

PERIODICALLY DRIVEN ATOMIC SYSTEMS

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neutral atoms, ions and biomolecules

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Dimitrios Trypogeorgos: *Periodically driven atomic systems*, neutral atoms, ions and biomolecules, © Trinity Term 2014

για την Άννα, το Φάνη και τη Χριστίνα

ABSTRACT

Periodically driven atomic systems: neutral atoms, ions and biomolecules

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This thesis is concerned with a variety of topics grouped together under the general theme of *periodically driven atomic systems*. Periodic driving is ubiquitous in most techniques used in atomic physics, be it laser cooling, ion trapping or AC magnetic fields. An in-depth understanding of the behaviour of such systems can be provided through Floquet theory which will develop as a central theme in the following chapters.

The thesis is divided in two parts: neutral atoms, and ions and biomolecules. In the first part I discuss a new ^{41}K - ^{87}Rb mixture experiment, built during the first year of my DPhil. This species combination has some very broad and low-loss interspecies Feshbach resonances that are instrumental for carrying out the experiments discussed in the first chapter. Unfortunately, the mixture experiment had to be put aside and our attention was shifted to Time-Averaged Adiabatic Potentials (TAAPs) and how these can be extended using multiple Radio-Frequency (RF) fields. This technique opens up the way for precise interferometric measurements. Lastly, the peculiar behaviour of Modulation Transfer Spectroscopy (MTS) of ^{39}K is investigated and a linearising transformation for four-wave mixing processes is presented.

In the second part we turn our attention to charged ions and biomolecules and the techniques of ion trapping. We propose a novel technique for co-trapping charged particles with *vastly different mass-to-charge ratios* and thoroughly explore its consequences. The behaviour of the trap and the stability of equations with periodic coefficients in general is studied using Floquet theory. The normal modes and symmetries of the system also need to be considered in relation to the effectiveness of the sympathetic cooling of the ions. Small systems were simulated using a Molecular Dynamics (MD) approach in order to capture the effect of micromotion and other heating processes.

PUBLICATIONS

Some ideas and figures have appeared previously in the following publications:

Dimitris Trypogeorgos, Christopher Foot, A two-frequency ion trap confining ions with widely different charge-to-mass ratios, *arXiv:1310.6294v2* 2014

Dimitris Trypogeorgos, Christopher Foot, The theory of an ion trap operating with two radio-frequencies, *in preparation*

Elliot Bentine, Dimitris Trypogeorgos, LIon: using LAMMPS for simulating trapped charged particles, *in preparation*

Tiffany Harte, Dimitris Trypogeorgos, Elliot Bentine, Christopher Foot, RF dressed potentials using multiple frequencies, *in preparation*

The first two can be found in the Appendix. The rest are not included in the thesis:

Dimitris Trypogeorgos, Tiffany Harte, Alexis Bonnin, and Christopher Foot, Precise shaping of laser light by an acousto-optic deflector, *Optics Express*, Vol. 21, Issue 21, pp. 24837-24846 (2013)

D Trypogeorgos, S D Albright, D Beesley and C J Foot, Design of a millimetre-scale magnetic surface trap for cold atoms, *J. Phys. B: At. Mol. Opt. Phys.* 47 075302, 2014

Martin Shotton, Dimitrios Trypogeorgos, and Christopher Foot, Enhancement of on-site interactions of tunnelling ultracold atoms in optical potentials using radio-frequency dressing, *Phys. Rev. A* 78, 051602(R) 2008

M. Landini, S. Roy, L. Carcagni, D. Trypogeorgos, M. Fattori, M. Inguscio, and G. Modugno, Sub-Doppler laser cooling of potassium atoms, *Phys. Rev. A* 84, 043432, 2011

Elliot Bentine, Dimitris Trypogeorgos, Christopher Foot, Orientation of large trapped ions, *in preparation*

Μια αστραπή η ζωή μας... μα προλαβαίνουμε.

— N. Καζαντζάκης

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ACRONYMS

AOM	Acousto-Optic Modulator
BH	Bose-Hubbard
BEC	Bose-Einstein Condensate
DAVLL	Dichroic Atomic Vapour Laser Lock
DSMC	Direct Simulation Monte-Carlo
EOM	Electro-Optic Modulator
FQHE	Fractional Quantum Hall Effect

FMS Frequency Modulation Spectroscopy

LAMMPS Large-scale Atomic/Molecular Massively Parallel Simulator

LLL Lowest Landau Level

MMFT Many-Mode Floquet Theory

MTS Modulation Transfer Spectroscopy

MD Molecular Dynamics

MOT Magneto-Optical Trap

ODE Ordinary Differential Equation

RF Radio-Frequency

RWA Rotating Wave Approximation

SAS Saturation Absorption Spectroscopy

SOC Spin-Orbit Coupling

TA Tapered Amplifier

TAAP Time-Averaged Adiabatic Potential

TOP Time-Orbiting Potential

TOF Time of Flight

VSWR Voltage Standing-Wave Ratio

INTRODUCTION

Periodic driving has been ubiquitous in atomic physics, particularly after the invention of the laser [1] which ushered atomic physics into its modern era. Atomic physics was redefined yet another time with the development of laser cooling techniques and a few years later the achievement of a new state of matter — a Bose-Einstein Condensate (BEC) of neutral atoms. The development of ion traps saw a similar benefit from laser cooling methods and are now the leading platform in quantum computation experiments.

In recent years, external driving or modulation of the parameters of atomic systems have lead to a wealth of new experimental handles or novel approaches to quantum simulation of condensed matter systems. The superfluid to Mott insulator transition in bosonic systems was demonstrated [2, 3] in an optical lattice (spatial rather than temporal periodicity). The value of the hopping term J in the Bose-Hubbard (BH) model can be changed by modulating the intensity of the beams forming the lattice [4]. Momentum-dependent magnetic fields have been generated through Raman induced Spin-Orbit Coupling (SOC) [5]. The time averaged description of such systems leads to artificial gauge fields. Some form of driving is always necessary and various proposals include modulated quadrupolar potentials [6] and shaking optical lattices [7]. An even broader class of Hubbard models can be studied through additional modulation of the interparticle interaction strength in dual species experiments [8].

Periodic driving is even more intimately connected to ion traps, since it is involved in the trapping mechanism itself — though this is true only for Paul traps since Penning traps employ a magnetic field. At this point a distinction between driving a system with an external force and parametric driving must be made. Ion traps and modulation of the various parameters in the previous paragraph fall under the second category. Both cases are amenable to description through Floquet theory which is extensively discussed throughout this thesis.

1.1 THESIS OVERVIEW

The thesis is divided in two parts concerning neutral atoms and ions respectively. A theoretical introduction chapter on the physics of cold atoms has been deliberately omitted due to length considerations. The reader is referred to many excellent books, reviews [9, 10] and other theses in the field covering the topic. Similarly, the

S. Chu, C. Cohen-Tannoudji, W. D. Phillips 1997 Nobel Prize.

E. A. Cornell, W. Ketterle, C. E. Wieman 2001 Nobel Prize.

N. F. Ramsey, H. G. Dehmelt, W. Paul 1989 Nobel Prize.

D. J. Wineland, S. Haroche 2012 Nobel Prize.

introduction to ion traps mainly focuses on the kinematics of a cloud of ions which does not necessary reveal the huge impact they have had in quantum computation and metrology experiments.

Chapter 2

During my first year I built a ^{41}K - ^{87}Rb experiment, planning to extend some of our rotation experiments to boson-boson mixtures. The potassium-rubidium combination is particularly appealing since the interspecies scattering length is large and there are many wide, low loss Feshbach resonances. The properties of both species have been extensively studied [11]. The technical experimental details are presented along with an outline of a measurement this experiment is uniquely poised to do.

Chapter 3

The exploration of Floquet theory led to a deeper understanding of the TAAP potentials, first demonstrated in [12]. A natural extension of this mechanism comes from the application of multiple RF fields. Multiple potential minima can be generated in this way. This opens up the possibility of spatial interferometric measurements e. g., two ring shaped potentials with a persistent current flow induced by rotating one or both of them, forms a Sagnac interferometer. A calibration procedure for the rotation frequency based on the interference fringes as they appear after Time of Flight (TOF) expansion is discussed.

Chapter 4

A few interesting aspects, namely the appearance of a crossover signal, of MTS of ^{39}K are investigated. The ability to change the lock point by adjusting the spectroscopy parameters offers some freedom in designing a laser system capable of addressing all three potassium isotopes with minimal reconfiguration of the optics. Initially we set out to solve this problem using Floquet theory but a transformation that leads to time independent, linear optical Bloch equations was later found.

Chapter 5

We consider the stability of damped periodically driven systems. The equations of motion of a trapped ion are used to introduce the various characteristic properties of periodic equations. Although a multitude of methods exist to tackle such equations, we find Floquet theory to be the most straightforward and insightful mainly because of its connection to the physics of condensed matter systems. Unfortunately there is no analytic solution to the Mathieu equation so the Meissner equation is used instead to discuss the Floquet analysis.

Chapter 6

The two-frequency ion trap has the potential to extend ion trapping to vastly different parameter regimes. We claim that co-trapping of ions with charge-to-mass ratios different by many orders of magnitude is possible, as well as efficient sympathetic cooling of the heavy ion by the atomic one. A rescaling of the equations of motions is necessary to understand the behaviour of the trap as two independent traps. This picture does not hold when the charge-to-mass ratio of the ions is similar, but the addition of a second RF field can still lead to improvements in the efficiency of sympathetic cooling. The capability the two-frequency trap offers to adjust the spring constants of the ions independently can immediately be used in mass spectrometry.

Chapter 7

Normal modes complete the picture of a system of ions below its crystallisation temperature. The theory of non-classically damped modes is presented and a state-space model is used to reliably compute the complex eigenvalues of the modes. The various symmetries of the system need to be broken for effective sympathetic cooling. An example of a Coulomb molecule comprising one very large ion and two smaller ones is discussed, and we identify some modes which involve a large amplitude of motion of the heavier ion and hence are not effectively cooled. Nevertheless, their characteristic cooling time is still experimentally reasonable. The theoretical approach is consolidated with MD simulations. Instead of writing yet another MD code, we opted to use Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS). A Matlab wrapper was written to translate the lingo of the various communities using LAMMPS, to be more ion trap friendly. The superior efficiency and configurability of LAMMPS allowed for simulation of relatively large systems and validation of the theoretical results. Some of the main characteristics of the code are presented in Appendix C.

Part I

NEUTRAL ATOMS

A new ^{41}K - ^{87}Rb experiment is built but not pursued further due to lack of time and resources. [TAAP](#) potentials are extended to multiple frequencies and we take a closer look into the [MTS](#) line shape in ^{39}K .

THE DUAL SPECIES MACHINE

Dual species systems have the capability of accessing a whole new class of experiments. The main important differences between two spin states of the same species and a two species configuration come from their mass imbalance and the possibility of tuning the interspecies scattering length via a Feshbach resonance. Single species systems can exhibit these characteristics as well, e.g. periodic driving leads to a band structure picture and hence an effective mass which can be different for different spin components [5]. Additionally, there exist Feshbach resonances between the different hyperfine ground states [13] or can be induced using microwaves [14]. Technical difficulties aside, the main limitation of a single species system comes from the fact that the experiments we are considering involve a magnetic trap, hence only low-field-seeking states can be trapped. The new machine aims to bring ^{87}Rb and ^{41}K to quantum degeneracy. This isotope combination is very appealing due to the large interspecies scattering length and an easily accessible, wide Feshbach resonance [15].

*The widest
resonance is at
515 Gauss with
 $\Delta B = 83$ Gauss.*

2.1 LASER SYSTEM

Several frequencies are required for laser cooling of dilute alkali gases. For most species a strong cooling light is required, red detuned by a few MHz from the $F = 2 \rightarrow F' = 3$ transition in the D_2 line. Although this is seemingly a closed transition there is the possibility of off-resonant excitation of the $F' = 2$ state which can decay to the $F = 1$ ground state hence depleting the population. Repumping light is used, resonant with the $F = 1 \rightarrow F' = 2$ transition, to prevent this from happening and keep the atoms cycling on the cooling transition where the isotropic scattering of photons reduces their temperature to (less than) the Doppler limit. The collection speed and efficiency of a Magneto-Optical Trap (MOT), and thus the experimental cycle time, is mainly dependent on the size of the beams and the available optical power. The design of the laser system for both species is motivated by this simple fact and the size of the beams was chosen to be as large as possible given the available optical power.

2.1.1 Laser system for ^{87}Rb

Two external cavity diode lasers (Toptica DL100) are used, fitted with Eagleyard anti-reflection coated diodes (EYP-RWE-0790-02000-1300-SOT12-0000). The DL100 is an industry standard laser diode mount in a Littrow external cavity configuration. The coated diodes have been found to be much more reliable than their uncoated counterparts since, due to the absence of a preferred laser mode, they have a much wider mode-hop-free range.

*All schematics are
drawn using the
gwOptics library.*

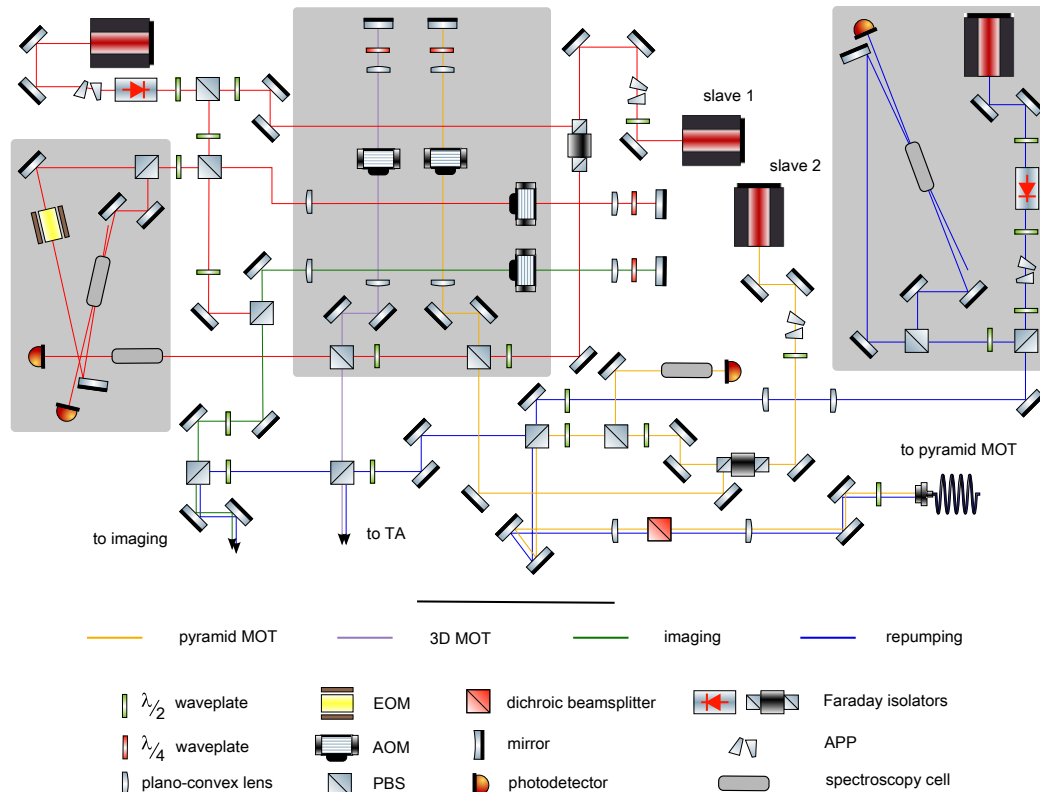


Figure 1: The laser system for cooling ^{87}Rb involves two master lasers for addressing the cooling and repumping lines. The cooling laser is locked on resonance using **MTS** and subsequently frequency shifted using various **AOMs**. Two slave lasers are used to produce more power to seed the pyramid **MOT** and the **TA** that produces the light for the 3D **MOT**. The repumping laser is locked to resonance using **FMS** and distributed to all the optical paths.

