labeled 111 enters the trapping region through the four access ports shown in the inset. The low NA beams are for global cooling, optical pumping, state reset (369 nm), and repump (935 nm and 760 nm).

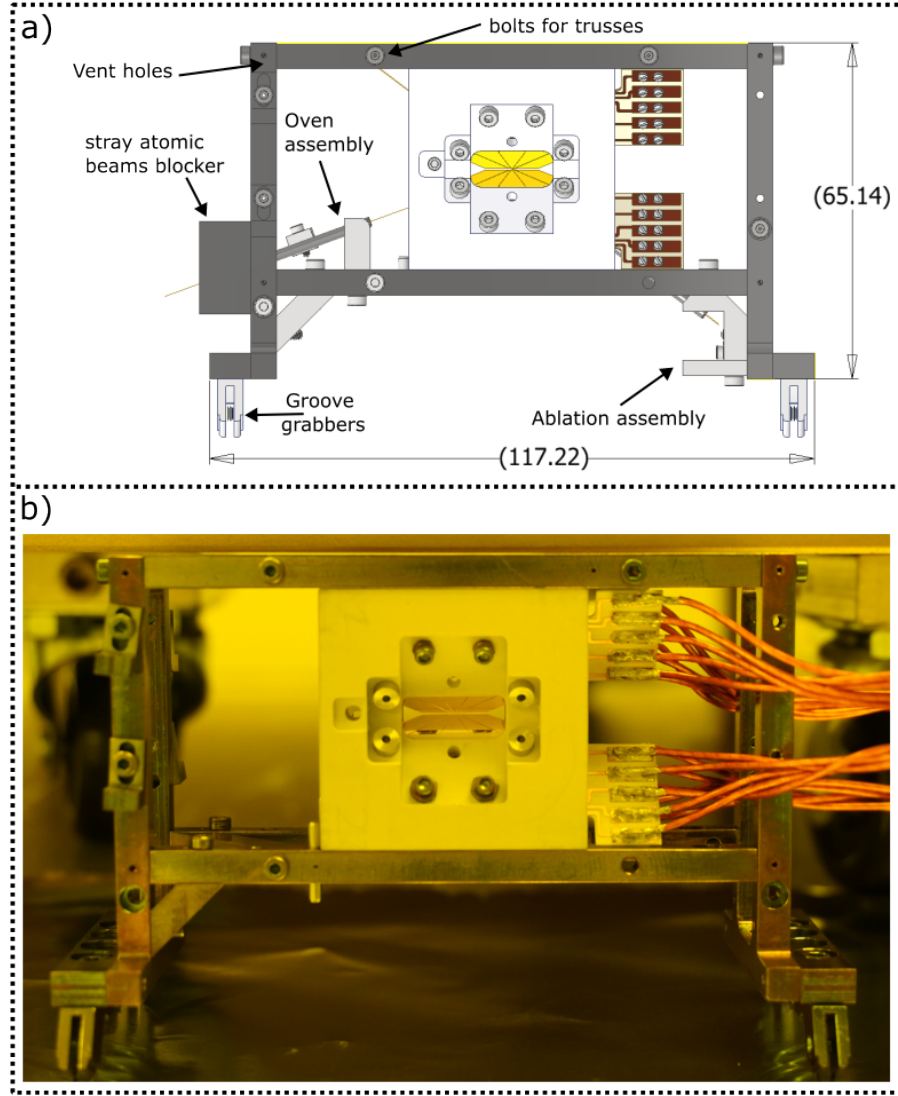


Figure 5.17: Bridge Assembly for Blade Trap Mount

a) CAD model of the bridge assembly for mounting the blade trap mount and the atomic sources. All dimensions denoted in mm. The oven mount has two atomic oven, one is natural abundance Ytterbium and another enriched for the ^{171}Yb isotope (95%). The ablation target assembly has three ablation targets which are Ytterbium foils, two of which are enriched. b) The assembled bridge assembly before attaching the atomic sources. The stray atomic beam blocker was not used in the real assembly.

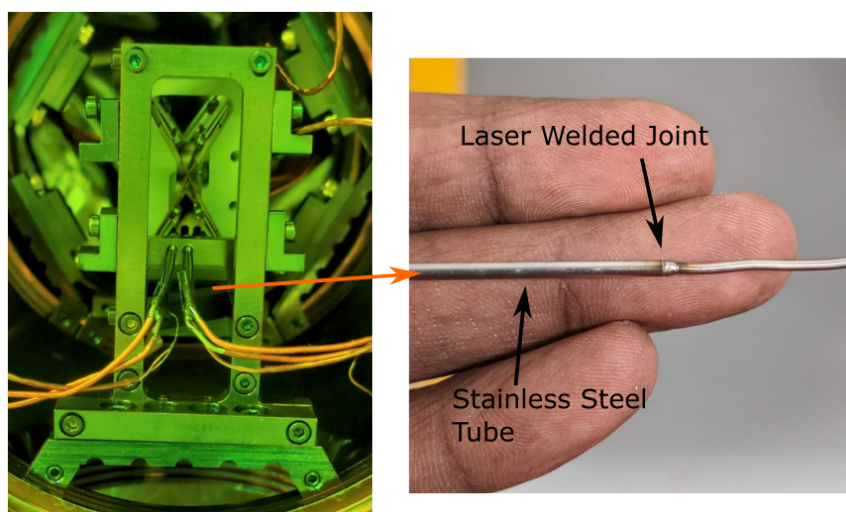


Figure 5.18: Atomic Oven Weld Joint

The atomic oven is a stainless steel tube that houses chunks of Ytterbium, which is very close to the weld joint. The weld joint is between the stainless steel tube and a wire to pass current through the tube to heat the Ytterbium sample. The return current wire is not attached to the picture on the right. A weld ensures a tight seal and avoids spraying Ytterbium in the opposite direction onto the glass viewport.

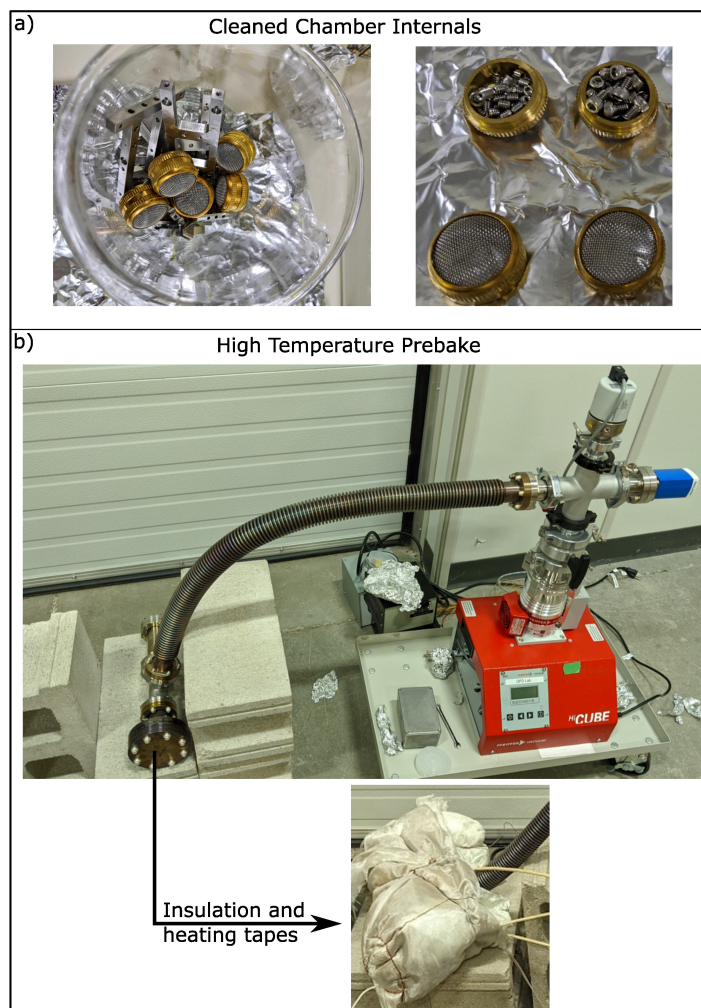


Figure 5.19: Internals Pre-Bake

a) Stainless steel internals in the science chamber were cleaned using soap + DI water sonication for 20 minutes before pre-bake. The Small components, like the nuts, bolts, etc., were packed into small metallic containers for ease of handling. The prebake was performed along with these containers. b) Prebake setup comprising of a 4.5 inch conical reducer along with a 2.75 inch nipple to pack all the internals for prebaking. After pumping down with the turbo, we baked these for three days and another 24 hours after turning OFF the turbo pump and allowing atmospheric air to backfill.



Figure 5.20: Science chamber internals: cube side view

Picture of chamber internals from the rear viewport of the central cube. The wires go toward the feedthrough, which allows for the connection to the outside vacuum. The three cylindrical tubes in the center guide the neutral flux from the ablation targets towards the trapping region.

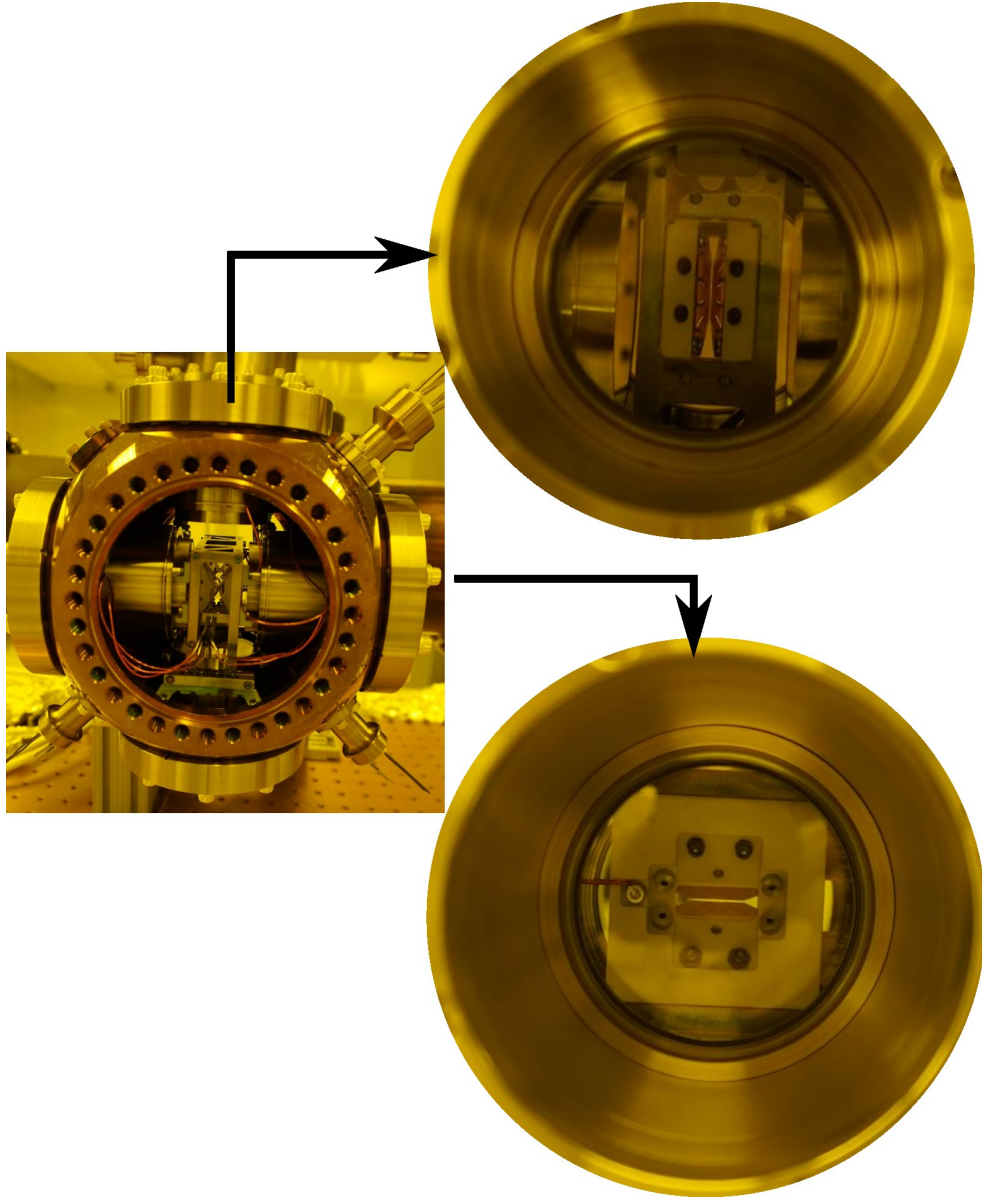


Figure 5.21: Science Chamber Assembled

Pictures of the science chamber before assembly and closing the final viewport. The two insets are top and side views of the trap as viewed from the reentrant windows. The wire attached to the shapal mount, as seen in the bottom picture, is a thermocouple that allows temperature measurements of the trap while in operation.