Due to their semiconductor manufacturing process, the output of the emission profile of the laser diodes is elliptical so anamorphic prisms are used to reshape it to circular. A 60 dB optical isolator (FI-780-5TVInj-1) is in place in order to avoid induced optical noise from back-reflections (see Fig. 1). A few hundred μ Ws of laser power are split off at the first polarising beam-splitter to seed the first slave laser. The light from the master laser is frequency shifted with an Acousto-Optic Modulator (AOM) at 110 MHz from the D_2 line and locked using MTS which pro-

duces a clean error signal with no Doppler background — we discuss [MTS](#) in detail in Sec. 2.1.4. The first slave laser is used to seed the Tapered Amplifier ([TA](#)) (EYP-TPA-0780-01000-3006-CMT03-0000 from Eagleyard) which produces the light for the 3D [MOT](#). The light for the pyramid [MOT](#) is produced by the second slave laser. The repumping light is co-propagating along the optical paths that lead to the two [MOTs](#) and the imaging fibres. As the repumping light is resonant, very little power is needed.

The repumping laser is locked on resonance using Frequency Modulation Spectroscopy ([FMS](#)) since [MTS](#) gives a signal only for closed transitions. The current of the laser diode is weakly modulated at 20 MHz by the Pound-Drever-Hall module supplied with the Toptica laser system. The local oscillator is phase-shifted and mixed with the output of the photodetector to produce an error signal which is fed to the PID module. Part of the error signal is AC-coupled to the laser diode current through a FET to increase the bandwidth of the lock. The spectroscopy cell is heated to 54 °C to give a higher vapour pressure that improves the signal-to-noise ratio of the error signal.

2.1.2 Laser system for ^{41}K

The approach taken for ^{41}K is somewhat different since the hyperfine splitting of the ground state is only 254 MHz. This frequency separation is well within the range of [AOMs](#), hence we use a single master laser for both cooling and repumping light. In addition, the dominant feature of [MTS](#) is the ground state crossover of ^{39}K . This is seemingly contradictory to the fact that [MTS](#) only produces a signal for closed transitions. A detailed explanation of this peculiarity is given in Ch. 4.

A DL100 laser, fitted with the same coated diode as above, is locked using [MTS](#) to the ground state crossover of ^{39}K . The rest of the light is amplified with a [TA](#) and coupled to the frequency management section via an optical fibre. The cooling and repumping transitions for ^{41}K are 83.1 MHz and 337.2 MHz blue detuned from the locking point respectively. All of the [AOMs](#) are arranged in a single-pass configuration which somewhat restricts the available tuning range (see Fig. 2). This is undesirable since it has been shown that sub-Doppler cooling of potassium can only be achieved by ramping the frequency and amplitude of the [MOT](#) beams [16]. However, quantum degeneracy can also be reached through sympathetic cooling with ^{87}Rb [17] or employing two spin states for the fermionic isotope [18].

Due to the very narrow excited state structure of potassium, the distinction between repumping and cooling light is somewhat artificial [19]. Both laser beams are far detuned from all the excited levels and have a similar power — cf. ^{87}Rb where the repumping light is resonant and only needs to be a small fraction of the intensity of the main laser cooling.

^{39}K is the most abundant isotope of potassium at 93.3%.

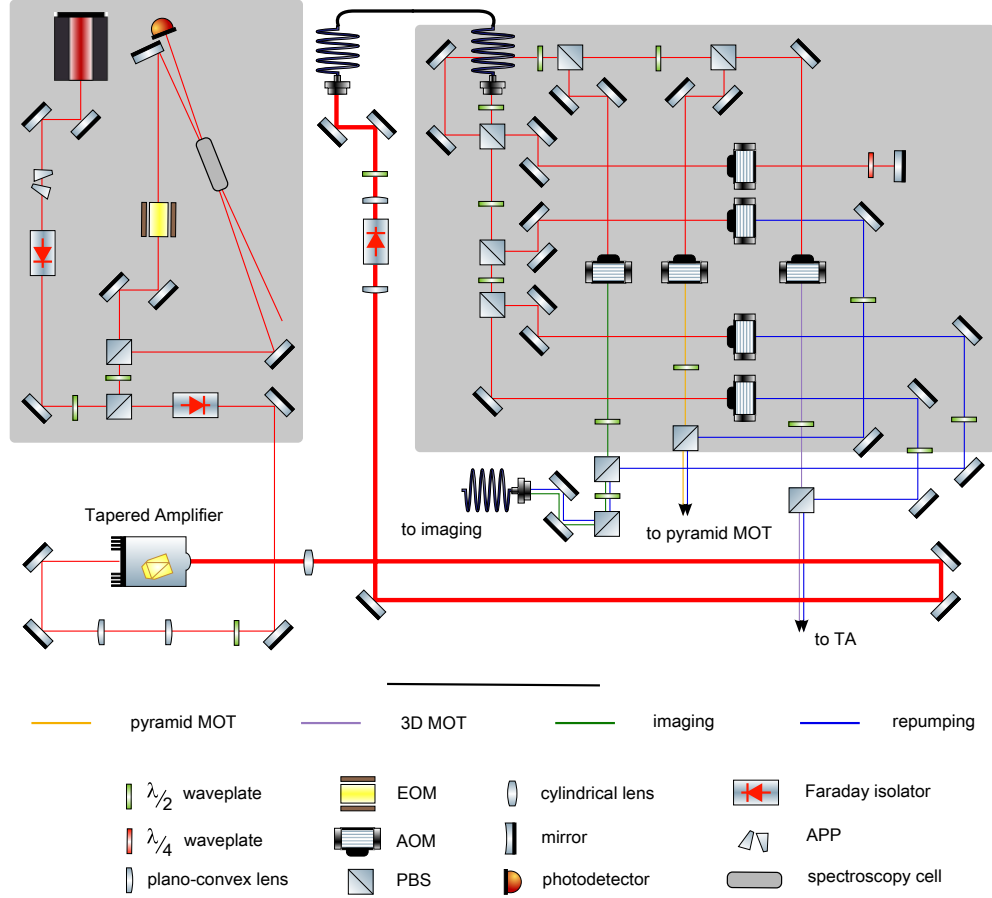


Figure 2: The laser system for ^{41}K involves a single master laser for addressing both the cooling and repumping lines. The master laser is locked on the ^{39}K crossover transition using MTS and subsequently frequency shifted using various AOMs in a single pass configuration. There is an intermediate amplification stage using a TA to produce enough power for the frequency management section.

2.1.3 Tapered Amplifiers

A number of TAs are used to increase the optical power of the beams forming the pyramid and 3D MOTs. Their arrangement is similar for both species (see Fig. 3). The Eagleyard chips are mounted on custom designed mounts based on a design from Institut d'Optique [20] with no moving parts. The current and temperature leads are mounted on the top of the TA box using standard DE-9 connectors, thus reducing the footprint of the TA mount. We use commercial current (LDC8040) and temperature drivers (TED8040) from Thorlabs inside a PRO800 chassis to drive the chips. The temperature is monitored with an AD590 transducer mounted as close to the chip as possible and controlled with a peltier element on the side of the copper mount. This arrangement was meant to prevent heat-induced misalignment effects but the heat capacity of the side wall proved to be insufficient, so the peltier was repositioned under the chip.

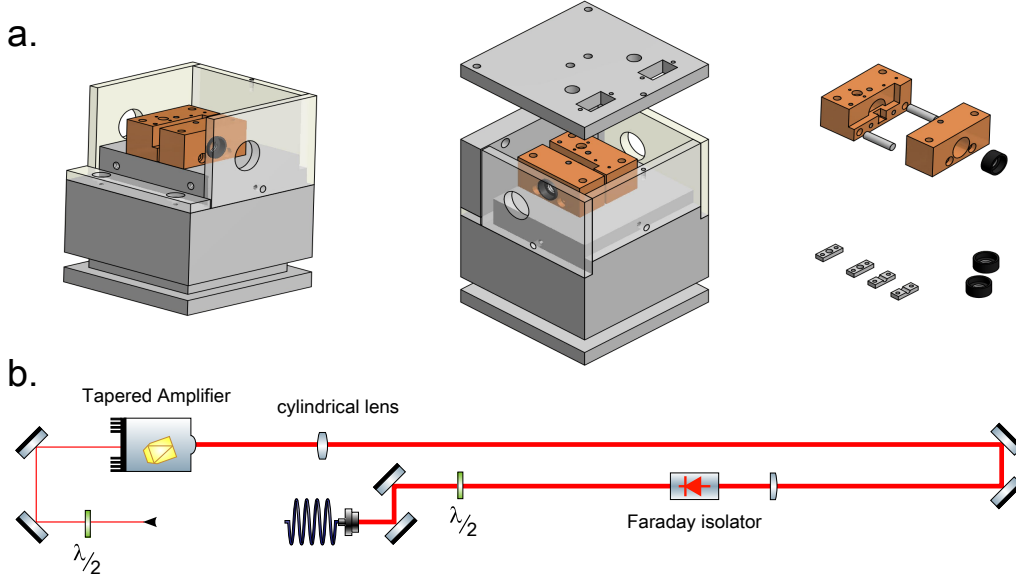


Figure 3: The mechanical design of the TA mounts (a) is based on a design from Institut d’Optique (see text for details). The TA is seeded with a two-colour beam (b) and a half-waveplate is used to adjust the power ratio of the two beams; the efficiency of the TA is polarisation-dependent. The output of the TA is collimated using a spherical collimator (vertical axis) and a cylindrical lens (horizontal axis). It is subsequently coupled into a photonic band gap fibre with about 50% efficiency.

All TAs are seeded with the cooling and repumping light for each species. The power ratio of the different seed colours at the output can be adjusted with a $\lambda/2$ waveplate since the amplification of the TA is polarisation dependent. A beam linearly polarised along the vertical is amplified roughly by a factor of 4 more than if polarised along the horizontal. The TA output diverges by differing amounts along the vertical and horizontal directions. A 6.5 mm collimator is used to collimate the vertical axis and a 15 cm cylindrical lens for the horizontal. After reshaping, the beam is coupled into an LMA-PM-10 photonic band gap fibre from Crystal Fibre which can handle up to a few Watts of power. The maximum coupling efficiency we were able to achieve is 54%.

2.1.4 Modulation Transfer Spectroscopy

Several spectroscopy techniques are used for locking the lasers in atomic physics experiments such as Dichroic Atomic Vapour Laser Lock (DAVLL) and FMS. The single beam techniques are Doppler limited but can have a capture range of several hundred MHz. The pump-probe schemes on the other hand have sub-Doppler resolution but with the cost of limited capture range <1 MHz. Among the latter, MTS has two main advantages: firstly, it readily generates dispersive-like signals that sit on a flat, zero background. This means there is no need to subtract the Doppler

The dominant peak in ^{39}K corresponds to the ground state crossover.

profile and the zero crossings are accurately centred on the atomic transitions. Secondly, the dominant signals come from closed transitions. This is especially useful if there are many closely spaced transitions. MTS in ^{39}K behaves slightly differently to the process described above. A full treatment is given in Ch. 4.

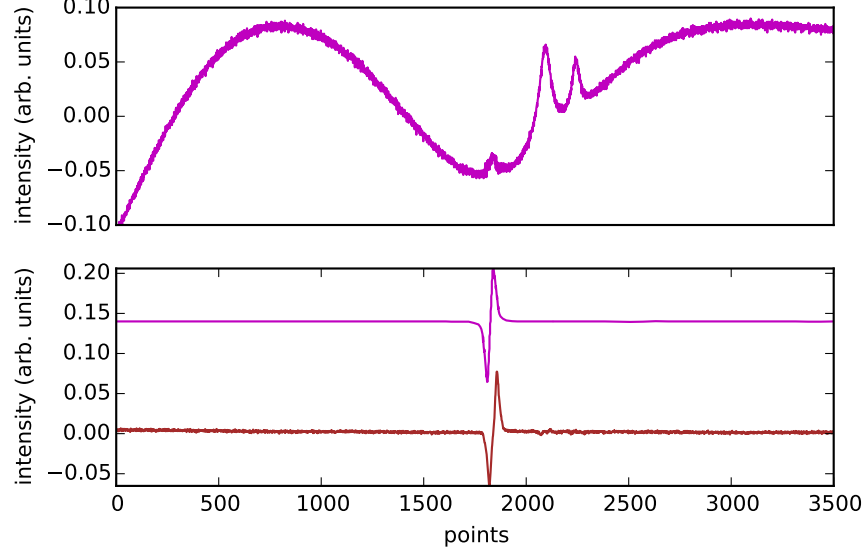


Figure 4: A typical SAS trace for ^{87}Rb is shown (upper) along with the corresponding MTS signal (lower). The measured curve MTS curve (brown) is contrasted with the theoretical curve (magenta) calculated using the model presented in Ch. 4. The pump beam is modulated with an EOM at 10 MHz and the spectroscopy cell is heated to about 40 °C to increase the vapour pressure. The MTS signal arises from the $F = 2 \rightarrow F' = 3$ since it is the only closed transition in the system.

MTS has been successfully demonstrated for ^{87}Rb [21]. The pump beam, with carrier frequency ω_c , is strongly modulated by an Electro-Optic Modulator (EOM) to generate sidebands separated by ω_m which is of the order of a few MHz. The electric field can be expressed as:

$$\begin{aligned} E &= E_0 \sin(\omega_c t + \delta \sin \omega_m t) \\ &= E_0 \left(\sum_{n=0}^{\infty} J_n(\delta) \sin(\omega_c + n\omega_m)t + \sum_{n=1}^{\infty} (-1)^n J_n(\delta) \sin(\omega_c - n\omega_m)t \right) \end{aligned} \quad (1)$$

where δ is the modulation depth and $J_n(x)$ is the n^{th} order Bessel function. The MTS signal arises from a non-linear four-wave mixing process [22] with the carrier frequency and one sideband interacting with the probe beam to give rise to a fourth wave. The probe beam, which now carries a sideband as well, is incident on a photo-detector and the beat signal that is measured is of the form:

$$\begin{aligned} S(\omega_m) &= \frac{C}{\sqrt{\Gamma^2 + \omega + m^2}} J_0(\delta) J_1(\delta) \times ((L_{-1} - L_{-1/2} + L_{1/2} - L_1) \cos(\omega_m t + \phi) \\ &\quad + (D_1 - D_{1/2} - D_{-1/2} + D_{-1}) \sin(\omega_m t + \phi)) \end{aligned} \quad (2)$$

with

$$L_n = \frac{\Gamma^2}{\Gamma^2 + (\Delta - n\omega_m)^2} \quad \text{and} \quad D_n = \frac{\Gamma(\Delta - n\omega_m)}{\Gamma^2 + (\Delta - n\omega_m)^2} \quad (3)$$

where Γ is the atomic linewidth and Δ the detuning from resonance. The above equations are true as long as the modulation strength $\delta < 1$ so that only first order sidebands need to be considered. A typical trace for the $F = 2$ manifold in ^{87}Rb is shown in Fig. 4.

2.2 VACUUM SYSTEM

Most of the vacuum components were recycled from a dismantled experiment except for the 3D MOT chamber. The design is a standard double MOT design with the second MOT being a traditional 3D MOT and the first a less widely used pyramid MOT (see Fig. 5). The pyramid MOT is made by using four mirrors that form an inverted pyramid with a hole in its centre. The main advantage of this configuration is that only a single beam is required to operate the MOT. The incident beam has two colours corresponding to the two species. It is launched from a bare fibre and enlarged to a radius of 24 mm.

A 2D MOT is more popular in similar vacuum designs [23].

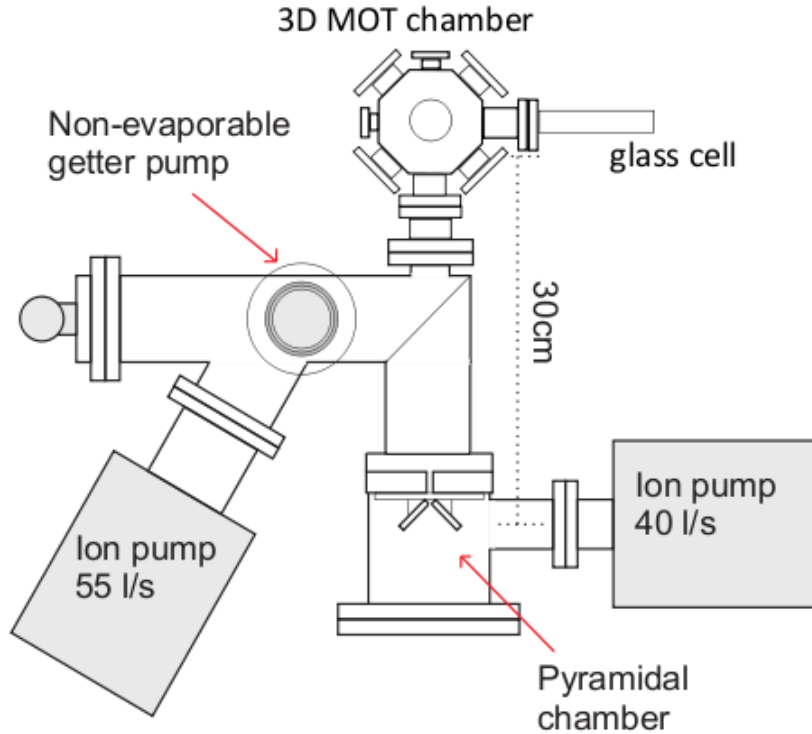


Figure 5: The atoms are collected in the pyramid MOT chamber which is pumped with a 40 l/s ion pump. The pyramid MOT beam acts as push beam as well, which sends the atoms on a free flight to the 3D MOT chamber. The pressure in the two chambers differs by about two orders of magnitude.

The atom flux achieved is comparable to a 2D MOT and done so with much less optical power — 45 mW:8 mW and 45 mW:45 mW of cooling:repumping light for ^{87}Rb and ^{41}K respectively. Both species are introduced into the vacuum by a couple of SAES dispensers connected in series and mounted in the pyramid MOT chamber, while vacuum is maintained at about 10^{-9} mbar by a Varian Triode 40 l/s ion pump. A choice of using standard un-enriched potassium dispensers was made but this might prove to be problematic if the fermionic ^{40}K isotope is to be used. Although loading from natural abundance sources using a Zeeman slower has been recently demonstrated [24] using an enriched source is much more straightforward. These are available commercially from Alvatech or alternatively one can buy enriched potassium powder (Trace Sciences) and make home made dispensers [25].

^{40}K has a natural abundance of just 0.01%

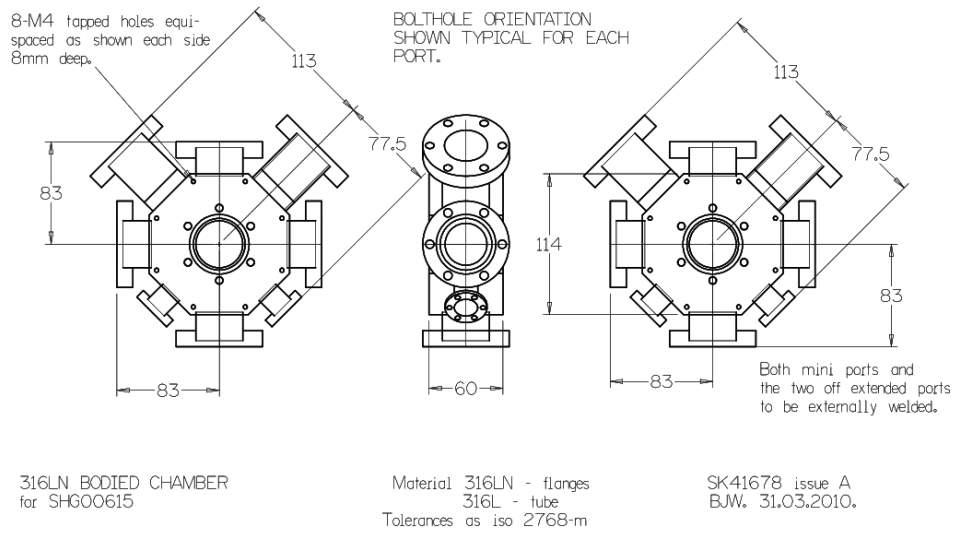


Figure 6: The 3D MOT chamber is manufactured by VG Scientia using 316LN non-magnetic steel. Its dimensions have been optimised so that the vertical dimensions is as small as possible while still allowing for CF40 viewports.

The pyramid MOT beam provides transverse cooling and also acts as a push beam that directs the atoms into the 3D MOT chamber. The pressure in the 3D MOT chamber is practically impossible to measure with the ion pumps due to charge build-up in the pump cathode [26]. Without a lifetime measurement available we can do some simple calculations to get an idea of what is expected. The differential pumping tube is $L=17$ mm long and has a diameter $D=5$ mm. The conductance between the two chambers, at low pressure, is determined by two parameters: the number of atoms entering the tube ($\propto D^2$), and the average number of collisions with the walls as the atom goes down the tube ($\propto L/D$) assuming free molecular

flow, i.e. mean-free path $\ll D$. At very low pressures this leads to the formula for molecular flow F down a thin tube [27]

$$F = \frac{65}{\sqrt{M}} \frac{D^3}{L} \text{ l/s} \quad (4)$$

with D and L expressed in cm. M indicates the relative molecular weight of the gas. For ^{87}Rb we get $F = 0.51/\text{s}$. The ratio between this flux entering the second chamber and the $551/\text{s}$ pump speed of the ion-pump leads to the two orders of magnitude difference in the vacuum attained in the two systems. The non-evaporable getter pump was fired only once, right after bake-out, and did not lead to a measurable difference in the vacuum pressure.

The main requirement for the 3D MOT chamber was to have the smallest possible footprint while still allowing for CF40 viewports to be fitted (Fig. 6) which give an optical access of 34 mm. It was made by VG Scienta using 316LN steel which was tested to be indeed non-magnetic. The powers of the 3D MOT beams are 25 mW:3 mW and 25 mW:25 mW of cooling:repumping light for ^{87}Rb and ^{41}K respectively; larger and higher power beams lead to faster loading times. The beams are fibre coupled to the main optical table of the experiment using two high power photonic band-gap fibres for each species. Each colour is split in 6 beams with a series of polarising beam-splitters and directed to the 3D MOT windows via various telescopes. The lower mirror in the telescopes can be rotated to redirect an incident beam at any angle. The whole vacuum apparatus is mounted on a separate bread-board in case it needs to be moved out of its current position for baking-out or cleaning the glass cell. It can be realigned using guiding brackets mounted on the optical table. Its height, measured at the centre of the windows, is 425 mm which allows for comfortable three level layering of the optics. The whole apparatus was aligned and levelled horizontally using a guiding beam from a He-Ne laser.

The chamber is based on a design by Simon Cornish.

2.2.1 Magnetic transfer

After the atomic cloud has been loaded onto the 3D MOT, it is transferred over a distance of 23 cm to a glass cell where the main experimental sequence takes place. The glass cell provides much better optical access and a metal-free region so that eddy currents do not affect the switching times of the magnetic fields. There are various methods of transferring a cloud of atoms, e.g. using a dipole trap [28], a pair of coils on a translating stage [29, 30, 31] or multiple pairs of overlapping coils [32]. A fair comparison depends on the details of the implementation of each method but broadly speaking the pros and cons of each category can be itemised as follows:

Another paradigm was recently demonstrated using a pair of deformable lenses [33].

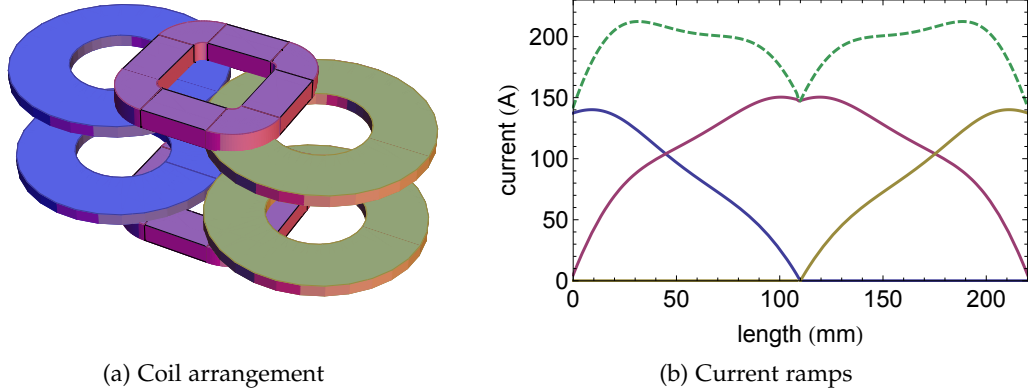


Figure 7: The coil arrangement around the vacuum system (a) involves two identical coil pairs for the 3D MOT and glass cell respectively. A rectangular coil pair facilitates the magnetic transfer of atoms between the two chambers. The current ramps for the transfer (b) are symmetric as expected (the colours correspond to the respective coil pairs). This means they can be ran backwards as well, which will allow for loading of two species without significantly deforming the magnetic potential. The total current is kept well below 400 A which is the maximum output of Lambda ESS 15 kW power supply which is capable of 40 V-375 A.

- A pair of quadrupole coils, or a single lens, on a translating stage is very straightforward to implement. The optical transport requires a relatively high power laser and can be cumbersome to align to the centre of the magnetic quadrupole. The translating coil pair significantly limits the optics placement around the vacuum. Also, the translating stage produces significant acoustic noise which can affect the laser stability if they are mounted on the same optical table.
- Translating large distances with overlapping coil pairs normally involves winding a few tens of coils and switching the current between them while controlling three pairs at a time which can be cumbersome. On the other hand, everything is stationary and no realignment is needed. Moreover, the atomic cloud can be transported along the vertical direction which is not as easy to do with the previous methods.

In the original demonstration of the overlapping coils method [32], about 15 quadrupole pairs were used to cover a distance of 60 cm (going around a corner). Our implementation is capable of transporting the cloud of atoms by 23 cm using only 3 coil pairs. Moreover only two pairs need to be driven at the same time. In

order to keep the gradient and aspect ratio constant during the transfer we need to satisfy the following system of equations:

$$\sum_{i=1}^3 I_i b_{x,i}(x, 0, 0) = 0 \quad (5)$$

$$\sum_{i=1}^3 \partial_z I_i b_{z,i}(x, 0, 0) = \text{gradient} \quad (6)$$

$$\sum_{i=1}^3 \left(\frac{I_i \partial_y b_{y,i}(x, 0, 0)}{I_i \partial_x b_{x,i}(x, 0, 0)} \right) = \text{aspect ratio} \quad (7)$$

where $b(x, y, z)$ is the unitary magnetic field, i.e. with the coil current set to 1 A. If all the above constraints are to be satisfied, 3 pairs need to be driven at the same time. This only breaks down at the first and last part of the transport process where one is forced to use only two pairs and thus let the aspect ratio change uncontrollably. Our implementation is similar to the endpoint situation since we only use 3 pairs in total (Fig. 7a) and thus we can only satisfy the first two equations. However, with a carefully designed geometry of the coils, this is not a problem and in fact the aspect ratio variations in our system are significantly smaller than in the original demonstration.

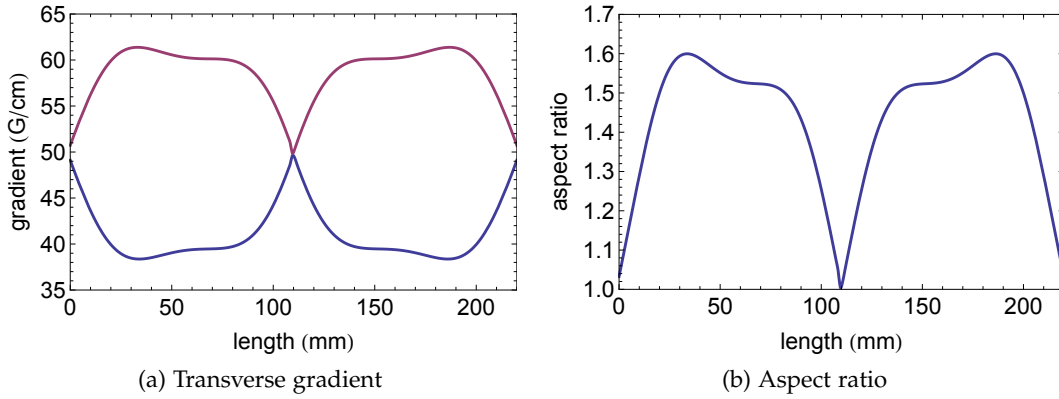


Figure 8: (a) The transverse gradient of the quadrupole magnetic field fluctuates by 20% (symmetrically in x and y directions) during the transport process but the axial gradient is kept at 100 G/cm. (b) The aspect ratio changes by less than a factor of 2 so heating of the atomic cloud is expected to be negligible.