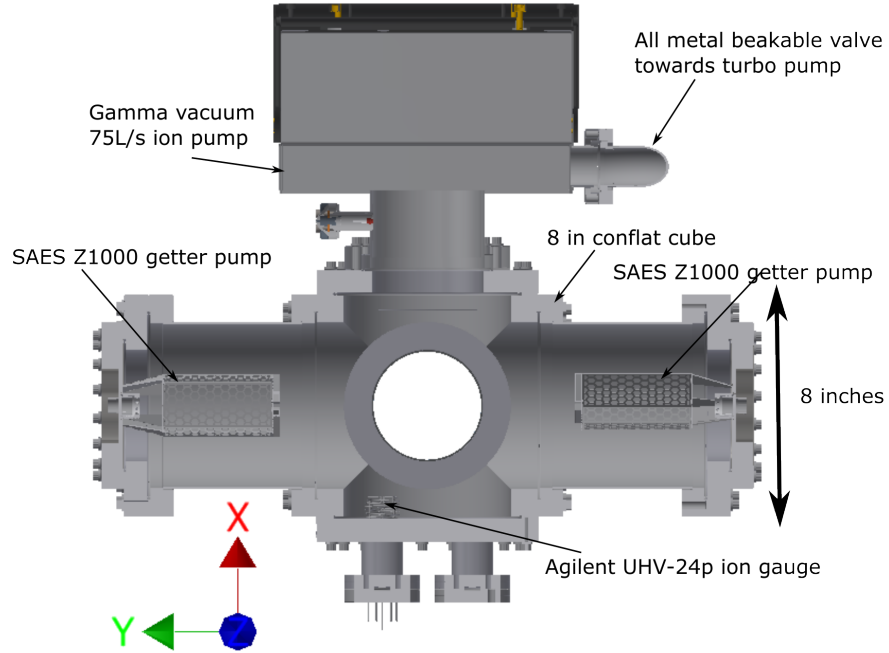


Figure 5.22: Blade Trap Pumping Internals

Cross-section of the CAD model of the vacuum system showing the vacuum-specific internals. Two getters (SAES getters, Z1000) for the getterable load. One ion pump for non-getterable load (Gamma Vacuum, 75S DIX). The DIX ion pump element was chosen because it was optimized for XHV and has a high pumping speed for noble gases. The UHV24p gauge was chosen for its low ($P < 6.66 \times 10^{-12}$ mbar) x-ray limit. We found the x-ray limit to be below 1.5×10^{-12} mbar (see Section 5.6.4 for details).

5.6 Vacuum System Design and Construction

As described in the Introduction, the pressure in the blade trap chamber is below 1.5×10^{-12} mbar. The pressure is likely lower since we are limited by the measurement capability of the pressure gauge. This is among the lowest, if not the lowest, achieved pressure in a room-temperature ion-trapping apparatus and was possible because of the optimization of every single component in the design. Fig. 5.22 shows the cross-section of the CAD model of the vacuum system showing the vacuum-specific internals. There are three main pumps in the system, two of which are ‘getter’ pumps (SAES getters, Z1000), and one is

an ion pump (Gamma Vacuum, 75S DIX)⁹. The pressure gauge (UHV24P) is a Bayert-Alpert (BA) gauge from Agilent. It might come to the reader’s notice that the part of the vacuum system, which is not the science chamber, is mostly empty space, and this is true. This is because, as we shall see later, this geometry optimizes for the highest pumping speed at the science chamber. However, before we get into the design details, it might be prudent to brush up on the basics of vacuum design. In this section, we will go over the relevant fundamentals of vacuum science, some concepts required to simulate vacuum system performance, and how these principles were used in optimizing the design and construction of our vacuum system.

5.6.1 Ultra/Extreme High Vacuum Fundamentals

The term “vacuum” generally refers to a space where the pressure is significantly lower than the atmospheric pressure. This definition encompasses a wide range of pressures, spanning approximately 17 orders of magnitude on Earth including modest vacuum created by a vacuum cleaner to the ultra-high vacuum achieved in advanced particle accelerators, and atomic physics experimental apparatuses comparable to the vacuum of interplanetary space. Scientists have traditionally categorized this pressure range into five broad categories: low, medium, high, ultra-high, and extreme ultra-high vacuum. Table 1 summarizes the pressure range in these categories. Although somewhat arbitrary, this classification has proven to be convenient for describing the various physical phenomena observed within each pressure range.

The use of the unit mbar above is consistent with recent vacuum literature; however, both torr and mbar are common units. The advantage of using mbar is that it can be easily converted into equivalent SI units, $1 \text{ mbar} = 1 \text{ hPa} = 10^{-2} \text{ Pa}$. Most modern AMO experiments operate in UHV. The primary reason for this is that the mean free path of particles λ is inversely proportional to the pressure.

$$\lambda = \frac{1}{\sqrt{2}d^2N/V} = \frac{k_B T}{\sqrt{2}d^2P}, \quad (5.23)$$

UHV allows unimpeded travel of the atomic beams for the experiments and low background gas collisions for trapped atoms and ions in the vacuum chamber. At atmospheric

⁹The constituent gases in a vacuum system are usually categorized into two types: getterable and non-getterable. The pumping action of a getter pump is through a chemical reaction that binds gas molecules to its surface and effectively removing them from the chamber volume. Gases that do not bind to the getter surface, like methane and argon, are referred to as non-getterable, and these are pumped by the ion pump.

Region	Pressure range
Low vacuum	Atmospheric pressure to 1 mbar
Medium vacuum	1 to 10^{-3} mbar
High vacuum (HV)	10^{-3} to 10^{-8} mbar
Ultrahigh vacuum (UHV)	10^{-8} to 10^{-12} mbar
Extreme high vacuum (XHV)	Less than 10^{-12} mbar

Table 5.3: Pressure ranges for vacuum categories
(1 atm = 1013.25 mbar)

pressure, the mean free path of a nitrogen molecule is $\mathcal{O}(100\text{nm})$, and at XHV pressure, it is greater than 5000 km.

In vacuum engineering, an important concept is gas flow. At low pressures, the ideal gas law,

$$PV = nk_{\text{B}}T, \quad (5.24)$$

applies well to describe the gas dynamics where P is the pressure, V is the volume of the container, k_{B} is the Boltzmann constant, T is the temperature and n is the number of gas molecules present inside the volume V .

Gas throughput Q_{PV} , which describes the number of gas molecules entering or leaving a system, is defined as

$$Q_{PV} = \frac{d(PV)}{dt}. \quad (5.25)$$

Usually, the PV subscript is omitted, and the symbol Q is used to describe the total gas throughput. The common units for specific outgassing are mbar l/s. In UHV, most of the gas originates inside the chamber from the chamber's surfaces and components. Different surfaces in a chamber 'outgas' differently, i.e. they emit gas at different rates and therefore their throughput/outgassing is denoted as a specific outgassing rate q which is the total outgassing rate of the surface per unit area

$$q = \frac{Q}{A}. \quad (5.26)$$

The flow of gas through an element of a system, for example a pipe or an orifice, is only possible when there is a pressure difference between the two sides of an element. To quantify the ability of a vacuum component to sustain/impede the flow of gas, the concept of conductance is used. Conductance, C is defined as the ratio of the throughput (gas flow) through the element and the pressure difference across it,

$$C = \frac{Q}{\Delta P}. \quad (5.27)$$

In UHV, the calculation of the flow properties does not need to account for inter-particle collisions and hence the conductance of an element is independent of the pressure difference across it. The conductance of an element is simply a function of the geometry of the element and is usually measured in units of liters per second (l/s). The conductances of multiple elements can be converted to a combined or effective conductance depending on how the elements are connected. Sequential connections or series connections lead to a higher impedance to gas flow than parallel connections, and the effective conductance of elements connected in series and parallel are

$$\begin{aligned} C_{\text{eff}} &= C_1 + C_2 + \dots + C_n \quad \text{for parallel connection,} \\ \frac{1}{C_{\text{eff}}} &= \frac{1}{C_1} + \frac{1}{C_2} + \dots + \frac{1}{C_n} \quad \text{for series connection.} \end{aligned} \quad (5.28)$$

The gas inside a vacuum system is evacuated by means of a vacuum pump, and the rate at which the gas is evacuated is denoted as the pumping speed (S), also measured in liters per sec (l/s). The pump is usually connected to the vacuum chamber through multiple pipes and fittings, which have conductance C_{eff} . The effective pumping speed (S_{eff}) available at the chamber can then be calculated as:

$$S_{\text{eff}} = \frac{C_{\text{eff}}}{1 + \frac{C_{\text{eff}}}{S}}.$$

To calculate the pressure in a chamber, with volume V , pumped at an effective pumping speed S_{eff} , we simply have to apply the principle of mass conservation and balance the amount of gas entering the chamber from the chamber walls and the amount of gas leaving the chamber due to pumping,

$$V \frac{dP}{dt} = Q - P \cdot S_{\text{eff}}.$$

If the initial pressure is P_0 , then the pressure as a function of time is given as

$$P = \frac{Q}{S_{\text{eff}}} + \left(P_0 - \frac{Q}{S_{\text{eff}}} \right) \exp \left(-\frac{S_{\text{eff}}}{V} t \right). \quad (5.29)$$

The ultimate pressure, then, is

$$P_{\text{ult}} = \frac{Q}{S_{\text{eff}}} = \frac{qA}{S_{\text{eff}}}, \quad (5.30)$$

where A is the surface area of the walls of the chamber. Note that the ultimate pressure of a chamber is maintained till the system is being pumped; this means that in UHV, the pumps are always functioning.

From Eq. (5.30), it should be clear that there are only two ways to reduce the ultimate pressure in a system: reducing the outgassing and increasing the effective pumping speed.

In general, the local pumping speeds for different gas species range from approximately 1 l s^{-1} to order of 1000 l s^{-1} , and the outgassing rates for different elements span at least eight orders of magnitude from $10^{-7} \text{ mbar l s}^{-1} \text{ cm}^{-2}$ to $10^{-15} \text{ mbar l s}^{-1} \text{ cm}^{-2}$. Therefore, simply increasing the pumping speed is not always the preferred solution for achieving low pressures; the reduction of outgassing rate of components is equally essential to vacuum performance.

5.6.2 Optimizing Vacuum system design using Monte Carlo simulations

Vacuum system design and electrical design have much in common. Eq. (5.30) is analogous to Ohm's law¹⁰, $U = IR$ with the substitutions $P \Rightarrow U$, $C \Rightarrow Y = 1/R$ and $Q \Rightarrow I$. There are elaborate formulae [180] available for calculating the conductances of vacuum elements of various geometries such as an orifice, a tube, etc. However, like electrical circuits, not all vacuum components have geometries that are determined by these formulae. There are more complications in vacuum circuits, for example, the outgassing comes from all walls of the chamber, and there is no localized current source. To obtain accurate predictions of system performance, it is therefore necessary to use more sophisticated means such as simulations.

Monte Carlo-based methods for simulating vacuum systems launch a large number of test particles in the system, and when a particle's trajectory encounters a surface, the

¹⁰I have used the symbol U for voltage to avoid confusion. In this chapter, V is reserved for volume. In this analogy, also the volume $V \Rightarrow C$ is analogous to the capacitance.