The magnetic field arising from the currents ramps (Fig. 7b) was simulated using the Radia package from ESRF. The symmetric design of the coils allows for running the transport backwards and mixing the atoms of different species at the half-way point if needed. In this way the problem of one species deforming the potential while the transport of the second species is taking place can be circumvented. Through optimisation of the geometry of the coils we were able to minimise the aspect ratio variations to a factor less than 2 (Fig. 8b) — cf. factor of 6 in [32].

Any variations of the size of the cloud are along the transverse direction (Fig. 8a) and the axial gradient is kept constant at a value of 100 Gauss/cm.

The coils are wound using hollow tubing bought from Wolverine Tube and wrapped in Kapton by S&W Wire. With an external (internal) diameter of 4 mm (3 mm), they can be efficiently cooled by running water through them. The main water line in the lab has a pressure of 2 bar and its temperature is stabilised at 12 °C. The simplest heat exchange model for water flowing in contact with a conductor leads to a steady-state temperature estimation:

$$T = P \left(\frac{1}{\rho Q c_p} + \frac{1}{kA} \right) + T_{\text{room}} \quad (8)$$

where

- P dissipated power (W)
- c_p specific heat of water ($\text{Jkg}^{-1}\text{°C}$)
- ρ density of water (kg/m^3)
- Q water flow (l/s)
- k water-to-copper thermal conductivity ($\text{Wm}^{-1}\text{K}^{-1}$)
- A total area of the coil (m^2)

The water flow Q was calculated for each coil by solving the standard hydrodynamic equations and later measured to be 7.7 ml/s and 5.0 ml/s for the circular and square coils respectively, in complete agreement with the calculations. The final steady-state temperatures for the coils are about 41 °C for the first and last pair and 109 °C for the middle pair. The middle pair is allowed to go to such high temperatures since it is only used for a few ms during transporting the atomic cloud, thus it does not have time to achieve its steady-state temperature. The first and last pairs though provide the quadrupole field for the MOT and final evaporation stage respectively, so their temperature is limited to less than 50 °C.

2.2.2 Magnetic trap

Two more coil pairs are used for a bias field and an additional quadrupole field (see Fig. 9a). The bias field is produced by a pair of coils arranged in a Helmholtz configuration and provides access to the interspecies Feshbach resonance of ^{87}Rb and ^{41}K . The achievable magnetic field is about 550 G at 330 A which is adequate for making use of most of the interspecies resonances. It is necessary for the magnetic field to be as uniform as possible throughout the cloud so there is no residual trapping term. The optimal Helmholtz configuration dictates coils with a square profile and separation equal to their diameter. Nevertheless, since the positioning of the coils can only be accurate down to about 1 mm, an extra pair of coils can be

used to make the field more uniform [34]. In this case, this can be either any of the two quadrupole pairs connected to the high power MOSFET bank via an H-bridge [35].

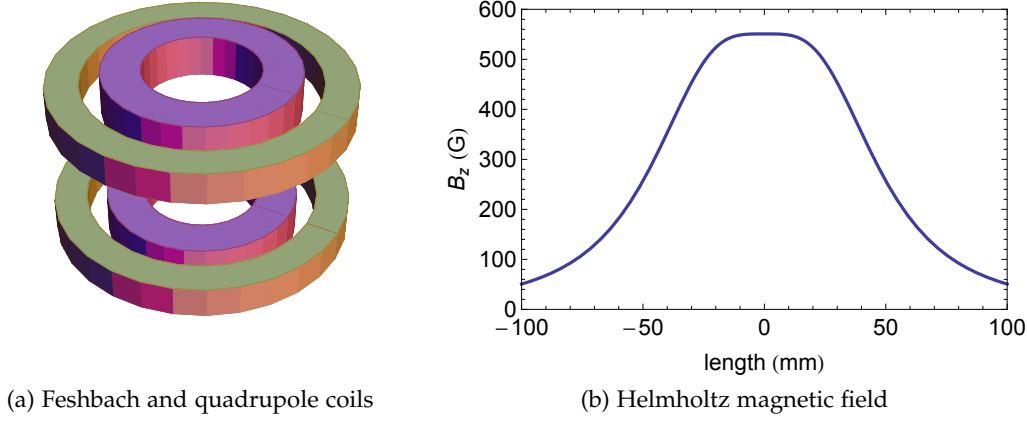


Figure 9: (a) The Feshbach (outer) and quadrupole coils (inner) are fitted in between the transport coils and the glass cell. (b) The magnetic field produced by the Feshbach coils is uniform over a large region in the centre of the trap and its maximum value is about 600 Gauss.

The additional quadrupole pair can reach much higher gradient values than the one involved in the transport. With 610 G/cm at 330 A it can significantly accelerate the magnetic evaporation of the atoms and also push the TAAPs to a more interesting regime [12]. Due to their small size, both pairs of coils are cooled very efficiently leading to steady-state temperatures of around 32 °C.

Lastly, an AC coil array similar to the one used in our ^{87}Rb experiment [29], will be fitted around the glass cell for the purpose of making a Time-Orbiting Potential (TOP) trap and coupling RF radiation to the atoms to implement TAAP for dual species.

2.3 FUTURE MEASUREMENTS

Unfortunately, the experimental progress was interrupted shortly after the completion of the building phase of this experiment while the MOT sequence was being tested. Thus, instead of a BEC sequence, this section records proposed future measurements that could be carried out with a two-species apparatus. Experiments involving optical lattices and the observation of the Mott insulator state were instrumental in solidifying the connection between atomic and condensed matter physics [3]. Such a system is described by the BH hamiltonian where the role of the

hadronic lattice is assumed by the optical potential and the condensed atoms are trapped at the minima of the periodic potential [2]:

$$H = -J \sum_{\langle i,j \rangle} b_i^\dagger b_j + \sum_i \epsilon_i \hat{n}_i + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) \quad (9)$$

The Hubbard parameter U is the onsite repulsion strength between two atoms and J corresponds to the hopping matrix element between adjacent sites i, j . The number of atoms per site is $\hat{n}_i = b_i^\dagger b_i$ where $b_i^\dagger, b_i$ are the creation and annihilation operators respectively. Also included in the model is an energy offset ϵ_i for each lattice site to account for an external trapping potential. It is well known that the standard BH model does not exhibit exotic behaviours such as a supersolid phase which appears on extended soft-core models [38, 39, 40]. The interest in such models was renewed with the condensation of ^{52}Cr [41] which has a very large magnetic dipole moment and long range interactions need to be taken into account.

Our approach for creating soft-core BH models involves rotating a cloud of two co-trapped atomic species. The behaviour of dual species vortex lattices has been studied extensively [42, 43, 44, 45, 46] with respect to the interspecies interaction strength. The Abrikosov lattices phase-separate for large repulsive interaction and overlap at the opposite extreme. Interesting nematic phases have been predicted to appear for intermediate interaction strengths. Most of these studies assume similar density for both species and rotation frequency at a regime where they both form Abrikosov lattices. In the regime we are interested in, the heavier species (^{87}Rb) has appreciable density while there are only a handful of atoms of the other species (^{41}K). For adequate repulsive interspecies interaction strength the ^{41}K atoms should arrange themselves in the vortex cores of the Abrikosov lattice, giving rise to a system described by a soft-core BH model. The “softness” of such a configuration comes from the back-action of the trapped species to the Abrikosov lattice which makes the Hubbard parameters depend on the occupation number of the lattice sites. A Feshbach resonance between the two species can be used to control the Hubbard parameters. The phase diagram of such systems is much richer than the standard BH model and they are also thought to be linked with high temperature superconductivity. This is being studied theoretically by the research team of Prof. Dieter Jaksch in Oxford Physics and can form the basis of a future research proposal.

Moreover, one of the main challenges in observing ordered states in optical lattices (mainly for fermions) is the extremely low temperatures required. The lattice arrangement provides a very appealing cooling method where the trapped species can be cooled through Raman transitions to the first excited Bloch band while the other species serves as a cold reservoir [47, 48]. Atoms with high quasi-momentum q are selectively removed from the lowest band and subsequently decay to ground

Since then ^{164}Dy
and ^{168}Er have also
been condensed
[36, 37].

Three-body
collisions limit the
stability of the
system.

motional state via collisions with the atoms in the reservoir. Since the excited atoms can only decay by releasing a phonon with the assistance of the Raman process, they collect in the dark state region around $q = 0$ after several cooling cycles.

ATOM TRAPPING WITH MULTIPLE RADIO FREQUENCIES

The dressed atom picture was originally introduced by Claude Cohen-Tannoudji to explain the scattering of optical and radio frequency photons by an atom and later the absorption spectra of atoms in intense laser beams [49, 50]. It became the preferred method of giving a physical picture to explain neutron experiments [51] and cold atoms coupled to microwave fields [52]. Coupling resonant RF radiation to an ensemble of trapped atoms to shape the field-induced adiabatic potential was first proposed by Zobay and Garraway [53]. The concept was extended in [54] by incorporating a slowly varying magnetic field to time average the potential, and was first demonstrated in [29]. Time and again, new conceptual paradigms of trapping have launched the field of ultra cold atoms to new directions. The previous concepts can be naturally extended to using multiple RF fields to further shape the magnetic potential.

In this chapter, we outline the fundamentals of Floquet theory [22] and show how it can be applied as a general method to compute the eigenergies of a periodically driven system. As an example, we demonstrate the creation of N magnetic shell traps using $2N-1$ RF fields.

While writing this chapter a similar work appeared on the arXiv [55].

3.1 SPIN-1/2 COUPLED TO AN RF FIELD

We begin by considering a simple two-level driven system described by the Hamiltonian:

$$H(t) = -\frac{\Delta}{2}\sigma_z - \frac{\epsilon_0}{2}\sigma_x + \Omega \cos(\omega t)\sigma_x \quad (10)$$

where Δ is the detuning from resonance, ϵ_0 an energy offset term and Ω the Rabi frequency of the RF driving field. In the absence of an external bias field ($\epsilon_0 = 0$) the Hamiltonian can be written explicitly as:

$$H(t) = \begin{pmatrix} \Delta/2 & 0 \\ 0 & -\Delta/2 \end{pmatrix} + e^{i\omega t} \begin{pmatrix} 0 & \Omega/2 \\ \Omega/2 & 0 \end{pmatrix} + e^{-i\omega t} \begin{pmatrix} 0 & \Omega/2 \\ \Omega/2 & 0 \end{pmatrix} \quad (11)$$

Using the Hermitian matrix $R(t) = \omega t \sum_j |j\rangle\langle j|$, we form the rotating matrix $U(t) = \exp(-iR(t))$ and use it to transform the Hamiltonian to a frame rotating with angular velocity ω . Assuming near-resonant weak driving, we employ the Rotating Wave Approximation (RWA) and drop the rapidly oscillating off-resonant

terms $e^{-2i\omega t}(\cdot) \rightarrow 0$. The resulting Hamiltonian is now stationary and its eigenvalues are simply:

$$E = \pm \sqrt{\Delta^2 + \Omega^2} \quad (12)$$

demonstrating that the dressed states form an avoided crossing on resonance with an energy gap equal to the Rabi frequency. The [RWA](#) approach offers an intuitive picture of the system but cannot be used for multiple frequencies since there is no single rotation that leads to a stationary frame. Moreover, it ignores the Bloch-Siegert shifts [\[56\]](#) which can be important for shaping the magnetic potential. Instead we can recast the Hamiltonian as a Floquet matrix using Floquet's theorem. Since the Hamiltonian $H(t+T) = H(t)$ is periodic with period T we assume there exist solutions of the form:

$$\Psi_\alpha(t) = \exp(-i\epsilon_\alpha t/\hbar)\Phi_\alpha(t) \quad (13)$$

where the periodicity of the system has been absorbed into the Floquet states $\Phi_\alpha(t) = \Phi_\alpha(t+T)$ and ϵ_α are the quasienergy levels. The modes are constant in time, but only uniquely defined up to multiples of $2\pi/T$. By substituting the expression for the Floquet modes into the Hamiltonian we get a time-independent eigenvalue problem involving an infinite matrix:

$$H_F = \begin{pmatrix} \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \Delta/2 + \hbar\omega & 0 & 0 & \Omega/2 & 0 & 0 \\ 0 & -\Delta/2 + \hbar\omega & \Omega/2 & 0 & 0 & 0 \\ 0 & \Omega/2 & \Delta/2 & 0 & 0 & \Omega/2 \\ \Omega/2 & 0 & 0 & -\Delta/2 & \Omega/2 & 0 \\ 0 & 0 & 0 & \Omega/2 & \Delta/2 - \hbar\omega & 0 \\ 0 & 0 & \Omega/2 & 0 & 0 & -\Delta/2 - \hbar\omega \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix} \quad (14)$$

By examining the block structure of the matrix we immediately see the terms that were dropped in the [RWA](#) couple 2×2 blocks of angular frequency that differ by a single quantum of the oscillating field ($\hbar\omega$). The Hamiltonian in this form is stationary and its eigenvalues can be computed by truncating the determinant. Infinitely many manifolds are created, but in practice we can always chose the one that has the largest overlap with the diabatic states. The number of terms that need to be included before truncating are judged by the convergence of the eigenvalues as the dimensions of the determinant are increased.

*Piecewise models
lead to artificial
discontinuities [\[55\]](#).*

*In close analogy to
band structure
calculations.*

3.2 FLOQUET QUASIENERGY SPECTRUM

Time-dependent Hamiltonians generally require special treatment since the time propagator does not always work out to be a simple phase factor. Methods like expanding the time propagator into a Dyson series, perturbation theory or the adiabatic approximation can be used for a limited range of parameters. In various cases, e.g. for an atom interacting with light, the time dependence can be treated analytically and exact solutions for the transition amplitudes can be calculated [56]. Asymptotic solutions can also be found for some cases as in the Landau-Zener problem [57]. We saw in the previous section that when the interaction term is near resonant and for small coupling strengths the RWA can be employed. This was recently extended to systems with arbitrarily large coupling [58].

When the time-dependence of the Hamiltonian is periodic, a very powerful tool for calculating the eigenenergies is Floquet theory as introduced by Shirley [59]. Floquet developed his theory around the end of the 19th century [60] and it is a substantial branch of the mathematics of dynamical systems, however it is perhaps more familiar to physicists in its incarnation as Bloch's theorem for the wave functions of spatially periodic systems such as lattices in solid state physics. Note however that Bloch extended the principle to all three spatial dimensions whereas only one time dimension is commonly used. The typical way of presenting Floquet theory is through matrices (as in Section 3.1), but given the physical system at hand a propagator method seems more appropriate. Let us assume a time-dependent Schrödinger equation:

$$H(t)\Psi(t) = i\hbar \frac{\partial}{\partial t} \Psi(t) \quad (15)$$

where the Hamiltonian $H(t+T) = H(t)$ is periodic with period T as before. We saw how substituting the modes from Eq. 13 leads to a stationary problem involving infinite determinants. To avoid this we can use an alternative method [61] by considering the propagator of the system:

$$U(T+t, t)\Psi(t) = \Psi(T+t) \quad (16)$$

Inserting the Floquet modes in the above equation we get:

$$U(T+t, t)\Phi_\alpha(t) = \exp(-i\epsilon_\alpha T/\hbar)\Phi_\alpha(t) = \eta_\alpha \Phi_\alpha(t), \quad (17)$$

The Floquet quasienergies $\epsilon_\alpha = -\hbar \arg(\eta_\alpha)/T$ can be directly calculated from the eigenvalues of the propagator. Since any two solutions whose Wronskian is zero will do for initialising the system we choose $U(T, 0) = I$. The Floquet modes for any arbitrary time can also be calculated but we are only interested in the quasi-energy spectrum of the system.

3.2.1 Many-mode Floquet theory

Calculations are performed using the QuTiP [62] and ADM [63] packages.

Floquet theory can be formally extended to multiple driving frequencies [64]. The generalisation is referred to as the Many-Mode Floquet Theory (MMFT). The calculations follow in the spirit of Shirley's original paper, but using a Fourier representation of the driving field. This ultimately leads to an infinite determinant having a different structure than before, with more diagonals, above and below the main one, populated. In contrast, there is no need to explicitly consider individual frequency components when using propagators. The periodicity of the system simply needs to be extended to the least common multiple period of all the driving fields.

The last thing to keep in mind is that Floquet theory and the RWA can be combined when treating a system with multiple driving. Consider the case of just two driving fields. We first rotate the Hamiltonian to a frame oscillating at the mean angular frequency $\bar{\omega}$ and drop the rapidly oscillating terms $e^{-2i\omega_1 t}(\cdot) \rightarrow 0$, $e^{-2i\omega_2 t}(\cdot) \rightarrow 0$ and $e^{-i(\omega_1+\omega_2)t}(\cdot) \rightarrow 0$. Then, we apply Floquet theory to the Hamiltonian which is still time-dependent but the frequencies involved are now much slower. The effective coupling is reduced to $(\Delta - \hbar\bar{\omega})/2$ and the calculation proceeds as before. At the expense of an approximate solution we thus recover the previous intuitive physical picture.

3.3 THE DOUBLE-SHELL TRAP

The Zeeman sublevels in the $F = 1$ manifold of ^{87}Rb can be used as a representation of a spin-1 system when a constant bias field is applied. For small magnetic fields of the order of a few tens of Gauss, the energy spacing of the levels changes linearly with a slope of 0.7 MHz/G. RF radiation can be used to introduce couplings between the states via the interaction $H_{\text{int}} = g_F \mu_B \mathbf{F} \cdot \mathbf{B}$. The Hamiltonian describing the system can be written explicitly:

$$H = \begin{pmatrix} 0.7B'(r) & \Omega_i \cos(\omega_i t) & 0 \\ \Omega_i \cos(\omega_i t) & 0 & \Omega_i \cos(\omega_i t) \\ 0 & \Omega_i \cos(\omega_i t) & -0.7B'(r) \end{pmatrix} \quad (18)$$

where $B'(r)$ can be considered as a bias field for now, $\Omega_i = g_F \mu_B \mathbf{F} \cdot \mathbf{B} / (2\sqrt{2}\hbar)$ are the Rabi frequencies and the index i implies summation over all $2N-1$ RF driving fields. For $N=1$, the Breit-Rabi diagram of the $F = 1$ manifold simply changes to a dressed atom picture where the atomic trajectories follow the adiabatic states which are an admixture of the $|0\rangle$ and $|\pm 1\rangle$ states (see Fig. 10).

In our ^{87}Rb experiment we use a magnetic gradient field $B'(r)$ which translates the energy level diagram above into real space. The RF is resonant at a radius of

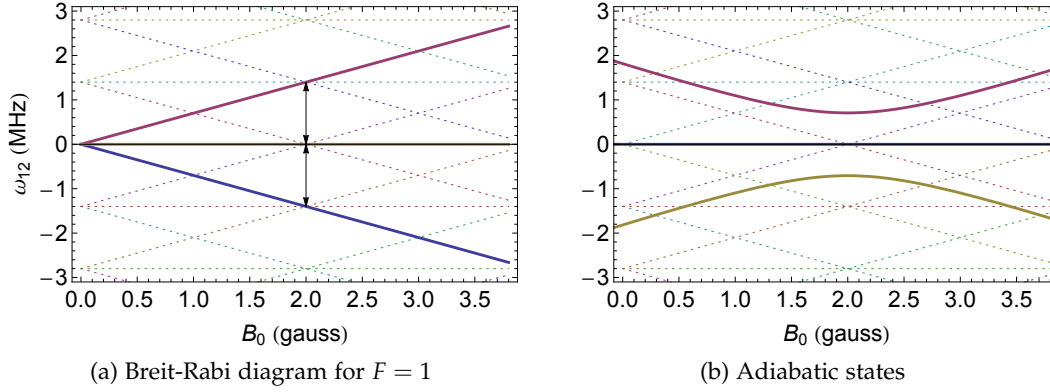


Figure 10: (a) The spacing between the Zeeman sublevels of the $F = 1$ manifold in ^{87}Rb increases by 0.7 MHz/G for small magnetic fields. An RF field with $\omega_1 = 1.4\text{ MHz}$ is applied which couples the states at a bias field of 2 G. (b) The coupling creates an avoided crossing in the diabatic states. The upper mixed state can be used to magnetically trap atoms. The dashed lines are the diabatic states shifted by $n\omega_1$ where $n = \pm 1, \pm 2, \dots$

$r = \hbar\omega_1 / m_F g_F \mu_B B'$ and in a spherical quadrupole field the avoided crossings lie on an ellipsoidal surface where the atoms can be trapped. The exact coupling strength depends not only on the Rabi frequency of the RF but the polarisation as well [29] but we neglect this complication for the rest of this Chapter. The lifetime of atoms trapped at the avoided level crossing is limited by Landau-Zener losses which scale exponentially with the square of the Rabi frequency [65]. Power broadening has also been taken into account, but in any case it is only important when $\Omega \simeq \omega$ which is much larger than the typical Rabi frequencies we can achieve in the lab, i.e. $\Omega \simeq 200\text{ kHz}$ while $\omega = 1.4\text{ MHz}$.

A natural extension of the experiments with the TAAP potentials is using multiple frequencies to generate more interesting trapping geometries. We begin by the simple observation that for $2N-1$ applied RF fields, N shells are created. The physical picture can be elucidated by the following: every applied RF field creates an adiabatic crossing at which the diabatic states bend upwards and downwards. To create a double well trap (two shells) the atoms need to be placed into the diabatic state that is bent upwards by the first and third RF fields while the middle frequency creates a maximum which acts as a barrier. The maximum barrier height is limited by the interfrequency spacing which also dictates the attainable Rabi frequencies.

To achieve a wide interfrequency spacing, RF coils with a wide frequency response (low Q) are required. For this reason, the RF coils were rewound to achieve an optimal balance between the opposing constraints of a strong magnetic field and a sufficiently high self-resonance. More details about the matching procedure can be found in Appendix A. Let us assume the values of the applied RF fields to be 1.4 MHz , 1.8 MHz and 2.2 MHz and their Rabi frequencies about 200 kHz . The

A great introduction to TAAP potentials can be found in [29].

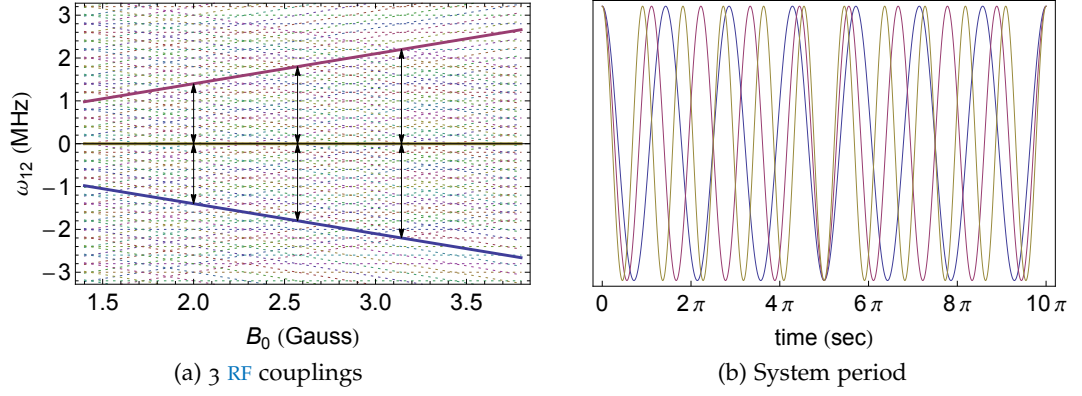


Figure 11: (a) The Zeeman sublevels are coupled with 3 RF frequencies at 1.4 MHz, 1.8 MHz and 2.2 MHz. The values are chosen so that the period of the system does not become too large. This is a computational rather than physical constraint. (b) The period of the system is 10π which corresponds to the least common multiplier of the RF fields.

period of the system is 10π so that 7:9:11 Floquet manifolds are created for every physical RF field (which leads to the dense grid of dotted lines in Fig. 11a). Using Floquet theory as described previously we can calculate the structure of the adiabatic states which is shown in Fig. 12.

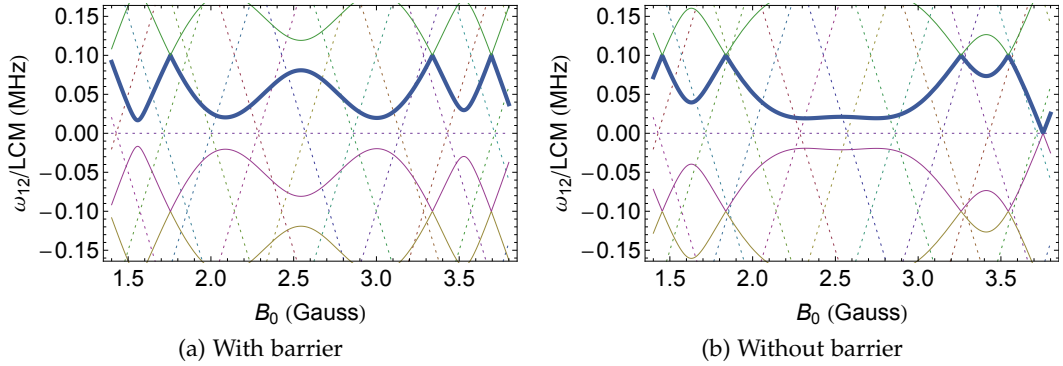


Figure 12: The eigenenergies of a system coupled with 3 resonant fields with (a) and without (b) a barrier at a position corresponding to 2.5 Gauss. The height of the barrier can be controlled by adjusting the Rabi frequency of the middle RF field which can be used to facilitate loading of the atoms or create a double well interferometer.

*Keep in mind that
we are using a
gradient rather than
a bias magnetic field.*

The double shell structure is immediately visible. A shift of the resonances is also noted which is due to the Bloch-Siegert effect [66, 67]. Since the effect depends on the applied frequency $\propto \Omega^2/\omega$, the adiabatic crossings become non-symmetric and their Rabi frequencies differ by about 10%. This is taken into account by adjusting the RF power accordingly. Gravity also needs to be considered for a vertically aligned system like ours, since it tilts the potential curves.

3.4 INTERFEROMETRIC MEASUREMENT OF ROTATION

A long standing goal of our ^{87}Rb experiment is to observe the Fractional Quantum Hall Effect (FQHE) by rotating a cloud of atoms in an optical lattice or in the shell trap. Rotation of a 2D BEC is akin to applying a perpendicular magnetic field as can be seen by starting from the Hamiltonian of a single particle in a 2D harmonic potential:

$$H = \frac{\mathbf{p}^2}{2m} + \frac{1}{2}m\omega^2(x^2 + y^2) \quad (19)$$

Transforming the above to a rotating frame $H_R = H - \boldsymbol{\Omega} \cdot \mathbf{L}$ gives rise to a Coriolis term that can be written explicitly as:

$$H_R = \frac{1}{2m} [(p_x + m\Omega y)^2 + (p_y - m\Omega x)^2] + \frac{1}{2}m(\omega^2 - \Omega^2)(x^2 + y^2) \quad (20)$$

The centrifugal term sets the limit on the rotation frequency which cannot be higher than the trapping frequency since the atoms would otherwise not remain trapped. In the limit $\Omega \rightarrow \omega$ the Hamiltonian is identical to that of a charged particle in a magnetic field. By direct comparison, the rotation-induced magnetic field has magnitude $B = 2m\Omega/e$. For typical experimental parameters, this can be analogous to fields of hundreds of Tesla which is much higher than any real magnetic field created in the lab and will allow us to probe such systems at previously inaccessible regimes.

For high enough rotation frequencies, the vortex lattice is predicted to melt and the more exotic states associated with the Lowest Landau Level (LLL) appear, such as the Laughlin state which is the ground state of the system at filling factor $\nu = 1/2$ [46]. The filling factor ν is defined as the ratio of the number of particles to the number of magnetic flux quanta. Precise balancing of the trap frequency and rotation frequency is needed to reach the Laughlin state and any small residual trap anisotropies will cause the atoms to fly out. This can be partly remedied by time averaging the trapping potential to smooth any imperfections.

Detecting these states once they are formed is as challenging as forming them in the first place. There are various proposals on how this might be possible by simply studying the density distribution from TOF pictures, making a Ramsey-type interference measurement using a sequence of Raman pulses or imaging the shot noise correlations which for the Laughlin state are predicted to be completely anti-correlated [68]. We plan to use the latter method in the ^{87}Rb experiment and a near-resonant lock-in imaging lattice has been integrated in the experiment to hold the atoms still while fluorescent imaging takes place. Nevertheless, an interferometric measurement, although it cannot be used in the FQHE regime, can still be useful in the intermediate stages. We propose a scheme based on the double-shell trap to

*Spatial rather than
temporal
interferometry.*

measure the angular momentum of a rotating cloud by interfering it with a static cloud which serves as a phase reference.

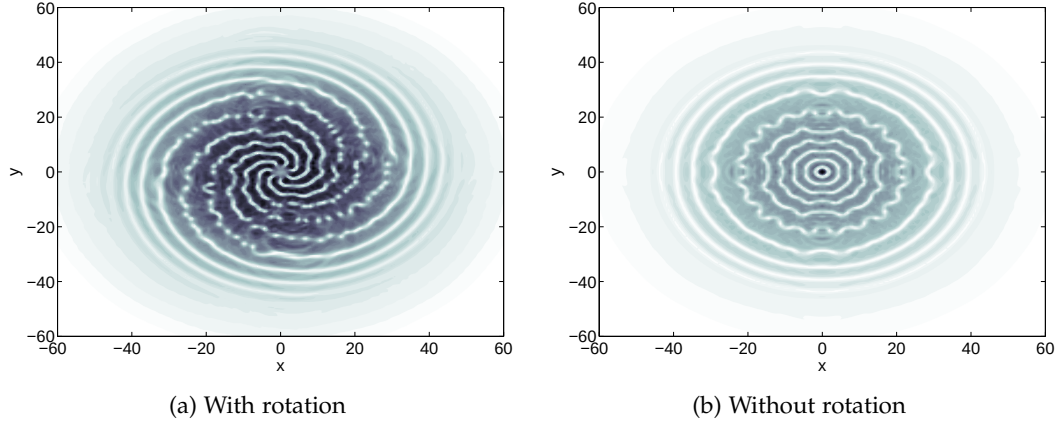


Figure 13: (a) A rotating cloud is made to interfere with a static one which provides the phase reference. A typical interference pattern appears after a few ms TOF from which the rotation speed of the cloud can be extracted, e.g. this cloud has a winding number equal to 7. (b) Similar plot with no rotation induced on the outer ring. The fringe pattern consists of concentric circles as in a Mach-Zehnder interferometer.