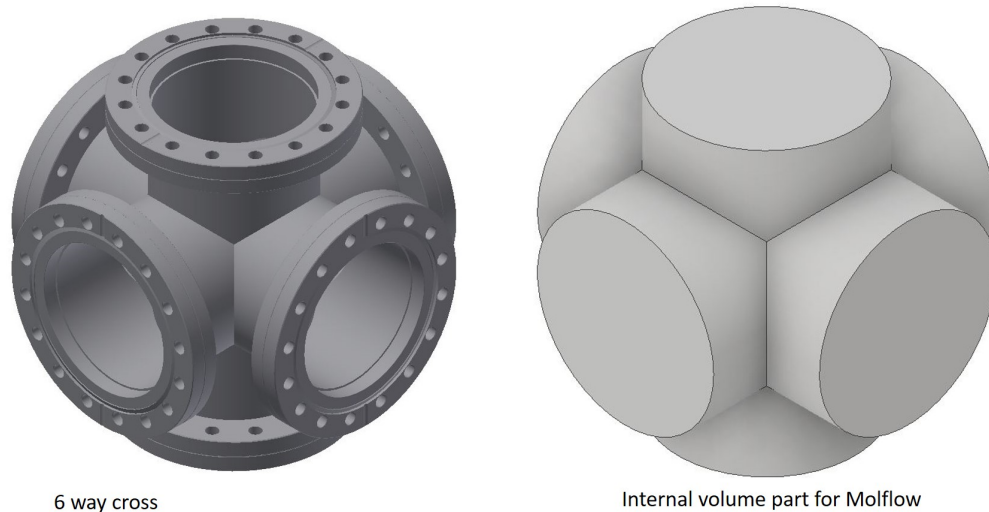


Figure 5.23: Geometry Definition for Vacuum Simulations

The beginning of any vacuum simulation requires the creation of the negative geometry i.e. the model that represents the vacuum system volume and not the walls.

particle is reflected based on known laws of reflection, which in this case is Knudsen's cosine law [181]. The particle is removed from the vacuum system once it encounters a pump, which is a surface with a sticking coefficient that determines its pumping speed. With a large number of particles simulated, the statistics of these particles show the quantities of interest in the vacuum system, such as pressure, conductance, effective pumping speeds, etc. MolFlow is a simulation software developed by CERN for analyzing molecular flow in ultra-high vacuum (UHV) systems. It is particularly useful for designing and optimizing complex vacuum systems due to its user-friendly graphical user interface, the ability to process and mesh large CAD models, and highly optimized particle tracing module that works on minimal hardware requirements.

The first step to simulate a vacuum model in MolFlow¹¹ is to generate a negative CAD model of the vacuum component. Fig. 5.23 shows this negative model for a six-way cross, a common vacuum fitting in UHV systems. Once the negative geometry is constructed, it is imported into the simulation software, and the outgassing and pumping surfaces are selected. Like any simulation, MolFlow simulations for vacuum system design are garbage-in-garbage-out, and it is the designer's responsibility that the surface outgassing rates they

¹¹This is true in general for any vacuum simulation software, for example, COMSOL now has a UHV module.

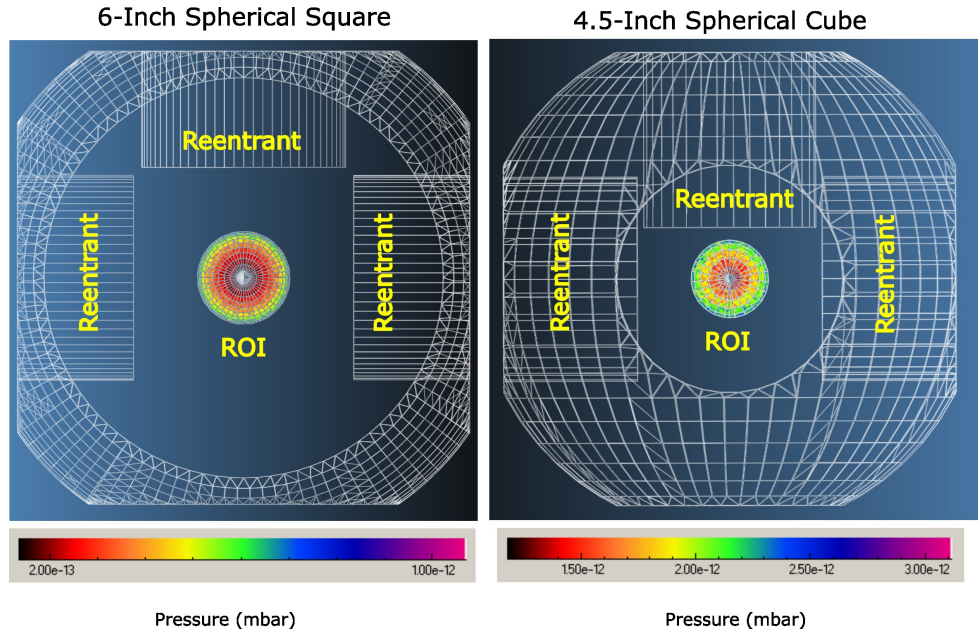


Figure 5.24: Ultimate Pressure in a Vacuum Chamber

Simulation of ultimate pressure in Kimball physics part number 53-140320 (spherical square) and 53-110400 (spherical cube) assuming sticking factor = 1 on the pumping flange. Average pressure in ROI 2.17×10^{-12} vs and 6.67×10^{-13} mbar respectively for a relatively high outgassing rate of 10^{-12} mbar $\text{l s}^{-1} \text{cm}^{-2}$, expected from non prebaked steel. The simulations show that even without the tedious and time consuming outgassing mitigation techniques, discussed in the following section, it is possible to achieve XHV.

select are representative of their systems. After this, the user simply needs to let the simulation run and extract the quantities of interest once the results have converged.

There are several strategies for optimizing vacuum system performance, but it generally prudent to divide the problem into three main steps: Chamber selection, pump and pump housing selection, and attachment selection.

Chamber Selection

Unless a fully custom vacuum chamber design is an option, the choice of the vacuum chamber is largely determined by the scientific requirements of the experiment. Usually, the requirements are satisfied by several commercially available options; however, from a vacuum point of view, all options are not alike. When optimizing designs using simulations,

it is good to know some analytical results that can serve as guidelines for optimal choices and avoid mindlessly simulating every available geometry. For example, the conductance of an orifice or a tube,

$$\begin{aligned} C_{\text{orifice}} &\propto D^2, \\ C_{\text{tube}} &\propto D^3/L, \end{aligned} \tag{5.31}$$

where D is the diameter of the orifice/tube. The Fig. shows the results of two chamber choices that could have satisfied the scientific requirements of the chamber in this work. One on the left has six 4.5-inch (CF63) flanges, and the other has four 4.5-inch (CF63) flanges and two 6-inch (CF100) flanges. The flange size for the reentrant windows in our chamber is 4.5 inches, and hence we could have used either, however, the first chamber allows for pumping through larger flange size. This drastically increases the available pumping speed at the region of interest (ROI). For comparing different geometries, it is useful to create a spherical measurement surface in the middle of the chamber where the average pressure can be recorded. Fig. 5.24 shows the results of simulations of the two chambers above available from Kimball physics, a six-inch spherical square and a 4.5-inch spherical cube¹². Assuming a high outgassing rate of 10^{-12} mbar l s⁻¹ cm⁻², the best achievable pressure in the above two chambers is 2.17×10^{-12} , 6.67×10^{-13} mbar respectively. Hence, we chose the chamber that allows pumping from a 6-inch port.

Pump and Housing Selection

The simulations for chamber selection make no assumptions about the type and pumping speed of the pumps used in the design. The only assumption is that the pumping speed available at the pumping flange is equal to the conductance of the flange, that is, a sticking factor of 1. The goal of the rest of the design is to maximize the pumping speed available at the pumping flange of the chamber.

The way pumps are placed in a vacuum system plays an important role in their effective pumping speed. The most prominent pumps in XHV designs are non-evaporable getter (NEG) pumps, and they are available at pumping speeds as high as 4000 l/s, which is achievable with a single pump. However, using a high pumping speed pump does not necessarily mean a high effective pumping speed. The effective pumping speed of a pump is determined by the pump's housing. For example, the NEG pumps used in this design

¹²I know, I know. The designers at Kimball have a peculiar naming convention.

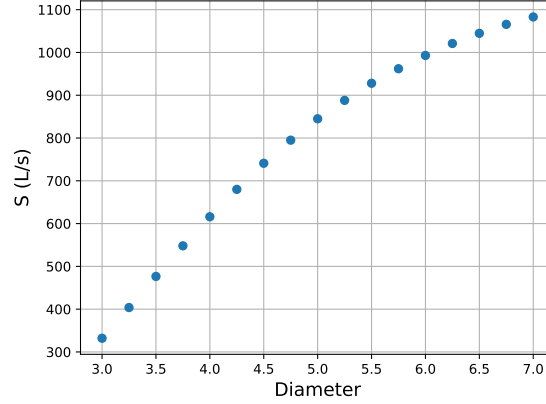


Figure 5.25: Effective Pumping speed of Z1000 vs Tube Diameter

The pumping speed available at the surface of the Z1000 NEG from SAES is 1250 l/s for hydrogen. The effective pumping speed is approximately 1000 l/s at 6-in, which is the internal diameter of the CF150 flange of our current design.

are the Z1000s from SAES getters, which provide a pumping speed of 1250l/s each for hydrogen. A Z1000 cartridge can be easily fitted into a tube of diameter, $D = 3$ in; however, this drastically reduces the effective pumping speed of the pump. Fig. 5.26 shows the results of simulations of a Z1000 NEG pump housed inside tubes of different diameters and just enough length, $L = 6$ in, to completely house the pump. It can be seen that even when the tube diameter is twice the minimum diameter in which the tube can be fit, the effective pumping speed is smaller than the pumping speed achievable at the pump surfaces. Similarly, the tube length in which the getter is placed should be no more than the minimum length necessary to house the getter. Fig. 5.26 shows the effect of using a longer tube on a SAES D1000 NEG pump.

Attachment Selection

The word attachment here refers to all components of the vacuum system that are used to connect the pumping flange of the chamber to the pump housing. From a vacuum point of view, the goal of the attachments is to allow for the maximum possible conductance between the pumping flange and the chamber. In our design, we had the option of using a cube or a six-way cross to connect the various pumps to the science chamber. Both alternatives work for the design; however, the cube offers much better conductance and,

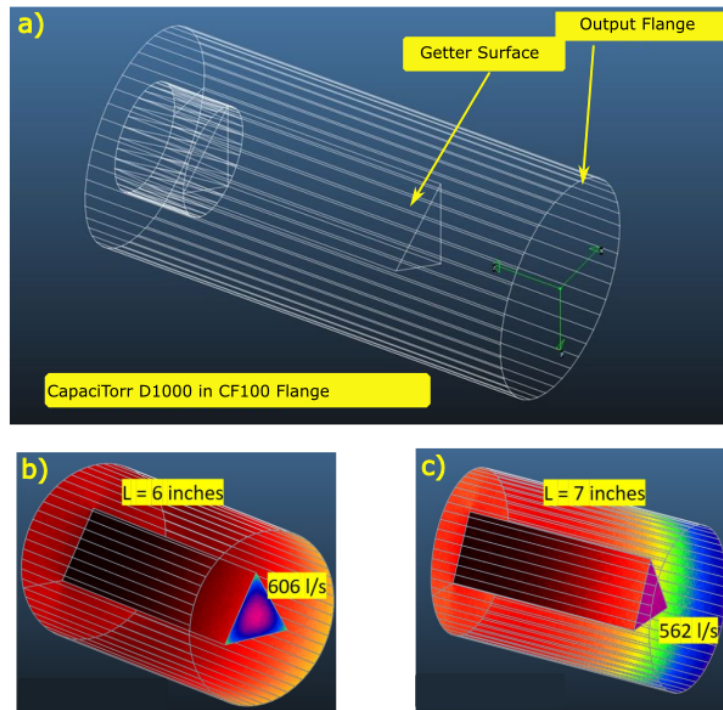


Figure 5.26: Caption

a) Simulation model of a NEG (D1000 from SAES) inside a tube of diameter 6 inches. The D1000 has a pumping speed of 1000 l/s for hydrogen. **b)** and **c)** the effective pumping speed drops by $\approx 8\%$ with just one inch increase in the tube length.