For short TOF times a characteristic fringe pattern appears that has azimuthal symmetry (see Fig. 13). It is possible to extract the rotational frequency¹ from such patterns by counting the number of spiral arms [69]. Since these are simply mean-field simulations, they are not expected to be accurate at larger rotational frequencies where the strongly correlated nature of the system becomes important.

The versatility of the multiple-shell trap allows for various experiments to be envisaged, such as double-well interferometers and Sagnac interferometers. The middle frequency can be replaced with a microwave field that couples the two ground hyperfine states. This will create two wells where atoms in the $F = 1, F = 2$ are respectively trapped. Alternately imaging each state can be used to overcome the diffraction resolution limit. Miscibility experiments and the investigation of boundary instabilities are also possible [72].

*All simulations were
done using octBEC,
GPELab [70, 71].*

¹ The code used to produce the graphs and verify our own implementation using octBEC was kindly provided by Steve Eckel.

OPTICAL BLOCH EQUATIONS APPLIED TO MTS

Laser cooling techniques require laser light at precisely controlled frequencies (<1 MHz) relative to the resonance transitions of the atoms or ions. This is commonly achieved using Doppler-free spectroscopy, in particular for alkali metals that have sufficient vapour pressure at room temperature — in our work with ^{41}K and ^{87}Rb the glass cells may be heated to tens of $^{\circ}\text{C}$ above room temperature. Techniques that have been previously used include, e.g. [DAVLL](#) — this is essentially polarisation spectroscopy of the wide Doppler and Zeeman broadened line which gives a very large capture and scanning range. However, the broad line width makes it subject to frequency drifts on the MHz level and when it was implemented on an experiment in Oxford it required an additional Doppler-free saturated absorption setup to check the drifts and periodically reset the offsets in the electronics. This additional part negated the simplicity of the arrangement for [DAVLL](#). [FMS](#) produces dispersion-shaped Doppler-free signals at the relevant transitions in ^{39}K and ^{87}Rb , but the spectrum for these elements is somewhat cluttered because there are several hyperfine levels and isotopes. Also Saturation Absorption Spectroscopy ([SAS](#)) gives rise to crossover resonances at half the frequencies of the transitions between atomic energy levels which adds further complications, with the relative strengths of the various resonances varying with the intensity and polarisation of the laser light. [MTS](#) has a number of characteristics that make it attractive: there is no Doppler background, it has reasonable capture range and a steep slope and an error signal exists only for closed transitions which is advantageous if there are many closely spaced transitions. In this Chapter we show that this last statement is not exactly correct by exploring the [MTS](#) of ^{39}K using the optical Bloch equations.

[MTS](#) is routinely used to generate error signals suitable for the frequency control of lasers (locking) to an atomic line and it involves a typical counter-propagating pump-probe setup where the pump beam is frequency modulated. Building on the well understood theory of [SAS](#) [73, 74], [MTS](#) can be described as a four-wave mixing process in which the main mechanism of transferring the frequency modulation from the pump laser beam to the probe beam through a sufficiently non-linear medium is referred to as modulated hole burning [22]. A thorough model based on the optical Bloch equations is required to capture the exact dependence of the intensity profile (demodulated in-quadrature) depending on the various parameters of the system, e.g. the polarisation state of the pump and probe beams. Originally, we set out to describe this process using Floquet theory but a transformation

Or for systems with observable ground state crossovers in general.

was later found that linearises the system [75, 76, 77]. Other similar systems that have been studied (without linearisation) include phase modulated electromagnetically induced transparency signals [78], frequency modulation in microwave spectroscopy [79], spectra of coherently driven systems [80], coherent pulse trains [81], coherent population trapping [82] and dark resonances [83].

4.1 THEORETICAL DESCRIPTION

Let us consider a typical MTS configuration and the signal that corresponds to the D_2 transition of an alkali atom. The polarisation of the pump and probe beams can be changed between three configurations: $\text{lin} \perp \text{lin}$, $\text{lin} \parallel \text{lin}$ (or any arbitrary angle ϕ) and $\sigma^+ \sigma^-$.

The temporal part of the exciting electric field for the pump and probe beams can be written as:

$$E_{\text{probe}} = \frac{E_p}{2} e^{-i\omega t} + c.c. \quad \text{and} \quad (21)$$

$$\begin{aligned} E_{\text{pump}} &= \frac{E_c}{2} e^{-i(\omega t + \alpha \sin \Omega t)} + c.c. \\ &= \frac{E_c}{2} \left[\sum_{n=0}^{\infty} J_n(\alpha) e^{-i(\omega + n\Omega)t} + \sum_{n=1}^{\infty} (-1)^n J_n(\alpha) e^{-i(\omega - n\Omega)t} \right] + c.c. \\ &\simeq \frac{E_c}{2} \left(J_0(\alpha) e^{-i\omega t} + J_1(\alpha) e^{-i(\omega + \Omega)t} - J_1(\alpha) e^{-i(\omega - \Omega)t} + c.c. \right) \end{aligned} \quad (22)$$

where

- E_p, E_c amplitude of the probe and the carrier of the pump respectively
- Ω modulation frequency
- J_n n^{th} -order Bessel function
- α modulation depth
- ω frequency of the D_2 line in the lab reference frame

The modulation depth is assumed to be $\alpha \ll 1$ so that the second order sidebands are negligible. The Doppler effect needs to be included in the reference frame of an atom moving at velocity v along the propagation axis of the pump beam (opposite to the probe beam).

$$E_{\text{probe}} = \frac{E_p}{2} e^{-i\omega_2 t} + c.c. = E_p e^{-i(\omega_1 + 2kv)t} + c.c. \quad (23)$$

$$E_{\text{pump}} = \frac{E_c}{2} \left(J_0(\alpha) e^{-i\omega_1 t} + J_1(\alpha) e^{-i(\omega_1 + \Omega)t} - J_1(\alpha) e^{-i(\omega_1 - \Omega)t} \right) + c.c. \quad (24)$$

where $k = \omega/c$ is the wave-vector of the beams, $\omega_1 = \omega + kv$ the angular frequency of the probe beam as seen by an atom moving at velocity v and $\omega_2 = \omega - kv$ the angular frequency of the pump beam as seen by an atom moving with the same velocity.

4.1.1 The Liouville equation

The dynamics of the system are encapsulated in the density matrix ρ whose equation of motion can be written as:

$$\dot{\rho} = i[\rho, H_{at} + H_e] + \dot{\rho}_{sp} + \dot{\rho}_{tr} \quad (25)$$

where H_{at} is the static Hamiltonian corresponding to an isolated alkali atom, H_e is the Hamiltonian corresponding to the non-quantised electric field and $\dot{\rho}_{sp}$, $\dot{\rho}_{tr}$ are relaxation terms accounting for spontaneous emission processes and the finite interaction time of an atom with the beam respectively. Written in the basis of its own eigenstates, the atomic Hamiltonian can be expressed as:

$$\begin{aligned} H_{at} = & \sum_{F_g} \sum_{M_g=-F_g}^{F_g} \Delta_{F_g, M_g}^g |F_g, M_g\rangle \langle F_g, M_g| \\ & + \sum_{F_e} \sum_{M_e=-F_e}^{F_e} (\omega_0 + \Delta_{F_e, M_e}^e) |F_e, M_e\rangle \langle F_e, M_e| \end{aligned} \quad (26)$$

where ω_0 is the angular frequency of the D_2 transition, F_g, M_g (F_e, M_e) are the total atomic angular momentum and magnetic quantum numbers for the ground (excited) levels respectively and Δ_{F_g, M_g}^g (Δ_{F_e, M_e}^e) is the frequency separation between the zero-frequency reference of the ground (excited) state and the corresponding ground (excited) hyperfine level. The expression has been rearranged to make the fine structure frequency transitions appear explicitly. Cast in the same basis, the electric field Hamiltonian in the reference frame of the moving atom can be written as:

$$\begin{aligned} H_e = & \sum_{F, F'} \sum_{M, M'} C_{F, M}^{F', M'} G(t) |F, M\rangle \langle F', M'| \quad \text{with} \\ G(t) = & \left(\Omega_c e^{-i\omega_1 t} + \Omega_p e^{-i\omega_2 t} - \Omega_s e^{-i(\omega_2 + \Omega)t} + \Omega_s e^{-i(\omega_2 + \Omega)t} \right) \end{aligned} \quad (27)$$

where Ω_c , Ω_p and Ω_s are the Rabi frequencies of the pump carrier, probe, and sidebands respectively. The transition strength coefficients $C_{F, M}^{F', M'}$ express the normalised transition strength between any two eigenstates; they can be conveniently

calculated using the Wigner-3j and 6j symbols which make the symmetries more obvious (the transition selection rules follow directly from their properties):

$$C_{F,M}^{F',M'} = (-1)^{2F'+I+J+J'+L+S+M+1} \sqrt{(2L'+1)(2J'+1)(2J+1)(2F'+1)(2F+1)} \\ \times \begin{Bmatrix} L & L' & 1 \\ J' & J & S \end{Bmatrix} \begin{Bmatrix} J & J' & 1 \\ F' & F & I \end{Bmatrix} \begin{pmatrix} F' & 1 & F \\ M' & M-M' & -M \end{pmatrix} \quad (28)$$

Finally, the relaxation terms need to be added to complete the Liouville equation. Expressed in the same basis as Eq. 27, the matrix elements of the spontaneous emission term $\dot{\rho}_{sp}$ are:

$$\begin{aligned} \langle F_e, M_e | \dot{\rho}_{sp} | F'_e, M'_e \rangle &= -\Gamma \langle F_e, M_e | \rho | F'_e, M'_e \rangle \\ \langle F_e, M_e | \dot{\rho}_{sp} | F_g, M_g \rangle &= -(\Gamma/2) \langle F_e, M_e | \rho | F_g, M_g \rangle \\ \langle F_g, M_g | \dot{\rho}_{sp} | F'_g, M'_g \rangle &= \Gamma \sum_{F_n} \sum_{q=-1}^1 C_{F_g, M_g}^{F_n, M_g+q} C_{F_g, M'_g}^{F_n, M'_g+q} \langle F_g, M_g | \rho | F'_g, M'_g \rangle \end{aligned} \quad (29)$$

where Γ is the spontaneous decay rate of the excited states. The finite transit time in the atom-light interaction region is taken into account through the term $\dot{\rho}_{tr}$:

$$\begin{aligned} \langle F_i, M_i | \dot{\rho}_{tr} | F_j, M_j \rangle &= -\gamma \langle F_i, M_i | \rho | F_j, M_j \rangle, \quad \forall i \neq j \\ \langle F_g, M_g | \dot{\rho}_{tr} | F_g, M_g \rangle &= \frac{\gamma}{N_{gr}} - \gamma \langle F_g, M_g | \rho | F_g, M_g \rangle \\ \langle F_e, M_e | \dot{\rho}_{tr} | F_e, M_e \rangle &= -\gamma \langle F_e, M_e | \rho | F_e, M_e \rangle \end{aligned} \quad (30)$$

where N_{gr} is the number of ground states and $\gamma = 8v/\pi^2 d_b$ the inverse of the interaction time between the atom and the light, which depends on the beam diameter d_b and the thermal velocity v of the atoms. The Liouville equation can now be written by combining the terms above:

$$\begin{aligned} -i\dot{\rho}_{ij} &= \sum_k \rho_{ik} (H_{at} + H_e)_{kj} - \rho_{kj} (H_{at} + H_e)_{ik} + (\dot{\rho}_{sp})_{ij} + (\dot{\rho}_{tr})_{ij} \\ &= \sum_k \rho_{ik} (H_e)_{kj} - \rho_{kj} (H_e)_{ik} + \rho_{ij} (\omega_j - \omega_i) + (\dot{\rho}_{sp})_{ij} + (\dot{\rho}_{tr})_{ij} \end{aligned} \quad (31)$$

4.1.2 Approximations necessary to solve the equations

The approximations necessary to solve this set of coupled differential equations are well described in an excellent review article by Minogin [84]. First, we intro-

duce slow oscillating variables that lead to the elimination of the rapidly rotating exponential terms in the interaction Hamiltonian.

$$\sigma_{ij} = \begin{cases} \rho_{ij}e^{-i\omega_1 t} & \text{if } i \in \{\text{excited states}\} \text{ and } j \in \{\text{ground states}\} \\ \rho_{ij} & \text{if } i = j \\ \rho_{ij}e^{i\omega_1 t} & \text{if } i \in \{\text{ground states}\} \text{ and } j \in \{\text{excited states}\} \end{cases} \quad (32)$$

For a system with a single frequency dependence this change of variables would be sufficient to reduce the problem to a readily solvable set of equations, however in our case exponential terms oscillating at frequencies $\pm(\omega_1 \pm \omega_2)$ and $\pm(2\omega_1 \pm \Omega)$ remain. The *RWA* is then made, dropping the frequencies $\pm(\omega_1 + \omega_2)$ and $\pm(2\omega_1 \pm \Omega)$ to leave only the slowly varying exponential terms $\pm(\omega_1 - \omega_2)$ and $\pm\Omega$, where $\omega_1 - \omega_2 = -2kv$. The frequency detuning is defined as $\Delta = \omega_1 - \omega_0 - kv = \omega - \omega_0$.

The system is now amenable to numerical methods, however calculations made with this set of equations are very resource demanding and prone to numerical errors due to the stiff nature of the system. To obtain a more reliable and manageable system, the variables σ_{ij} are replaced by new variables with fixed frequency dependence. The correct oscillation frequencies can be determined by considering the non-linear interactions of the two beams and the atomic vapour. The exact transformation depends on the polarisation of the pump and probe beams since the excitation-deexcitation cycle involves different Zeeman sublevels. Assuming both pump and probe are linearly polarised along the same axis and considering interactions involving up to 3 photons, the equations for the populations and the transition frequencies ω^{Zee} between the Zeeman sublevels with $\Delta M = 0$ have 11 distinct frequencies: 0, $\pm\Omega$, $\pm 2\Omega$, $\pm 2kv$, and $\pm(2kv \pm \Omega)$, whereas the optical coherencies ω^{Opt} have 20: 0, $\pm 2kv$, $\pm 2kv \pm \Omega$, $\pm(2kv \pm 2\Omega)$, $4kv$, $4kv \pm 2\Omega$, $\pm\Omega$, $\pm 2\Omega$, and $\pm 3\Omega$. A few examples explaining the choice of the frequencies are shown in Fig. 14.

During crossover transitions between two states whose energies are $\omega_0 + \Delta_i^e$ and $\omega_0 + \Delta_j^e$, atoms moving at velocity $(\Delta_i^e - \Delta_j^e)/2k$ are excited at $\omega + kv = \omega_0 + \Delta_i^e$ by the probe and $\omega + kv = \omega_0 + \Delta_j^e$ by the pump:

$$\begin{cases} \omega_1 = \omega + kv = \omega_0 + \Delta_i^e \\ \omega_2 = \omega - kv = \omega_0 + \Delta_j^e \end{cases} \Rightarrow \begin{cases} \omega = (\Delta_i^e + \Delta_j^e)/2 \\ v = (\Delta_i^e - \Delta_j^e)/2k \end{cases} \quad (33)$$

Different coherences can thus be non-zero and have to be taken into account. A similar process occurs between two ground states $\Delta_{i,j}^e \rightarrow \Delta_{i,j}^g$ as can be seen in the right-hand side of Fig. 14. Once all the frequencies corresponding to each element of the density matrix have been determined, we can make a variable change which imposes those oscillations on the slowly varying variables σ_{ij} . For parallel

The 24 transitions in ^{39}K lead to 576 Liouville equations which can be reduced further by symmetry considerations.

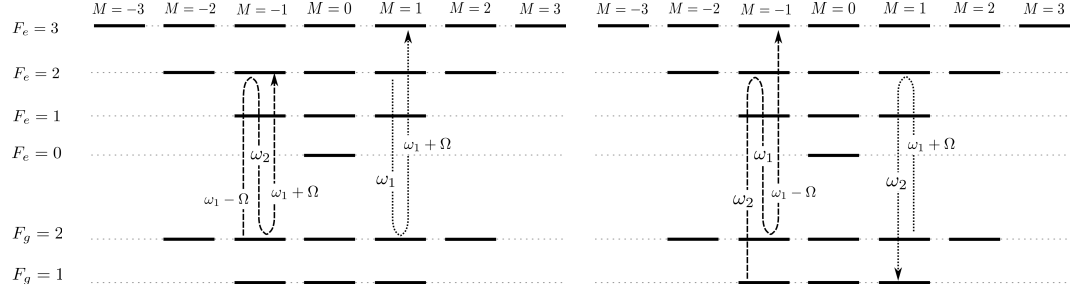


Figure 14: Energy level diagram showing an example of pump-probe interaction which couples a ground and an excited level (optical coherence, dashed line), and two excited states (Zeeman coherence, dotted line). This kind of Zeeman coherence can only be non-zero when the spacing between two excited levels is smaller than the natural linewidth of those levels (in ^{39}K $\Gamma \simeq 6\text{ MHz}$ and $\Delta_3^e - \Delta_0^e \simeq 5.4\text{ MHz}$, so this kind of coherence can be non-vanishing). Different couplings can occur during a crossover between the two ground states.

polarisation only $\Delta M = 0$ transitions are allowed and the variable change takes the following form [76, 75]:

$$\begin{aligned}
 \sigma_{ii} &= q_{1,ii} + (q_{2,ii} + iq_{3,ii})e^{-i\Omega t} + (q_{4,ii} + iq_{5,ii})e^{-2i\Omega t} + \dots \\
 &\quad + (q_{10,ii} + iq_{11,ii})e^{i(2kv+\Omega)t} + c.c. \\
 \sigma_{ij}^{Zee} &= (r_{1,ij} + is_{1,ij}) + (r_{2,ij} + is_{2,ij})e^{-i\Omega t} + \dots \\
 &\quad + (q_{11,ij} + iq_{11,ij})e^{i(2kv+\Omega)t} + c.c. \\
 \sigma_{ij}^{Opt} &= (r_{1,ij} + s_{1,ij}) + (r_{2,ij} + is_{2,ij})e^{-i\Omega t} + (r_{3,ij} + s_{3,ij})e^{i\Omega t} + \dots \\
 &\quad + (r_{20,ij} + is_{20,ij})e^{-2i\Omega t} + c.c. \\
 \sigma_{ji}^{Zee} &= (\sigma_{ij}^{Zee})^* \quad \text{and} \quad \sigma_{ji}^{Opt} = (\sigma_{ij}^{Opt})^*
 \end{aligned} \tag{34}$$

where all the new time-dependent variables $q_{n,ij}$, $r_{n,ij}$ and $s_{n,ij}$ are real. The expressions for the populations and the various coherences contain all the 31 frequencies listed previously. The obtained system is linearised but underdetermined. To obtain a consistent linear system it is necessary to isolate new equations for each new variable by considering only the terms whose exponential dependence corresponds to the oscillation frequency we are interested in. The set of linear equations obtained by this method is much larger than the original one but it can still be solved faster since the time dependence in the exponential terms has been completely removed. A similar process is used to linearise the system for the other polarisation configurations.

The quantum trajectories method could be used as an alternative since the complexity scales with N rather than N^2 , where N is the number of equations.

4.1.3 Velocity averaging of the detected signal

We begin by expressing the classical expression of the induced electric dipole $\langle d \rangle = \langle \Psi | X | \Psi \rangle$ in terms of the eigenstates $\Psi = \sum_n C_n |n\rangle$, where $|n\rangle$ is the n^{th} state of the electronic structure (previously denoted as $|F, M\rangle$). We can rewrite this in terms of the density matrix.

$$\begin{aligned} \langle d \rangle &= \sum_{i,j} \rho_{ij} \langle j | r | i \rangle = d_{eg} \sum_{i,j} C_{ij} \rho_{i,j} \\ &= d_{eg} \sum_{i,j} C_{ij} \left((r_{1,ij} + s_{1,ij}) + (r_{2,ij} + is_{2,ij}) e^{-i\Omega t} + \dots + c.c. \right) \end{aligned} \quad (35)$$

where the dipole element $d_{eg} = d_{i,j} = d_{j,i}$ only couples states that do not belong to the same manifold and is zero otherwise. The sum over i and j involves all the coherence frequencies defined above for parallel polarisations and C_{ij} is a short notation for the transition strength coefficients $C_{F,M}^{F',M'}$ defined in Eq. 28. Since different fields excite different transitions, the modulation depth coefficients a_q must be taken into account (here we assign the subscript q to the modulation depth α so it can be included in the sum — it holds true that $\alpha_0 = 0$ and $\alpha_1 = \alpha_{-1}$). Therefore, in the general case, the electric field arising from the electric dipoles of the atoms induced by the pump beam is given by:

$$E_{dip} = d_{eg} \sum_{q=-1}^1 a_q \sum_{ij} C_{q,ij} \rho_{ij} = d_{eg} \sum_{q=-1}^1 a_q \sum_{ij} C_{q,ij} \left(\sum_{n=1}^{\text{all possible frequencies}} (r_{n,ij} + is_{n,ij}) e^{i\omega_{ij,n}t} \right) \quad (36)$$

where the coefficient $C_{q,ij}$ is the relative transition strength between the state i and j induced by the a_q component of the field, ρ_{ij} is the optical coherence between the states i and j connected by an allowed transition and $\omega_{ij,n}$ is the n^{th} frequency of the coherence labelled by ij . The intensity detected by the photodiode is calculated from the beating of E_{dip} and the probe field E_{probe} expressed as $|E_{dip} + E_{probe}|^2$. To first order in amplitude, the signal observed at the frequency Ω has the form:

$$I_0(\Delta, v, t) \cos(\Omega t) + Q_0(\Delta, v, t) \sin(\Omega t) \quad (37)$$

with the in-phase and quadrature single velocity components:

$$\begin{aligned} I_0(\Delta, v, t) &= \sum_{q=-1}^1 a_q \sum_{i,j} C_{q,ij} (s_{a,ij} + s_{b,ij}) \\ Q_0(\Delta, v, t) &= \sum_{q=-1}^1 a_q \sum_{i,j} C_{q,ij} (r_{a,ij} - r_{b,ij}) \end{aligned} \quad (38)$$

where $r_{a,ij}$ and $r_{b,ij}$ ($s_{a,ij}$ and $s_{b,ij}$) are the real (imaginary) parts of the optical coherences between the levels i and j oscillating at frequencies $2kv - \Omega$ and $2kv + \Omega$ respectively. The system is numerically integrated for a time t_{eq} which is of the order of a few hundred lifetimes in order to make sure equilibrium is reached and then averaged over all velocity classes to obtain:

Convergence is somewhat ill defined for large modulation amplitudes.

$$\begin{aligned} I(\Delta) &= \int_{-\infty}^{+\infty} dv f_{MB}(v) I_0(\Delta, v, t_{eq}) \\ Q(\Delta) &= \int_{-\infty}^{+\infty} dv f_{MB}(v) Q_0(\Delta, v, t_{eq}) \end{aligned} \quad (39)$$

where $f_{MB}(v)$ is the Maxwell-Boltzmann distribution projected along the axis of the beams:

$$f_{MB}(v) = (\sqrt{\pi}u)^{-1} e^{-(v/u)^2} \quad \text{where} \quad u = \left(\frac{2k_B T}{m} \right)^{1/2} \quad (40)$$

In practice the averaging is carried out for a range of thermal velocities distributed over about 3 Doppler widths, i.e. for each of the velocities given by:

$$v_i = \frac{1}{N_v} \sqrt{\frac{k_B T}{m}} \left(3p + \frac{1}{2} \right) \quad (41)$$

where the integer p runs from 1 to N_v and the number of velocities included is about $N_v = 200$. The distribution is offset from zero since stationary atoms do not traverse the nodes and antinodes of the standing wave (for parallel polarisation) producing erroneous results for small velocity classes. Finally, the phase difference ϕ between the probe and the detected signal can be adjusted so that the in-phase or quadrature components can be selected:

$$I(\Delta) \cos(\phi) + Q(\Delta) \sin(\phi) \quad (42)$$

Using a phase-sensitive detection the angle ϕ is adjusted to get the maximum signal with the highest gradient. When $\Omega \leq \Gamma$ the in-phase and quadrature components have very similar characteristics and can be used interchangeably. On the other hand, when $\Omega > \Gamma$ (as in our case) the maximum signal arises from an admixture of both components [85].

4.2 SPECTROSCOPY OF POTASSIUM

Unlike the case of ^{87}Rb which is described in Section 2.1.4, the MTS signal for ^{39}K mainly comes from the ground state crossover transition for the parameters used in our experiment. However, experimental measurements on ^{39}K have been published

by Goldwin's group in Birmingham [86] which show the main signal coming from the cooling transition (as in ^{87}Rb) but their paper makes no attempt to explain this. This discrepancy arises because they chose a $\sigma^+\sigma^-$ polarisation configuration for the pump-probe beams which indeed leads to no MTS signal corresponding to the crossover as we have verified using our model. The ability to arrange for the maximum amplitude of the error signal to correspond to any of these two transitions raises the possibility of locking the laser to either one of them and designing a system for addressing all potassium isotopes with minimal reconfiguration of the optics.

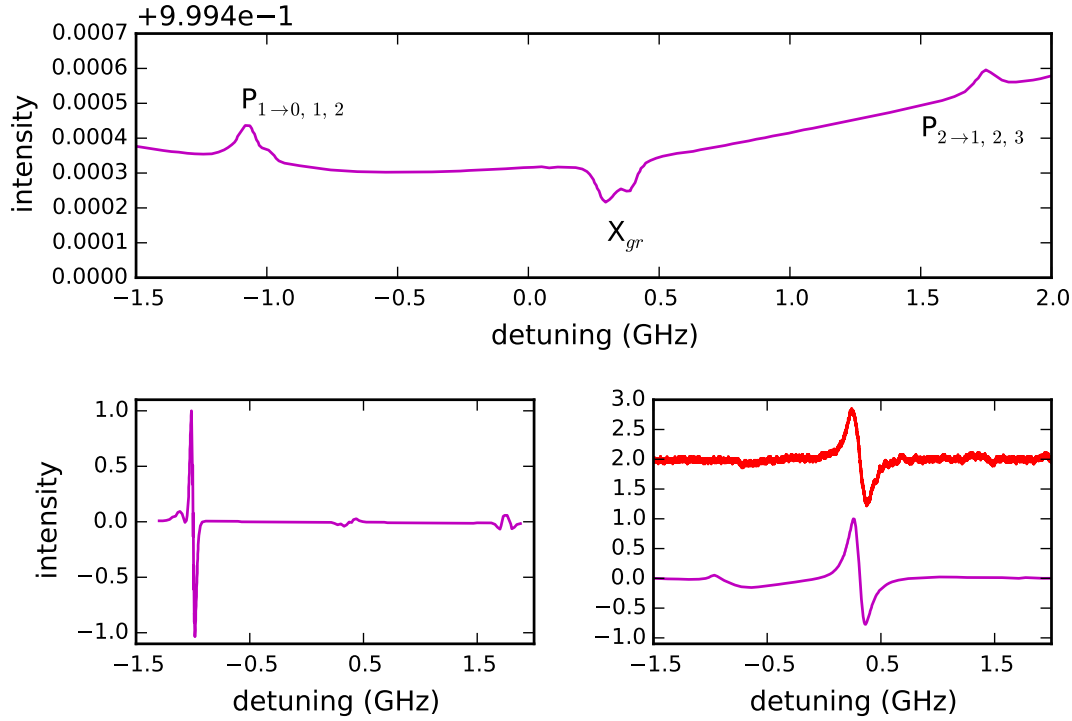


Figure 15: The top panel shows a typical SAS signal for potassium. All isotopes are present in the sample but only ^{39}K is visible since it is the most abundant. The width of the D_2 excited state is only 35 MHz so the allowed transitions cannot be distinguished. The bottom two panels show typical MTS signals for parallel polarisations for $\Omega = 10\text{ MHz}$ and $\Omega_p = \Omega_c = \Omega_s = \Gamma/2$ (left) or $\Omega_p = \Omega_c = \Omega_s = 10\Gamma$ (right). The cooling transition dominates for low powers while the crossover does so for higher ones. All intensities are normalised to unity. Measured data are shown in red.

Our MTS arrangement involves about 10 mW of optical power divided equally between the pump and probe beams which have a waist of 2 mm. The pump is modulated at 10 MHz using an EOM and the spectroscopy cell is heated to 50 °C. The pump beam is also shifted by 100 MHz using an AOM — this does not affect the signal in any way but can be used to change the modulation frequency by adding sidebands to the main driving frequency of the AOM instead of using the EOM. The pump and probe beams are not exactly collinear so that the probe intensity

can be measured on a photodiode without the use of a beam-splitter to pick it up which makes polarisation measurements much more straightforward. Preliminary investigations of the behaviour of the crossover peak show the following trends (see Figures 15 and 16) which agree well with the results from our theoretical approach.