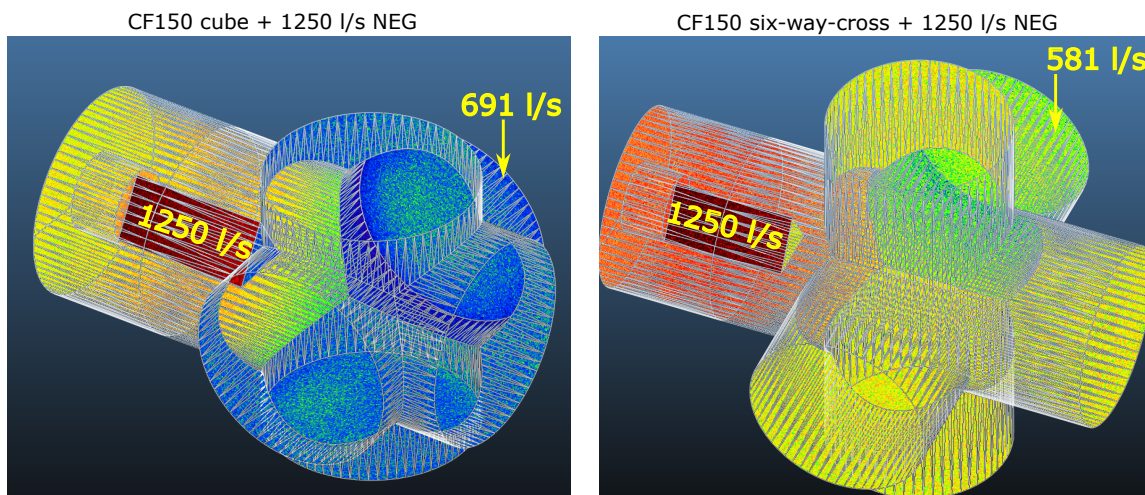


Figure 5.27: Vacuum Attachment Selection

Comparative study for selecting between different attachments available for connecting the science chamber and the pump.

hence, effective pumping speed at the chamber pumping flange. Fig. 5.27 shows the effective pumping speed available at one port of a cube and a six-way cross, respectively, when the NEG and the housing optimized in the previous step are used as the pump. An important point to note is that the attachments are also where the vacuum gauge is placed. A high conductance to the science chamber also ensures that the pressure read at the gauge location is indicative of the pressure in the region of interest.

Full System Simulation

With all the above optimizations completed, the entire system can be simulated with all the internal details to extract expected performance. These simulations are helpful for troubleshooting a constructed system, as the designer knows what pressure to expect during construction. Fig. 5.28 shows the CAD model used to perform the full simulations of the system and the expected pressure for the region of interest. The outgassing rate for the steel surfaces is set to 10^{-14} mbar l s⁻¹ cm⁻².

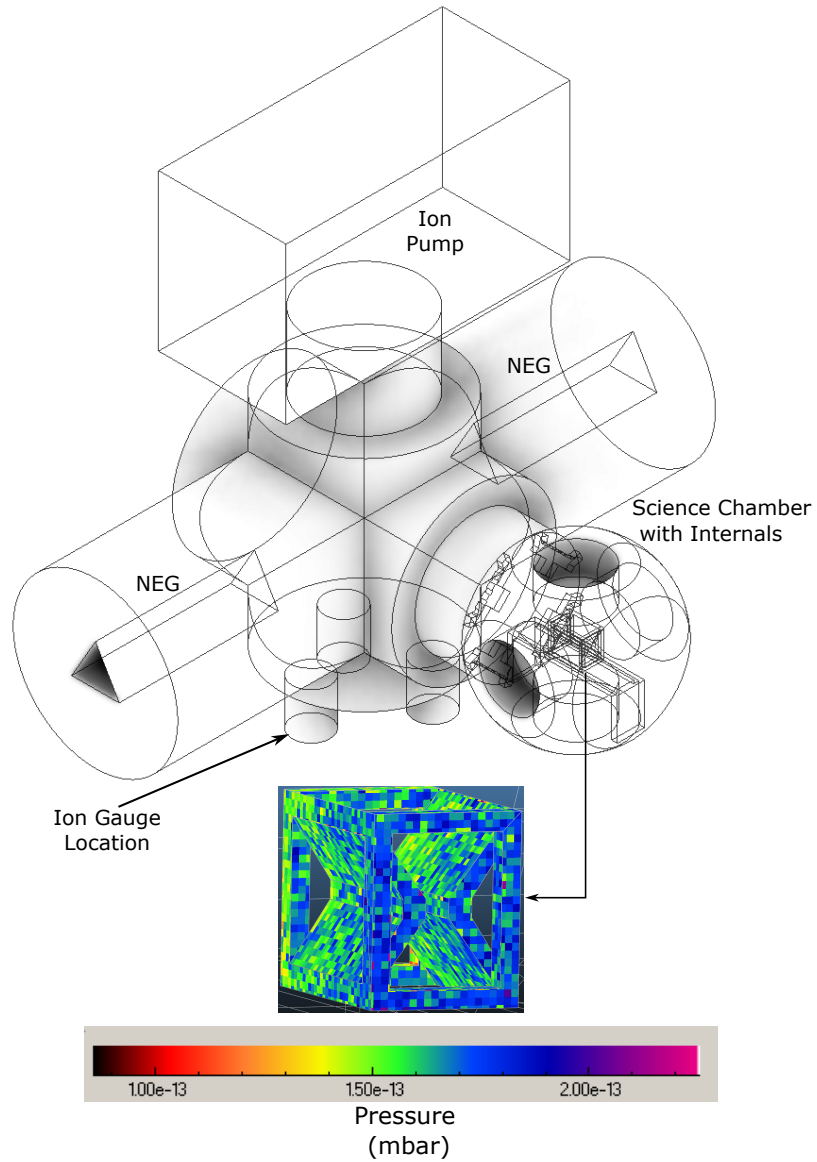


Figure 5.28: Full Vacuum System Simulation

Detailed negative CAD model of the vacuum system and pressure map for the region of interest (ROI). Simulation performed with stainless steel surfaces outgassing rate = 10^{-14} mbar $\text{l s}^{-1} \text{cm}^{-2}$. Extracted pressure at the gauge locations $\approx 5 \times 10^{-14}$ mbar.

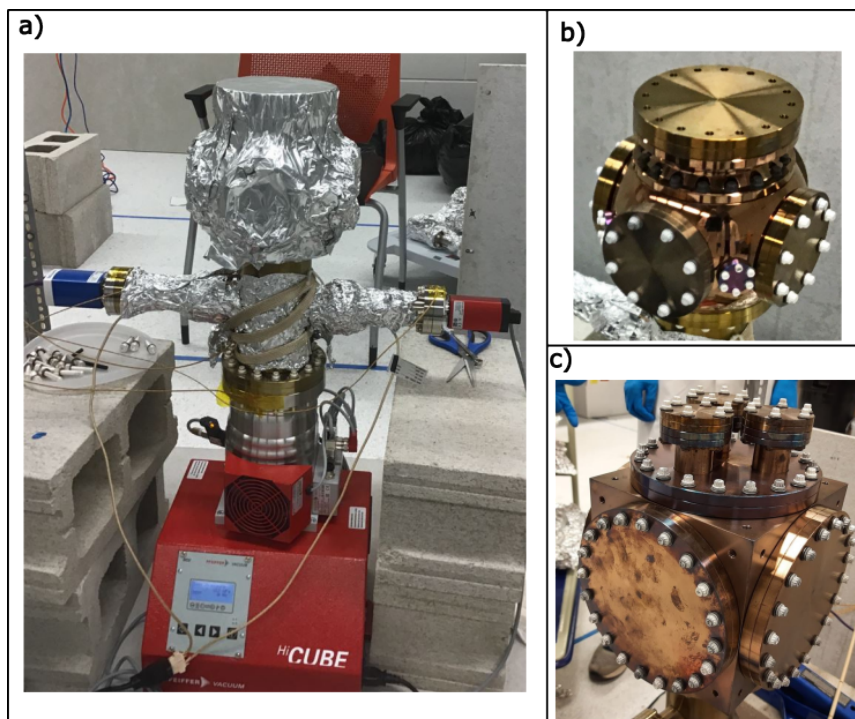


Figure 5.29: Prebake Setup for Stainless Steel

a) All components in the vacuum system were prebaked at 400°C and were mounted directly on the input flange of a turbo pumping station to achieve the highest effective pumping speed. **b)** Science chamber after the pre-bake was complete. **c)** Central cube after prebake was complete.

5.6.3 Outgassing Reduction

UHV and XHV systems have a pressure that is at least 13 orders of magnitude lower than atmospheric pressure. It is very rare in practice for any device to have such a wide span in its operating parameters, and such is the case for vacuum pumps. Pumping from atmospheric pressure to UHV is not achieved through a single pump. The pumps shown in the vacuum system in Fig. 5.22 are the internal pumps in the system; these pumps can only be activated when the pressure range is below 10^{-6} mbar. The pump that brings the vacuum system to the operating range of the internal pumps is usually a turbomolecular pumping station¹³ and the evacuation process involves baking the system, at temperatures between 150°C and 250°C while it is being pumped by the external pump. The pressures achieved after the evacuation phase is between 10^{-6} and 10^{-10} mbar depending on the duration of the bakeout and the effective pumping speed of the external pumps.

Almost all UHV systems are baked during evacuation, and the reason is to remove the adsorbed gas from the walls of the vacuum chamber. Assuming clean surfaces, the dominant gas species in an unbaked vacuum chamber is water vapor which is desorped from the vacuum chamber surfaces. The outgassing rate of an unbaked vacuum chamber with metallic walls is approximately [182, 183]

$$q_{H_2O} \approx \frac{3 \times 10^{-9}}{t_H}, \quad (5.32)$$

where t_H is the time in hours and q_{H_2O} is in units of mbar l s⁻¹ cm⁻².

The outgassing of baked stainless steel is in the range of 10^{-12} mbar l s⁻¹ cm⁻²; therefore, an unbaked chamber requires ≈ 40 days to achieve an outgassing rate of a baked chamber. Usually, every time a vacuum chamber is exposed to atmosphere, it is baked at least for a day, usually between 2 to 7 days. After the baking process has been completed and the vacuum chamber has cooled to room temperature, the outgassing from the walls of the vacuum chamber is now dominated by the inherent outgassing of the chamber walls and internal components and determines the ultimate pressure of the apparatus with the internal pumps activated.

For a clean, baked, and leak-free vacuum system, the main source of gas is the gas dissolved in the volume of the metal walls of the vacuum chamber. The dissolved gas diffuses to the surface of the chamber and is released into the vacuum environment. Usually in most metals used in UHV systems, the dissolved gas is usually hydrogen even though the

¹³Actually, just like the internal pumps, even the turbomolecular pump kicks in between 1 and 10^{-3} mbar and requires a backing pump usually referred to as a roughing pump.

solubility of hydrogen in solid metals is very low. Hydrogen is dissolved as single H atoms in molten metal during manufacturing and remains trapped in the bulk when the metal solidifies. In a UHV system, these single H atoms diffuse to the surface of the metal and, after recombination, are released as molecular hydrogen. For most metals used in UHV systems (copper, stainless steel, and aluminum alloys), the residual hydrogen content is between 0.1 and 10 ppm by weight [183].

The outgassing rate is therefore determined by two factors, the rate of diffusion of H atoms to the surface and the recombination rate at the surface. Depending on the concentration of hydrogen atoms in the bulk of the metal, the rate-limiting factor could be either of these two. For most UHV systems, the outgassing rate is above 10^{-14} mbar $\text{l s}^{-1} \text{ cm}^{-2}$, and in this regime, the rate-limiting factor is diffusion. For lower hydrogen concentrations (lower outgassing), recombination becomes the rate-limiting process [184].

Higher temperature leads to higher mobility of H atoms in metals, and the standard method for depletion of dissolved hydrogen from the bulk is heating the vacuum system at high temperature while maintaining the vacuum¹⁴. This process might seem very similar to the bakeout process described earlier, which reduces water outgassing due to surface desorption, but there is an important difference. Whenever the chamber is exposed to atmosphere, the water vapor is readsorbed on the surface; however, the recharging of the bulk of the metal with hydrogen does not happen. The reason is that the diffusion of molecular hydrogen from the atmosphere into the bulk of the steel is much more difficult than that of atomic hydrogen, and even for H atoms, the solubility in metals at room temperature is very low. The consequence of this is that the metals retain the effect of all of the temperature treatments that have been used to degas the bulk, even after exposure to the atmosphere, after the initial bakeout to remove the desorption effects has been completed.

Apart from metals, some ceramics and polymers are also used inside vacuum systems and these require degassing of the bulk, just like the metals. For most of the polymers used inside the chamber, for example, Kapton, the dissolved gas is water in molecular form [185, 186]. Because water vapor is a significant proportion of atmospheric gas, the degassing of polymers is not permanent, and subsequent exposure to the atmosphere and moist environments leads to re-absorption. Polymers, therefore, degas during the bakeout of the system.

To achieve UHV, most vacuum chambers undergo a temperature treatment under vac-

¹⁴For copper and aluminum alloys, a bakeout at 150-200 C for 24-48 hours is enough. For austenitic steel, much higher temperatures are required, and these are usually limited by the temperature rating of the vacuum flanges, which is 350-400 C

uum prior to the building of the apparatus, and this is standard practice, at least in the atomic molecular and optical physics community. There are several procedures for the heat treatment of stainless steel that are followed [187, 188] and involve heating the vacuum chamber to $\approx 400^\circ\text{C}$ in vacuum and/or in air. The outgassing rates achieved by these standard techniques result in $q_{H_2} \approx 10^{-12}$ to 10^{-13} mbar l s $^{-1}$ cm $^{-2}$. The surface area in a room temperature ion trapping setup is in the range of 100 and 1000 cm ^{2} , and the effective pumping speeds are between 10 and 100 l s $^{-1}$, leading to pressures in the range of $q \approx 10^{-10}$ to 10^{-11} mbar in room temperature systems. To achieve XHV, we need to push for $q_{H_2} \approx 10^{-14}$ to 10^{-15} mbar l s $^{-1}$ cm $^{-2}$ and to find a procedure that can achieve such low outgassing rates, we need to understand outgassing in a little more detail.

The diffusion-limited model of outgassing [189, 180, 190] allows us to estimate the outgassing rate of the diffused gas on the surface of a solid given some concentration of the dissolved gas in the bulk of the solid. The usual approach is to use Fick's laws of diffusion [191, 192] to estimate the diffusion flux, i.e. the amount of gas leaving the metal surface per unit area into the UHV environment. For the outgassing of hydrogen from a steel plate inside vacuum, the model predicts a specific outgassing rate,

$$\begin{aligned} q(t) &\approx \frac{4D_{H_2}(T)}{L} \times c_0 \sum_{n=0}^{\infty} \exp \left[-(2n+1)^2 \pi^2 \frac{D_{H_2}(T)t}{L^2} \right] \\ &= \frac{4D_{H_2}(T)}{L} \times c_0(t) \end{aligned} \quad (5.33)$$

where $q(t)$ is the specific outgassing as a function of time, L is the thickness of the sample, c_0 is the concentration of dissolved hydrogen in stainless steel in mbar l cm $^{-3}$ and

$$D_{H_2}(T) = 4.7 \times 10^{-3} e^{-\frac{0.56\text{eV}}{k_B T}}, \quad (5.34)$$

is the temperature-dependent diffusion coefficient of hydrogen in stainless steel [193] (see the Appendix 2 for details).

From Eq. 5.33, if we ignore the sum in the first line for a moment, the specific outgassing is proportional to the concentration of the dissolved hydrogen and the diffusion coefficient. Intuitively, this makes sense; larger dissolved hydrogen content should lead to higher outgassing, and similarly, if the diffusion to the surface is faster, we should get higher outgassing. The sum determines how fast the concentration of the dissolved gas, and hence the outgassing, decays with respect to time. The diffusion coefficient of hydrogen at room temperature $D \approx 1.59 \times 10^{-12}$ cm ^{2} s $^{-1}$ and at room temperature, the reduction

in the outgassing is practically negligible; especially for thick metal structures like our vacuum chamber. The reduction factor becomes useful when the temperature is increased, and therefore, steel pre-baking is done at high temperature $T \approx 400^\circ\text{C}$. We could use Eq. 5.33 to precisely calculate the reduction factor; however, to estimate the outgassing rate from the walls of the chamber and other vacuum components, we would still need to know their dissolved hydrogen concentration c_0 . This can be estimated, in principle, from an outgassing measurement after an overnight bakeout [183], and the estimated value could be used to calculate the time of the high-temperature pre-bake to achieve the desired $q_{H_2} \approx 10^{-14}$ to 10^{-15} mbar l s⁻¹ cm⁻².

However, we decided to follow a simpler approach to decide the time for pre-baking. We know that for a given concentration of hydrogen dissolved in steel, the temperature dependence comes only from the temperature dependence of diffusion. Hence, for a sample at different temperatures,

$$\frac{q_{\text{RT}}}{q_{\text{HT}}} = \frac{D(T_{\text{RT}})}{D(T_{\text{HT}})}. \quad (5.35)$$

For a $T_{\text{RT}} = 25^\circ\text{C}$ and $T_{\text{HT}} = 400^\circ\text{C}$ we have $q_{\text{RT}} \approx 5 \times 10^{-6} q_{\text{HT}}$. Assuming an effective pump speed S_{eff} during the pre-baking of a vacuum component at a temperature T_{HT} with a total surface area A of the component q_{HT} is straightforward to calculate from Eq. (5.30) and from this we can estimate the value of q_{RT} as follows

$$q_{\text{RT}} = \frac{P_{\text{HT}}(t) S_{\text{eff}}}{A} \times \frac{D(T_{\text{RT}})}{D(T_{\text{HT}})}. \quad (5.36)$$

Eq. (5.36) now gives the means to decide how long the pre-baking of a component needs to be performed. For the thick-walled vacuum components, that is, the science chamber and the central cube, we decided to bake the trays until $P_{\text{HT}}(t) < 5 \times 10^{-8}$ mbar. At the end of the prebake, we also performed an air bake by turning off the pumping station and letting atmospheric air backfill into the prebake apparatus still at high temperature. Such air bakes have been shown to lead to approximately two times reduction in the specific outgassing due to the formation of an oxide layer on the surface of stainless steel acting as a diffusion barrier for hydrogen on the surface [194, 188].

Fig. 5.29 shows the setup used to pre-bake the stainless steel components. For the science chamber and the central cube, we pre-baked for approximately 30 days each and stopped the bakeout at 1.1×10^{-8} and 4.8×10^{-8} mbar, respectively. From Eq. (5.36), the

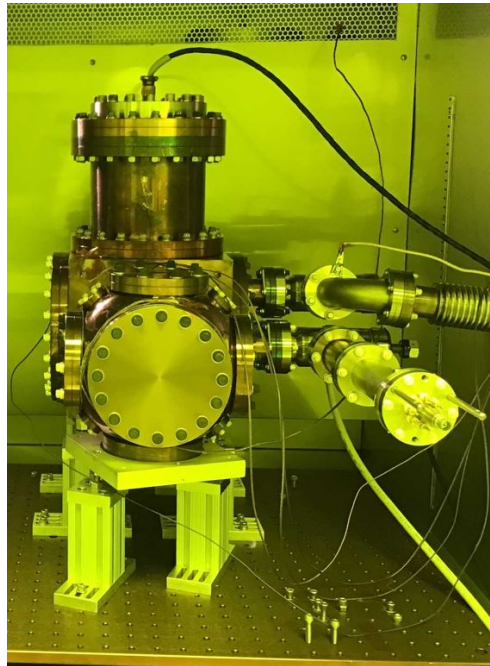


Figure 5.30: Base Pressure Test Setup

Base pressure measurement of empty vacuum chamber constructed from prebaked components. The pressure of the empty test chamber was consistently measured to be $P \ll 1 \times 10^{-11}$ mbar.



Figure 5.31: High-Temperature Prebake of Shapal Ion Trap Mount

Shapal trap mount inside a high-temperature oven (OTF-1200X by MTI Corp). Pre-bake was performed for 14 days at 900°C.

respective surface areas of the components in the pre-bake, and including the factor of two from the oxide layer formation [194, 188] we estimate

$$\begin{aligned} q_{\text{chamber}} &< 4.58 \times 10^{-15} \text{ mbar l s}^{-1} \text{ cm}^{-2} \\ q_{\text{cube}} &< 8.34 \times 10^{-15} \text{ mbar l s}^{-1} \text{ cm}^{-2} \end{aligned} \tag{5.37}$$

The above values seem very low; however, they are consistent with the measured outgassing rates using a similar technique [195] where outgassing rates of $q < 2 \times 10^{-15}$ mbar l s⁻¹ cm⁻² were achieved.

Once the components were prebaked, we checked the base pressure of the empty chamber constructed from these components with only a single getter pump (SAES Z1000) and a turbo pump to pump non-getterable load and consistently obtained $P \ll 1 \times 10^{-11}$ mbar within 6 hours of a three-day bakeout and subsequent cooldown. This chamber was later also used to test the outgassing of several components that would be part of the assembled chamber. In particular, the shapal holder that is used to hold the trap electrodes was a significant source of outgassing. We tested the base pressure of the above chamber with a test shapal piece of dimensions comparable to the shapal holder and found that even after a 400°C bake for several days, the base pressure of the above test chamber with the shapal

piece inside was higher than 3×10^{-10} mbar. Unlike hydrogen in stainless steel, there have been few studies done on the outgassing behavior of the shapal and hence could not come up with a concrete strategy for prebaking the shapal trap holder. However, outgassing in ceramics also comes from diffusion once the initial adsorbed gas is removed [196]; hence, the general idea that higher temperatures during pre-baking should lower outgassing applies. We decided to pre-bake the trap shapal holder at 900°C because this was the highest temperature we could obtain in any apparatus available to us. Fig. 5.31 shows the shapal holder inside a high-temperature oven (OTF-1200X by MTI Corp.). The shapal holder was baked for 14 days at 900°C, and the pre-bake was performed by Lewis Hahn and the details of the setup can be found in his master’s thesis [197]. After this high-temperature prebake, the base pressure test was repeated again and we were able to achieve the same low base pressures achieved earlier. Note that the bake time is highly dependent on the thickness of the sample and the initial concentration of the dissolved gas. No attempt was made to find an optimal prebake time or temperature since this would be outside the scope of the current project.

5.6.4 XHV Insights

Bakout procedure

The bakeout procedure followed after the construction of the set-up is quite similar to the procedures followed in most labs; however, we perform activation of the getters in the system twice. One activation is performed before the start of the bake during the upward ramp of pressure, and another activation is performed towards the downward ramp. The following is the sequence of operations that we followed after the system was ready to bake and placed inside the oven and connected to a turbo pump. The wires connecting the ion pump, pressure gauge, and NEG were high-temperature wires and, hence, were left connected during the entire duration of the bakeout.

1. Turn ON Turbo
2. After turbo side reaches 10^{-5} mbar turn ON the pressure gauge (UHV24p)
3. Wait for pressure in the chamber to reach 10^{-6} mbar
4. Degass both filaments of the ion gauge and wait for pressure to stabilize
5. Ramp temperature of the system to 110°C at a rate of 20°C/hour

6. Activate both NEG pumps simultaneously as per manufacturer recommendations (550°C for one hour)
7. Wait for getter temperature to stabilize to $\approx 110^\circ\text{C}$
8. Ramp temperature of the system to 180°C at a rate of $20^\circ\text{C}/\text{hour}$ (temperature limited by reentrant window specifications)
9. Leave system at 180°C for ≈ 7 days
10. Ramp temperature of the system to 110°C at a rate of $20^\circ\text{C}/\text{hour}$
11. Activate both NEG pumps simultaneously as per manufacturer recommendations (550°C for one hour)
12. Wait for getter temperature to stabilize to $\approx 110^\circ\text{C}$
13. Turn ON ion pump
14. Ramp temperature of the system to 25°C at a rate of $20^\circ\text{C}/\text{hour}$
15. Close valve to turbo once pressure has settled

Titanium Sublimation Pumps

Fig. 5.32 shows a previous version of our system in which we were unable to achieve XHV. The difference between the current design and the older version is the presence of a larger ion pump. Also, instead of two NEG, we had one NEG and a titanium sublimation pump. The lowest pressure recorded in that system was $3 \times 10^{-11}\text{mbar}$ after firing the titanium sublimation filament. The gauge used to record the pressures was the extractor gauge, IMR 430 from Pfeiffer Vacuum, with x-ray limit $< 10^{-12}\text{mbar}$. The extractor gauge was borrowed from another experiment, which was not used at that time. The constant observation with the system was that the pressure after a bakeout and NEG activation was lower than the pressure after firing (activating) the titanium sublimation pump (and, in principle, doubling the pumping speed). Additionally, we noticed that a bakeout of the system after firing the titanium sublimation pump resulted in lower pressures. After detailed analysis, we found that the reason for achieving the higher pressure was additional non getterable outgassing from the titanium sublimation pump.

This is also recorded in the literature, where methane outgassing from a titanium sublimation pump required a bakeout every time the pump was fired [198]. When a titanium

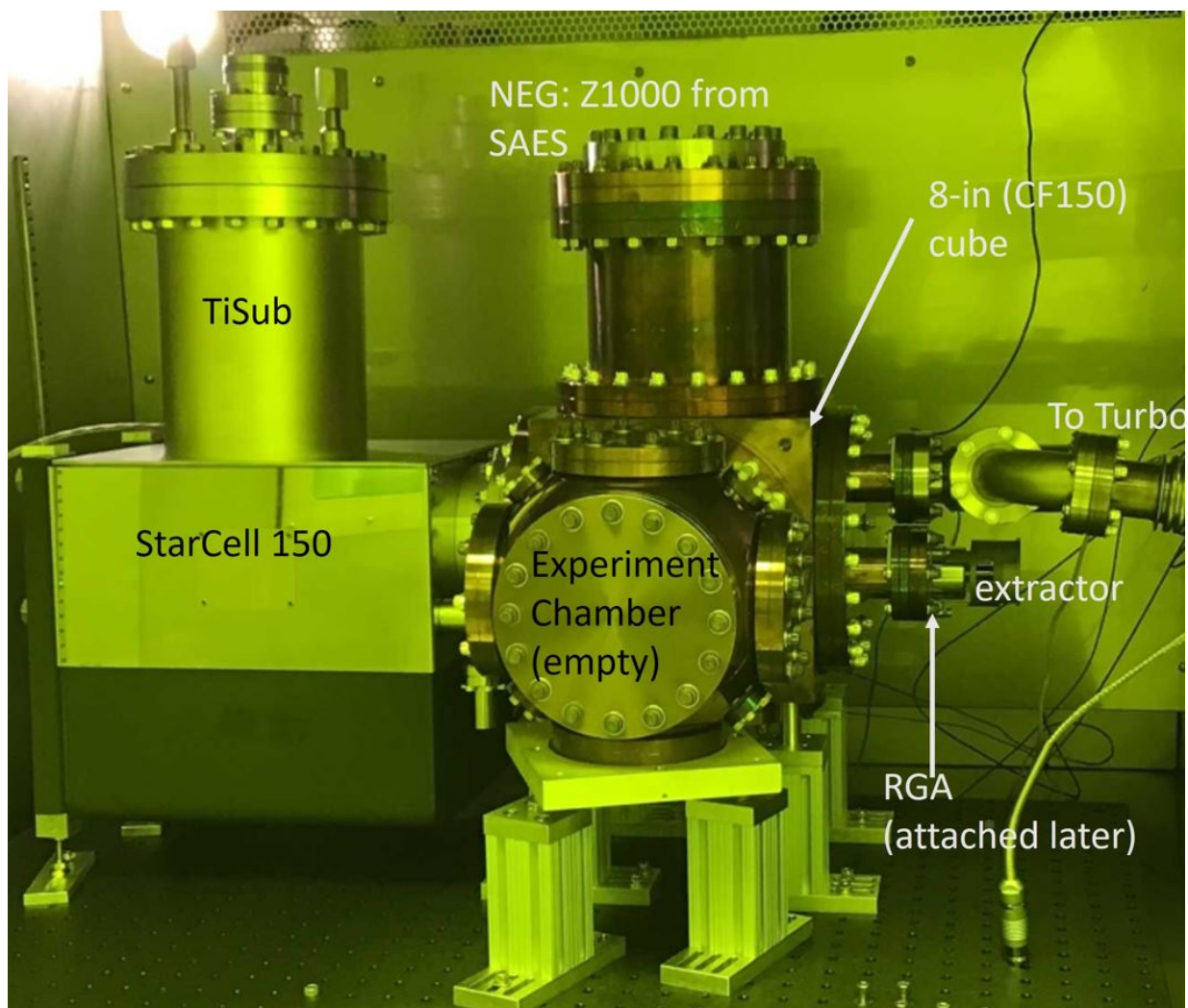


Figure 5.32: Failed XHV attempt

A previous version of our current design included an ion-TiSub combination pump from Agilent. The above picture is from a base pressure test for the system with an empty science chamber. The lowest pressure recorded in that system was 3×10^{-11} mbar after firing the titanium sublimation filament. The problem was diagnosed as non-getterable outgassing from firing the titanium sublimation pump. See text for more details.

sublimation pump is activated by running high currents through a titanium filament, the result is not only titanium sublimation but also the outflow of impurities in the bulk of the titanium filament. These impurities, especially carbon, react with the background hydrogen to produce methane, and since methane is not getterable, a drastic effect on the background pressure is seen. Although titanium sublimation technology is indeed XHV compatible, ensuring cleanliness of the titanium filaments is almost out of the hands of the end user. This is the main reason, in my opinion, that titanium sublimation pumps should be avoided in XHV systems.

Backup power for Turbo

While a system is in operation with the valve to the turbo pump open, a power failure could shut the turbo pump down. This is especially dangerous if the NEG's are in the middle of activation and are at high temperatures because any influx of atmospheric gas could render the NEG's useless. Additionally, if the ion pump or the ion gauges are not affected by the power failure, both devices could be damaged by exposure to atmospheric gas.

Is RGA useful?

In principle, residual gas analyzers (RGA) are useful especially to know the gas composition of a vacuum system and also to perform leak checks. However, in our experience, we could never extract useful information from an RGA (we used SRS RGA200 with the EM gain option). This was in part because switching the RGA filament on would always increase the system pressure by approximately three orders of magnitude from the base pressure, and there were several peaks in the RGA spectrum, especially hydrocarbons that were believed to be from the RGA itself, even though we never used the RGA in any other system. The main utility of the RGA was leak testing because the RGA can detect helium partial pressures of $\approx 10^{-13}$ mbar, but we found that if a proper tightening protocol is followed, CF flanges rarely lead to leaks.

During our final bake, we had a leak in one of our atomic oven feedthroughs, which limited the base pressure to 5×10^{-11} mbar, and there was no RGA in the system. We could point out the leak simply by spraying helium at different places around the chamber and looking for a pressure rise on the gauge and the ion pump. With helium sprayed directly on the feedthrough, we saw a pressure rise of up to 2×10^{-10} mbar within a few seconds of spraying. RGAs do allow for a much lower leak threshold in detecting leaks; however, other than that, we did not find much use for an RGA in our setup.

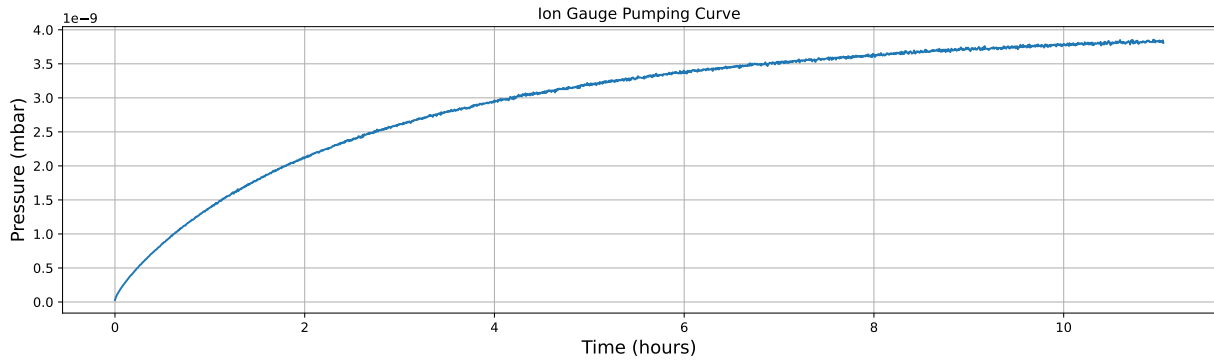


Figure 5.33: Pressure rise in vacuum system after turning off ion pump

UHV gauges have pumping effect which does not allow indefinite rise in pressure even with ion pump turned off (and zero pumping speed for non getterable load).

Change bolts after multiple heating cycles

In this work, we had to perform several vacuum tests and found that the leak tightness of the CF flanges was suspect after multiple bake-out cycles. This is common knowledge for people who have to bake their chambers often, especially scanning tunneling microscope operators, but for us AMO physicists, this is important information to know. In case some bolts of the chamber are loosened due to temperature cycling, it is also easy to check this since many times these bolts are loose enough to be loosened by hand. The best option is to replace the bolts and gaskets and re-tighten. If multiple tests are planned on a vacuum apparatus, annealed copper gaskets should be used.

UHV/XHV gauges

Most UHV and XHV system have a hot cathode pressure gauge also called a Bayert Alpert (BA) gauge. The pressure in a BA gauge is calculated by ionizing gas molecules in a small volume and measuring a collector current, I_c , proportional to the number of gas molecules that have been ionized. The ionization of gas molecules in the gauge is achieved by passing a current I_e through a filament, called an emitter, and heating it. The electrons ejected from the emitter's surface strike the gas molecules and ionize them. The collector current in a BA gauge depends on the pressure and the emission current,

$$I_c = SPI_e, \quad (5.38)$$

where S is the gas-dependent sensitivity factor, P is the background pressure. The BA gauge controller measures I_e , and the pressure is extracted from Eq. (5.38). In UHV and XHV systems, the dominant gas is hydrogen emanating from the walls of the chamber, and hence the sensitivity factor for hydrogen should be used. This is usually straightforward to find in the controller manual.

The ultimate pressure that can be read by the gauge is determined by two factors, the lowest current readout from the controller and the x-ray limit of the gauge. The electrons that are emitted from the emitter also impinge on the metal grid around the collector and lead to emission of x-rays, which are then intercepted by the collector. The x-rays striking the collector cause electrons to be photoelectrically ejected from the collector, leading to a photoelectron current from the ion collector. This photoelectron current is detected in the same way as positive ions arriving at the ion collector and consequently adds to the collector current. The x-ray limit depends on a lot of factors, including the gauge design, and UHV24p was chosen specifically due to its low x-ray limit with a manufacturer-specified value of $P < 6.66 \times 10^{-12}$ mbar. We found that the gauge x-ray limit is even lower in practice $\approx 1.5 \times 10^{-12}$ mbar since the pressure recorded after completion of the final bakeout of the system was $\approx 1.5 \times 10^{-12}$ mbar and this value was constant for approximately two weeks.

At $P < 10^{-11}$ mbar, the collector current $I_e < 1$ pA. Modern gauge controllers are designed to read such low currents; however, this assumes that the operator has taken the necessary measures to allow such low measurements. For example, at low pressures, it is best to set I_e to the maximum value allowed by the controller/gauge. This is also recommended by manufacturers. For UHV24p the typical operating value is $I_e = 4$ mA, but for pressure below 10^{-10} mbar, $I_e = 10$ mA is recommended. Similarly, electrical noise plays an important role in low-pressure measurements, and the bare minimum is to follow the manufacturer's recommended grounding practices. Care should be taken to avoid ground loops as much as possible. We found that a change of airflow around the gauge wires leads to charge build-up and an improper pressure readout, especially when the chamber is inside a convection oven.

Even with limitations imposed by the X-ray limit and electronic noise during measurement, BA gauges can be used to extract much more information about the system than just the pressure. The BA gauges also have a pumping effect while in operation, and this pumping speed depends on the value of the emission current I_e . This pumping effect can be used to extract the non-getterable load in a UHV/XHV system. Usually, the non-getterable load in a UHV/XHV system is pumped by the ion pump. With the ion pump switched off, the pressure would keep rising indefinitely due to the non-getterable load that does not get pumped by the getter; however, this does not happen. Fig. 5.33 shows the pressure in our vacuum chamber after the ion pump was turned off. Similarly

to the derivation of Eq. (5.30), it is easy to show that the pressure in the chamber should increase according to

$$P(t) = P_{\text{base}} + \frac{Q_{NG}}{S_g} \left(1 - \exp\left(-\frac{S_g}{V}t\right) \right), \quad (5.39)$$

Where P_{base} is the base pressure of the system, Q_{NG} is the non-getterable load in the system, S_g is the gauge pumping speed, and V is the volume. Fitting the data in Fig. 5.33 to Eq. (5.39) we found that $Q_{NG} = 6.15 \times 10^{-12}$ mbar l s⁻¹ cm⁻² and $S_g = 1.6 \times 10^{-3}$ l/s for $I_e = 4$ mA. The pumping speed of our ion pump for non-getterable gases is ≈ 10 l/s, and based on this, we expect the partial pressure due to non-getterable load in the chamber to be $P_{NG} < 1 \times 10^{-12}$ mbar. The partial pressure due to the getterable load is expected to be lower, and hence, we expect the limiting partial pressure to be likely from the non-getterable load. This technique is especially useful while performing vacuum tests and for knowing the non-getterable gas load of a component once the gas load from the empty chamber has been characterized.

Polymers in XHV?

Polymers are known to have much higher outgassing compared to metals [186, 185], and the general advice is to avoid using these. However, most ion trapping sets use polymers such as kapton mainly in the form of insulation on the electrical wires. Because the thickness of the polymers is very small, they are degassed very quickly and contribute minimally to the outgassing. Estimate $Q_{NG} = 6.15 \times 10^{-12}$ mbar l s⁻¹ cm⁻² was made in the fully constructed chamber after the final bakeout.

What is the right cleaning protocol?

When our previous system failed to achieve XHV, we investigated several aspects of the system, one of which was the cleaning protocol. Out of the several publications I found on the achievement of XHV, the most recent ones were from the Thomas Jefferson Accelerator Facility, and I reached out to Dr. Marcy Stutzman at the vacuum division. The usual cleaning protocol followed in several labs is thorough sonication in deionized water and detergent, followed by sonication in solvents such as acetone and isopropyl alcohol. The difference in the XHV cleaning protocol at Jefferson lab was that solvent cleaning was followed by a 400°C bake for several days. For cleaning out stainless steel vacuum parts, we baked them under vacuum for two days at 400°C. This does not include the reentrant windows because they can be baked at a maximum temperature of 180°C.

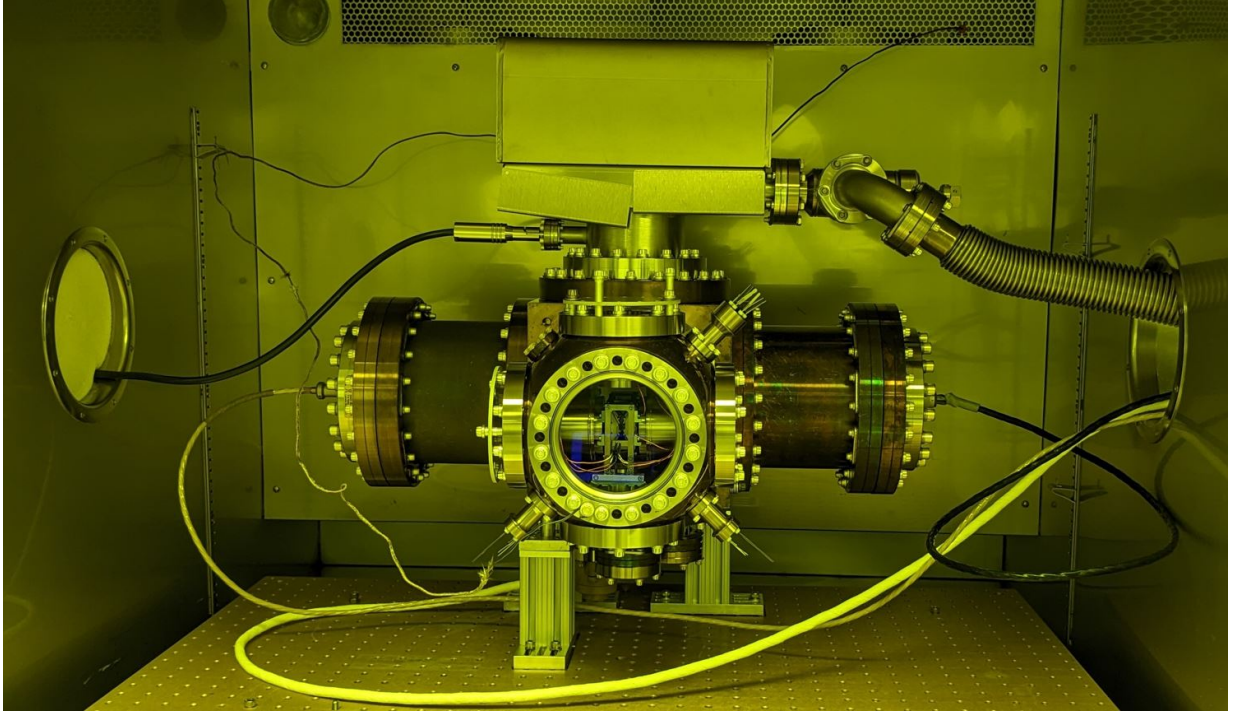


Figure 5.34: Blade Trap Chamber Current Status

Fully assembled blade trap vacuum setup inside TestEquity TE-1027C temperature chamber at the Quantum Nanofabrication and Characterization Facility (QNFCF) at the University of Waterloo. The complete assembly of the chamber was done inside the clean assembly area inside the QNFCF, and at the time of writing, we had just finished transporting the system to our lab.

5.6.5 Current Status

Fig. 5.34 shows the picture of the assembled system inside the high-temperature oven that was used for the final bakeout. The pressure in the chamber as measured by the UHV24p gauge is $P < 1.5 \times 10^{-12}$ mbar, and based on the procedure in Section 5.6.4, we estimate $P < 1 \times 10^{-12}$ mbar. This is the hydrogen equivalent pressure, and the nitrogen equivalent pressure, usually the value quoted in the literature, is approximately half. The final pressure at the ion location would have to be measured from the collision rates observed with the trapped ions.

The gauge pressure was measured to be $\approx 1.5 \times 10^{-12}$ mbar for roughly two weeks before we moved the chamber from the clean assembly space in the Quantum Nano Fabrication

and Characterization Facility at the University of Waterloo to our lab. During the transportation process, we had to turn off the ion pump and the BA gauge. After transporting the chamber to our lab and turning on the ion pump and the BA gauge, the pressure recorded on the BA gauge was $\approx 1.1 \times 10^{-11}$ mbar. At first, we thought this was because of a leak. A leak would certainly lead to an increase of the non-getterable load¹⁵ in the system, and hence we measured the non-getterable load in the system, by turning off our ion pump, using the procedure described in Section 5.6.4. A similar measurement was also performed on the system prior to transporting the chamber from the clean assembly space to the lab. Fig. 5.35 a) shows the pressure reading on the gauge during the measurement of the non-getterable load in the system. The two curves can be seen to match almost exactly, indicating that the non-getterable load had not changed. However, the pressure vs. time curves after ion pump switching were noticeably different as seen in Fig. 5.35 b). This suggests that the ion pump is somehow not ramping to its full pumping speed after the system has been moved to our lab.

After contacting the manufacturer, we learned that this behavior is not unexpected when ion pumps are turned on at extremely low pressures. Possible solutions to mitigate this problem are to use a higher voltage while turning the ion pump on or to perform a short bake of the pump. We are currently troubleshooting this issue. However, since we have verified that there is no leak in the system by measuring the total non-getterable load, we are confident that it is only a matter of time before we resolve this issue.

¹⁵Atmospheric gas has helium, argon, and methane the common non getterable gases and in presence of a leak the non-getterable load increases drastically

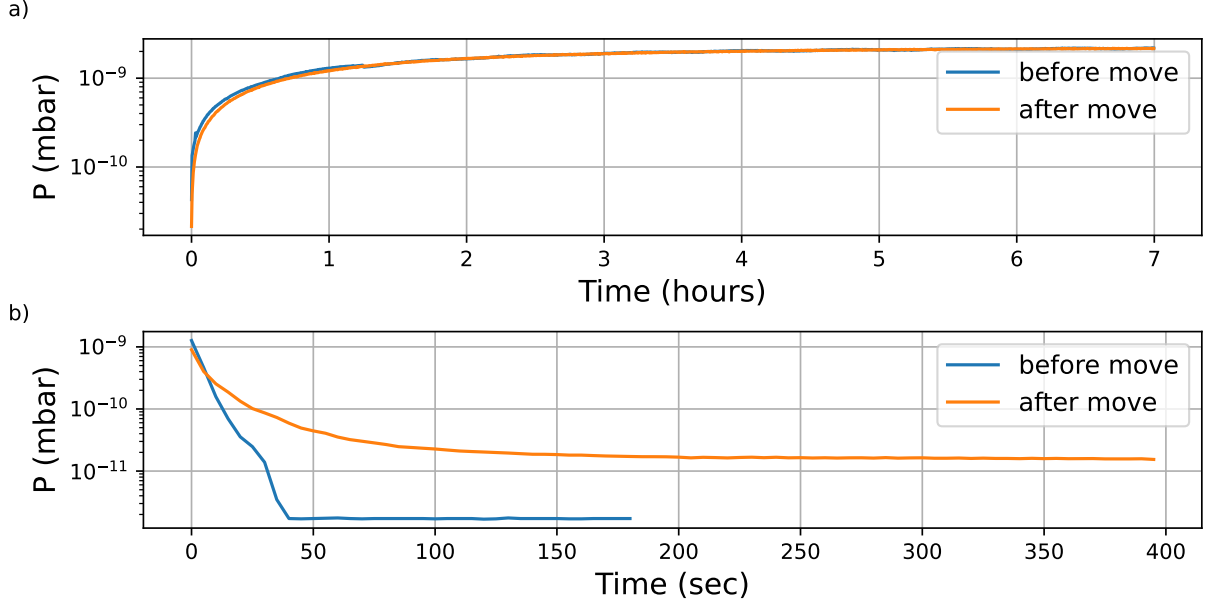


Figure 5.35: Non getterable load measurement before and after transportation

a) Pressure rise after turning off the ion pump gives an estimate of the non-getterable load in the system. Fitting the data to Eq. (5.39) we extracted $Q_{NG} = (6.824 \pm 0.029) \times 10^{-12} \text{mbar l s}^{-1}$ and $Q_{NG} = (6.913 \pm 0.018) \times 10^{-12} \text{mbar l s}^{-1}$ before and after transportation respectively. Similarly we found $S_g = 3.172 \pm 0.013 \times 10^{-3} \text{l s}^{-1}$ and $S_g = 3.222 \pm 0.008 \times 10^{-3} \text{l s}^{-1}$ before and after transportation respectively. In both cases, the pressure from the expected pumping speed of the ion pump is $< 1 \times 10^{-12} \text{ mbar}$.

b) The pressure drop after switching on the ion pump after acquiring the curves in a). The difference in the two curves shows clearly that the ion pump is not reaching its full pumping speed after transportation.

5.7 Conclusion and Outlook

The entire building process, including the vacuum chamber, the trap electrodes, and the assembly, took approximately three years. The large amount of time spent on this apparatus was due to the fact that we optimized every single aspect of the design in great detail. We also lost a little over a year trying to troubleshoot a failed XHV system, described earlier, and the restrictions imposed due to the COVID-19 pandemic. This chapter documents the design and construction of the blade trap apparatus.

The design and fabrication of the trap electrodes have been documented and allow for easy replication, which is especially useful for new experimental groups. The fabrication of electrodes in-house allowed us to achieve better surface quality compared to commercially available alternatives and also led to a large cost savings with the total cost of fabrication below 4000 USD (including the equipment usage cost at QNFCF). The vacuum system design has been thoroughly optimized using Monte Carlo techniques using the open source vacuum simulation software MolFlow. A three-step approach for optimizing vacuum system design is discussed using simulation software, and the application to the current design has been documented. The outgassing reduction techniques that lead to XHV have also been explained and documented. The final pressure in the system, as recorded on the Agilent UHV24p gauge, is $P < 1.5 \times 10^{-12}$ mbar. To the best of my knowledge, this is likely the lowest pressure achieved on a room-temperature ion-trapping apparatus.

As the number of ions in the quantum simulator grows, the vacuum requirements will become even more stringent. Cryogenic pumping systems offer very low pressures; however, they come with the added disadvantage of the size cost and the vibrations associated with closed cycle cryostats. In fact, at a recent conference (DAMOP 2024), engineers from a major trapped-ion quantum computing company were sharing plans about building a room-temperature vacuum system for their newer generation quantum computer due to noise induced by the closed-cycle cryostat. The current design is at the limit of achievable pressures in room-temperature vacuum systems made from standard components. However, with custom components, much lower pressures can be achieved. An important change to achieve lower pressures would be to use vacuum vessels with thin walls. Eq. (5.33) describes the effect of a high-temperature bakeout on the outgassing rate of the material under vacuum. For example, with the 400°C bake temperature used to degas stainless steel components, a 24-hour bakeout achieves $> 99\%$ reduction in outgassing for a stainless steel plate of thickness 2 mm, while outgassing for a 20 mm thick plate (representative of the thickness of our chamber walls) only reduces by $< 7\%$. Thin walls are easier to degas faster and achieve lower outgassing rates. Another approach to reduce outgassing would be to use NEG coatings on the walls of the vacuum chamber [199]. If these

types of coating are adopted, a thorough testing is required to ensure that the coatings do not flake from the chamber walls and deposit on the trap in the worst case. In any case, vacuum design would have to be carefully investigated when scaling the system to a larger number of ions.

An important bottleneck in assembling the current system was the alignment of the blade electrodes on the shapal electrode holder mount. Shapal is a ceramic, and usually the tolerances in the machining of ceramics are worse than the ones for machining metallic parts. Even with the optimized alignment procedure, which involved carefully selected spacers (blade plates), only one out of the three shapal holders we had recieved were suitable for use. A newer design could use a metallic holder, as the blade plates allow insulation of the blades from each other even on a metallic holder.

Chapter 6

Summary and Outlook

The work described in this thesis broadly serves towards building useful quantum technologies both for quantum simulations and quantum sensing. I have had to wear several hats during my PhD journey, the experimental physicist hat, the engineer hat, the theoretical physicist hat, and sometimes the just-do-it hat. Using the right hat for a given problem has probably been the biggest lesson I have learned from this journey. Being a first-generation graduate student and setting up the lab from scratch along with my colleagues naturally put me in an extremely advantageous situation, because I got to build the apparatus while also deeply thinking about the theory. This manifests itself in the type of results described in this thesis, both theoretical and experimental.

The results in Chapter 3 and the publication [102] describe how to simulate a new class of Hamiltonians on trapped ions. We have demonstrated for the first time, both theoretically and experimentally, how XY-type couplings

$$H_{\text{eff}} = \sum_{i < j} J_{ij}^x \sigma_x^i \sigma_x^j + \sum_{i < j} J_{ij}^y \sigma_y^i \sigma_y^j, \quad (6.1)$$

with individual control over J_{ij}^x and J_{ij}^y , are a part of the native interactions available on a system of trapped ions. The experimental demonstration was performed on two $^{171}\text{Yb}^+$ ions on our small-scale test bed quantum simulator the four-rod trap (described briefly in Chapter 2 and in detail in [88, 98, 101]). The main insight of this work is that spin-dependent forces, which have been the backbone of entangling operations on trapped ions [63], can also be applied in parallel on the same motional modes of trapped ions and the theory presented discusses when this is possible. The technique is also highly scalable with

straightforward generalization to a large number of ions in geometries other than a linear chain.

The proof-of-principle demonstration of XY-type couplings shown here could be extended to experiments with a larger number of ions, and in principle programmable lattice geometries [128, 127], to explore the ground-state order of frustrated XY-type models and to explore exotic quantum phases such as spin liquids [132]. An obvious next step in extending the theory would be to account for the corrections to the coupling matrices J_{ij}^x and J_{ij}^y that arise from the off-resonant terms in the spin-dependent force Hamiltonian. Similarly, a σ_z -spin-dependent force could be added and this would also require including the off-resonant terms and a good starting point could be to work in the interaction frame of the off-resonant terms [200]. In general, applying multiple spin-dependent forces on same or different motional modes can be explored in detail, and possibly there are several interesting interactions to be explored.

The results in Chapter 4 demonstrate the first sub-wavelength characterization of light intensity and polarization using a single trapped ion as a sensor and the compilation of a manuscript is in progress. What makes this work even more impactful is that the characterization was performed for ultraviolet radiation at wavelength $\lambda = 369$ nm. The technique utilizes the intensity and polarization-dependent optical pumping of $^{171}\text{Yb}^+$ ions as a signature to extract the light parameters and the resolution is only limited by the fundamental limit imposed by the absorption cross section of a resonant light detector. The achievable resolution can be further increased by using off-resonant detection if required.

Two methods for modeling the ion-light interactions have been discussed that allow us to simulate the ion internal energy level dynamics when light of known polarization and intensity is incident on the ions. In the first method, the full atomic density matrix for the relevant atomic energy levels interacting with light is evolved, and in the second method only the incoherent population dynamics of the ground state is taken into account. These techniques provide an efficient way to model multilevel ion-light interactions and can be easily generalized to other ion species for studying both coherent and incoherent dynamics.

An important insight provided in this work is that these interactions can also be ‘learned’ in some restricted sense. A deep neural network can be used to learn the functional form of the output-to-input relationship, i.e. the inverse of the model, for some specifically chosen set of initial states of the ion. The input here refers to the light polarization, and the output refers to the ion’s population in the ground-state manifold as a function of time. Learning the inverse of this function allows for an extremely efficient means of ‘intelligent sensing’ and makes the approach readily field deployable owing to the minimal computational overhead in light parameter extraction.

The light field characterization technique presented here opens new avenues for the characterization of complex optical systems capable of producing sub-wavelength optical features with unprecedented resolution. This is especially useful in characterizing light sources in optical lithography systems. The technique, originally invented for characterizing the fidelity of our individual addressing trapped ions for state reset and readout [101], also applies directly to characterizing the performance of large scale ion- and atom-based quantum computers. The possible next step in improving this technique would be to harness the several different transitions in a single trapped ion to achieve multi-wavelength characterization of optical systems. Similarly, there is scope for using multispecies ion traps to build subwavelength optical characterization tools.

Chapter 5 describes the design and construction of a large-scale ion trapping apparatus: the blade trap system. The trap design allows the trapping of more than 50 ions in a linear chain with a high degree of control of the trapping potentials. The design of the trap geometry and the construction of the trap electrodes have been thoroughly documented and should allow easy replication, especially helpful for new experimental groups. The vacuum system is an extreme high vacuum (XHV) chamber with background pressure $P < 1.5 \times 10^{-12}$ mbar. Usually, it is not standard practice in a trapped ions laboratory to spend several years building an experimental apparatus; however, we decided to optimize the design and construction meticulously at every step to achieve possibly the lowest pressure achieved in a room-temperature ion trapping apparatus. Devoting such a long time to a single device, especially vacuum engineering, was justified because, when working with a large number of ions, it is very important to achieve extremely low background pressure to minimize the chances of ion-neutral collisions while performing a quantum simulation. Even with 30 ions, uninterrupted data taking to observe just 100 ms of quantum evolution requires XHV. In addition, we already had constructed a functioning quantum simulator where we could test other ideas on a smaller scale and produce meaningful results¹.

The vacuum system design in Chapter 5 has been thoroughly optimized with Monte Carlo methods using the open source software MolFlow. Monte Carlo methods for vacuum engineering have been well adopted in the particle accelerator community but not widely adopted in the atomic molecular and optical physics community, and the current results would possibly lead to wide adoption. A three-step protocol for optimizing vacuum system design is discussed, which allows separate optimization of different elements in a design. In addition to geometry optimization, achieving XHV also requires decreasing the outgassing of the vacuum components. The outgassing reduction techniques used in the construction of the vacuum system have been carefully documented along with the required fundamentals

¹And write papers which is for good or for bad is extremely important for academics.

for further optimizations. Through this we hope that a room temperature XHV system would become a common feature in trapped ion laboratories around the world.

Once the peripherals around the blade trap setup for example, the optics and the control system etc. are constructed and assembled, this large-scale quantum simulator would be able to tackle problems far beyond the reach of the classical simulation. The Hamiltonians generated in Chapter 3 will truly present a quantum advantage at this scale. The intelligent sensing technique discussed in Chapter 4 will become an important calibration tool not only for the blade trap, but also for other systems. Together, these tools would contribute to the exploration of rich physics and would hopefully extend our understanding of nature.

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APPENDICES

.1 Rotating transforms

For the analysis in the last section, we applied a unitary transformation to the state $|\psi\rangle_s$ and saw how the any operator, including the Hamiltonian looks like in the new “rotated” frame. The form of the Unitary we chose was meant to remove the trivial time dependence coming from the Hamiltonian itself. However, for a general unitary U that induces the transformation $|\tilde{\psi}\rangle = U |\psi\rangle$, what is the corresponding transformation for the new Hamiltonian $\tilde{H}$? Assume that ψ is the solution of the Schrodinger equation with H and $|\tilde{\psi}\rangle$ is the solution of the Schrodinger equation with $\tilde{H}$, that is,

$$i\hbar\partial_t |\psi\rangle = H |\psi\rangle, \quad i\hbar\partial_t |\tilde{\psi}\rangle = \tilde{H} |\tilde{\psi}\rangle \quad (2)$$

We first note that $U^\dagger |\tilde{\psi}\rangle = |\psi\rangle$ and plug this into the first equation

$$\begin{aligned} i\hbar\partial_t(U^\dagger |\tilde{\psi}\rangle) &= \tilde{H}U^\dagger |\tilde{\psi}\rangle \\ \implies i\hbar\partial_t(U^\dagger) |\tilde{\psi}\rangle + i\hbar U^\dagger \partial_t |\tilde{\psi}\rangle &= \tilde{H}U^\dagger |\tilde{\psi}\rangle \\ \implies i\hbar\partial_t |\tilde{\psi}\rangle &= -i\hbar U \partial_t(U^\dagger) |\tilde{\psi}\rangle + U \tilde{H}U^\dagger |\tilde{\psi}\rangle \end{aligned} \quad (3)$$

Comparing the last equation with the schrodingers equation for $|\tilde{\psi}\rangle$ we get

$$\begin{aligned} \tilde{H} &= U \tilde{H}U^\dagger - i\hbar U \partial_t(U^\dagger) \\ &= U \tilde{H}U^\dagger + i\hbar(\partial_t U)U^\dagger \end{aligned} \quad (4)$$

The two equations above are equivalent because $\partial_t(UU^\dagger) = \partial_t(U)U^\dagger + U\partial_t(U^\dagger) = 0$

.2 Diffusion limited model of Outgassing

The diffusion limited model of outgassing allows us to estimate the outgassing rate of the diffused gas on the surface of a solid given some concentration of the dissolved gas in the bulk of the solid. The usual approach is to use Fick's laws of diffusion[191] to estimate the diffusion flux, i.e the amount of gas leaving the metal surface per unit area into the UHV environment.

The diffusion of a substance that is dissolved in another solid is governed by the two Fick's laws of diffusion. In one dimension these are the following:

$$\begin{aligned} J(x, t) &= -D \frac{\partial c(x, t)}{\partial x} \\ \frac{\partial c(x, t)}{\partial t} &= D \frac{\partial^2 c(x, t)}{\partial x^2} \end{aligned} \tag{5}$$

- J the diffusion flux, is the amount of substance that flows through a unit area during a unit time interval.
- D is the diffusion coefficient or diffusivity. Its dimension is area per unit time.
- C is the concentration, which is the amount of substance per unit volume.
- $\frac{dC}{dx}$ is the *concentration gradient*.
- x is position, the dimension of which is length.

If the concentration of the dissolved gas inside the solid is known, then the specific outgassing rate is simply proportional to the diffusion flux, i.e.

$$q = \alpha D \frac{\partial c(x_s, t)}{\partial x} \tag{6}$$

where x_s is the ordinate at the chamber surface and α is the recombination factor to account for any chemical change of the dissolved gas at the surface. For example, when H atoms dissolved in steel are released at the surface they first recombine to form H_2 molecules and hence for this specific case $\alpha = 1/2$.

Since the outgassing rate above is expressed in the form of a concentration gradient at the surface of the chamber, estimating outgassing requires solving the above differential equations with appropriate initial and boundary conditions. The initial concentration of the dissolved gas in the bulk can generally be assumed to be constant, that is, $c(x, 0) = c_0$ however the boundary conditions require a bit more analysis. The diffusion-limited model assumes that the rate-limiting factor in outgassing is gas diffusion in the solid and not gas release at the surface. This means that the gas concentration at the solid surface is always in equilibrium with the gas molecules in the gas phase. Calculating this equilibrium concentration requires us to use the Sievert's law of gas solubility.

.2.1 Sievert's Law of gas solubility

The Sievert's law pertains to the solubility of a gas in a solid or a liquid. When a gas is in contact with a solid/liquid solvent the concentration of dissolved gas molecules in the solid and the gas pressure in the gaseous phase are related by the following relation:

$$C_{\text{eq}}(P_g, T) = K_s(T) \sqrt{P_g} \quad (7)$$

Here, P_g is the pressure of the gas in the gaseous phase, C_{eq} is the concentration of the dissolved gas in the solid phase and K_s is given by

$$K_s(T) = K_0 e^{\frac{-E_s}{2K_B T}} \quad (8)$$

Where, E_s , the gas solubility energy and K_0 , a constant, both depend on the gas and the solid.

.2.2 Outgassing in the DLM

Based on the Fick's equation and the Sievert's law, we now have the ingredients to estimate the outgassing rate of a solid, as a function of temperature and time given a certain concentration of dissolved gas in the bulk. The solid is modeled as a slab that is inside vacuum with both sides of the solid exposed to vacuum ². In the slab approximation, the

$$q(t) = \frac{4(c_0 - c_w)}{L} D \sum_{n=0}^{\infty} \exp \left[-(2n+1)^2 \pi^2 \frac{Dt}{L^2} \right] \quad (9)$$

²for parts that are inside vacuum this is a valid model.. However, even for estimating the outgassing of the walls of the vacuum chamber, this model is reasonably accurate

for most cases the we have that $Dt > 0.05L^2$ and only the first term in the sum is required to approximate the outgassing

$$q(t) \approx \frac{4(c_0 - c_w)}{L} D e^{-\pi^2 \frac{Dt}{L^2}} \quad (10)$$