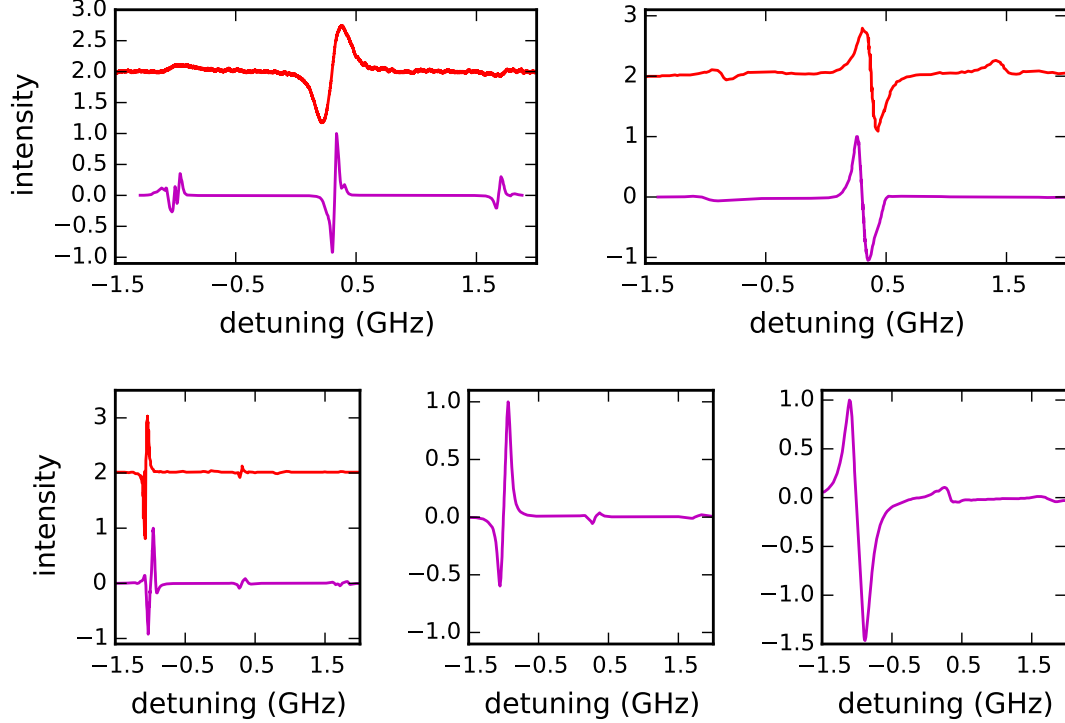


Figure 16: The top two panels show typical MTS signals for perpendicular polarisations. The crossover resonance does not saturate as the beam power varies from $\Omega_p = \Omega_c = \Omega_s = \Gamma/2$ (left) to $\Omega_p = \Omega_c = \Omega_s = 10\Gamma$ (right). The bottom row corresponds to circular polarisation. The crossover resonance completely vanishes at all beam powers ($\Omega_c = 2\Omega_p = 2\Omega_s = n\Gamma$ for $n = 1, 5, 10$ from left to right). All intensities are normalised to unity. The available data in red (from our apparatus and the Birmingham group) show good agreement with the model.

- It increases when more power is used for the MTS and shows no signs of saturation up to 25 mW/cm^2 . No appreciable power broadening is observed even at these intensities and the zero crossing stays fixed.
- It remains virtually constant when changing the temperature from ambient to about 70°C . This is to be expected since the probability of finding an atom in an velocity class that can participate in the crossover transition doesn't increase significantly. The increase observed in the experimental data is purely to the increase in vapour pressure which is not modelled in our approach.
- The optimal modulation depth is about $\alpha = 0.55$ where the height of the carrier and the sidebands is approximately equal.

- An equal pump-probe intensity maximises the peak signal. This is due to the same reasons as the previous point and can be traced back to the four-wave mixing interaction being optimal for electric fields of similar amplitude.

The behaviour of the crossover transition can be explained through a simple model which reveals the main processes that give rise to the [MTS](#) signal. Polarisation effects are not considered in this model.

4.2.1 Toy model

A minimal system that can reproduce the results from the previous section is shown in Fig. 17. The system can be excited in a number of different ways but only two of them correspond to the main signal coming from a crossover transition.

Selection rules allow for every transition between the four levels.

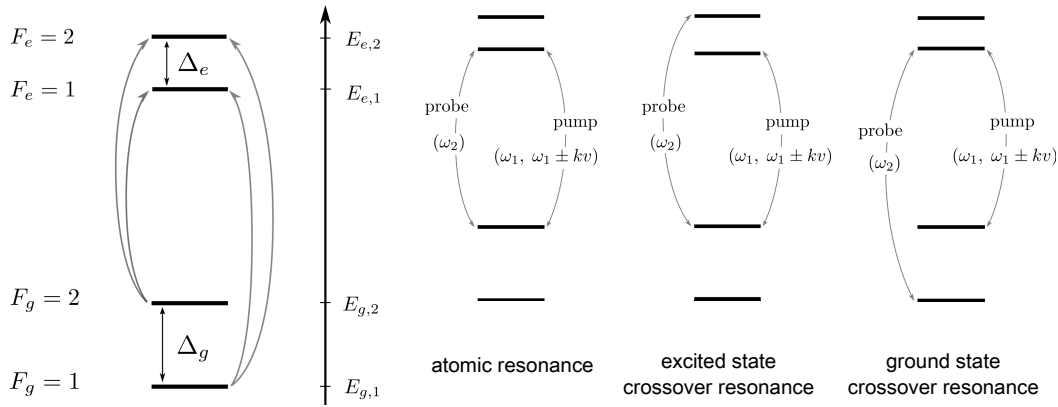


Figure 17: The possible transitions for the toy system are shown on the left. The three cases of interest correspond to real atomic transitions, excited state crossovers and ground state crossovers. The frequencies of the transitions are shown along with the velocity conditions that need to be satisfied for the transitions to be observed.

It is easy to see that a ground state crossover behaves effectively as a closed transition if the thermal energy of the atoms is larger than the ground state spacing, therefore it gives rise to a [MTS](#) signal (whereas an excited state crossover does not). However, the atoms involved in the crossover have a velocity $v_{cr} = (E_{g,1} - E_{g,2})/2k = \Delta_g/2k$, so that if the ground state energies are too far apart, then $f_{MB}(v_{cr})$ is negligible, and the crossover does not have an appreciable amplitude (see Table 1). For example an atomic velocity $v_{cr} = 2500$ m/s is needed for ^{87}Rb , cf. 190 m/s for ^{39}K .

The dependence of the peak height on the ground energy spacing was simulated with the toy system represented in Fig. 17. It was found that, the height of the simulated crossover peak is proportional to the number of atoms that have a large enough velocity to participate in the crossover. This is direct evidence that the thermal distribution of the atomic gas is solely responsible for the observed signal. This was shown by simulating how the peak height depends on varying Δ_g and Δ_e .

	atomic resonance	excited state crossover resonance	ground state crossover resonance
ω	$E_{e,1}$	$(E_{e,1} + E_{e,2})/2$	$E_{e,1} - (E_{g,1} + E_{g,2})/2$
v	0	$(E_{e,1} - E_{e,2})/2k$	$(E_{g,1} - E_{g,2})/2k$

Table 1: The various resonances that appear in the model have the frequencies listed in the first row while the atomic velocity has the values listed in the second row. The ground state crossover resonance will only appear as long as the energy gap of the ground states is narrow enough so that there are enough atoms with the necessary thermal velocity to excite it.

As expected, there is only very weak dependence on the width of the excited state Δ_e while it is linearly proportional to Δ_g .

Alternatively, it is easy to show that the height of the crossover peak for different temperatures is directly proportional to a $f_{MB}(v_{cr}, T)$ distribution. These results suggest that any alkali atom with a ground state hyperfine splitting of the order of 1 GHz will give a strong MTS signal on the ground state crossover.

Part II

IONS AND BIOMOLECULES

Floquet theory and Ordinary Differential Equations (ODEs) with periodic coefficients. A novel multifrequency ion trap and its applications. Normal mode spectrum analysis of sympathetic cooling and MD simulations.

THE THEORY OF PERIODIC EQUATIONS

We consider the stability of systems subjected to periodic parametric driving such that their equations of motion are ODEs with periodic coefficients with an arbitrary number of frequencies in their Fourier spectrum. Such equations are ubiquitous in physics. They describe the temporal behaviour of driven systems or the spatial character of the wavefunction in Hamiltonians of crystalline structures, e.g. atomic Floquet treatment, driven two level atom, Bloch theorem and band structure, mechanical vibrations [59, 87, 88]. In the next few chapters, the relevant concepts will be presented in the context of electrodynamic traps, whereby ions are confined by an oscillating electric field.

5.1 THE PAUL TRAP AND THE MATHIEU EQUATION

Earnshaw's theorem states that charged particles cannot be confined by electrostatic fields only [89]. Wolfgang Paul invented a way to confine ions using an oscillating quadrupole electric field. In the following we consider a linear Paul trap with AC voltage applied to opposite pairs of the four parallel rod-shaped electrodes and the end-caps at a constant DC voltage. The total electric field produced by such an arrangement is:

*Wolfgang Pauli
humorously referred
to him as his "real
part".*

$$\mathbf{E}(x, y, z, t) = -\frac{V(t)}{R_0^2} \begin{pmatrix} x \\ -y \\ 0 \end{pmatrix} + \frac{U_0}{Z_0^2} \begin{pmatrix} x \\ y \\ -2z \end{pmatrix} \quad (43)$$

where U_0 is the amplitude of the DC voltage of the endcaps and R_0, Z_0 the characteristic lengths along the radial and axial directions. For an applied AC voltage $V(t) = V_1 \cos(\omega_1 t)$ the equation of motion for an ion can be written as:

$$\frac{d^2 u_i(t_1)}{dt_1^2} + (a_i - 2q_i \cos(2t_1)) u_i(t_1) = 0 \quad (44)$$

where $i = x, y, z$ and time has been rescaled to $2t_1 = \omega_1 t$. This form is known as the Mathieu equation. Its application to the trapping of ions has been described in papers by Paul himself and other pioneering researchers in ion trapping such as Dehmelt and Wineland [90, 91, 92]. The dimensionless constants a_i and q_i depend

on the ratio of charge Q and mass M of the ion and the amplitudes of the static and oscillating components along the three Cartesian axes respectively.

$$a_x = a_y = -\frac{1}{2}a_z = -\frac{4QU_0}{MZ_0^2\omega_1^2} \quad (45)$$

and similarly for q

$$q_x = -q_y = \frac{2QV_0}{MR_0^2\omega_1^2}, \quad q_z = 0 \quad (46)$$

An approximate solution can be found [93] that has the form

$$u \simeq u_0 \cos At_1 (1 + B \cos 2t_1) \quad (47)$$

with $A, B \ll 1$. Thus, the function $\cos At_1$ corresponds to a much slower oscillation than $\cos 2t_1$ and the amplitude associated with the $\cos 2t_1$ term (micromotion) is very small. These assumptions constitute the *pseudopotential approximation* leading to the solution:

$$u \simeq u_0 \cos \left(\frac{\omega_i t_1}{\sqrt{2}} + \theta_0 \right) \left(1 + \frac{q_i}{2} \cos 2t_1 \right) \quad (48)$$

where θ_0 is an arbitrary phase. Although we assumed that $q \ll 1$ it turns out that this approximation works better than 1% even up to $q = 0.4$. It is evident from the above that the ion's centre of mass undergoes harmonic motion at angular frequency:

$$\omega_i \simeq \frac{\omega_1}{2} \sqrt{a_i + \frac{1}{2}q_i^2} \quad (49)$$

As shown below the ion has stable, bound motion for $q \leq 0.9$ along the $a = 0$ line. Note that in what follows we mainly consider motion and stability along the y -axis and drop the subscript on a_y and q_y but introduce other subscripts for frequency (and later mass as well) to describe the case of two species in a two-frequency trap.

5.1.1 Systems with periodic coefficients: the Hill equation

It is important to distinguish general mathematical properties of ODEs with periodic terms from results specific to the Mathieu equation (coefficient at a single frequency in addition to a constant term). This provides us with a general method that can be applied when the periodic function contains two separate frequencies. We are guided by the physical intuition that when the two frequencies are sufficiently different there should exist conditions for which one of the oscillating terms can be considered as a minor perturbation acting on the system dominated by the other. Linear second order homogeneous ODEs with periodic coefficients can be written in the form

$$\frac{d^2 u}{dt^2} + P(t) \frac{du}{dt} + Q(t)u = 0 \quad (50)$$

with $P(t + T) = P(t)$ and $Q(t + T) = Q(t)$ where T is the period of the system. We will refer to Eq. 50 without the velocity dependent damping term, i.e. $P(t) = 0$, as the Hill equation of which the Mathieu equation is a particular case. Since any function can be expressed in terms of even and odd functions, without loss of generality we choose $Q(-t) = Q(t)$ and rewrite the $Q(t)$ term in the Hill equation as a Fourier series of cosines.

$$\frac{d^2 u}{d\tau^2} + \left(c_0 + 2 \sum_{n=1}^{\infty} c_n \cos(2n\tau) \right) u = 0 \quad (51)$$

This form of the ODE was discussed by Mathieu in 1868 in connection with the problem of vibrations of an elliptic membrane [94, 95], and arises generally in situations with elliptical symmetry. The solutions that are non-singular, with period π or 2π in the variable τ , are the Mathieu functions. They are the elliptic equivalent of the sine and cosine functions that are the angular solutions for systems with circular symmetry. References [96, 97, 98] contain a wealth of applications of Mathieu functions.

The character of the solutions can be established through Floquet theory as we show later. However, for the remainder of this section we outline Hill's series solution method for obtaining an explicit expression for the solutions of the Hill equation. Floquet's theorem states that there is a solution of the form

$$u = e^{\mu\tau} \phi(\tau) \quad (52)$$

The characteristic exponent μ determines the stability of the system which is of key importance for ion trapping. Calculating $\phi(\tau)$ and hence the full solution follows straightforwardly once μ has been found. We assume a typical series solution to the equation, of the form

$$u = e^{\mu\tau} \sum_{n=-\infty}^{\infty} b_n e^{2ni\tau} \quad (53)$$

Substituting in equation 51 gives the system of equations

$$(\mu + 2ni)^2 b_n + \sum_{m=-\infty}^{\infty} c_m b_{n-m} = 0 \quad (54)$$

where $n = 0, \pm 1, \dots$ and $c_n = c_{-n}$. Dividing by $c_0 - 4n^2$ ensures convergence and leads to the usual form of Hill's determinantal equation from which μ can be found from the equation $\Delta(i\mu) = 0$. Whittaker managed to obtain a simple expression for Hill's determinant by mapping it to a function that has the same poles in the complex plane [95]. We sketch Whittaker's solution here, starting by rescaling the equations by $c_0 - (i\mu - 2n)^2$ rather than as before. We denote this form of the determinant $\Delta_1(i\mu)$ and note that it is absolutely convergent. Moreover,

it is an even periodic function of μ with period $2i$ and analytic everywhere except for the obvious poles. We can define a complex function of $\Delta_1(i\mu)$ containing an arbitrary constant K that does not have any poles and hence respects Liouville's theorem. This means that the function has to be constant throughout the analytic plane and by considering its behaviour when $\mu \rightarrow \infty$ we can show that it is equal to unity. We can then easily find the value of K for $\mu = 0$. This leads to:

$$\Delta(i\mu) = \Delta(0) - \frac{\sin^2(\frac{1}{2}\pi i\mu)}{\sin^2(\frac{1}{2}\pi\sqrt{c_0})} \quad (55)$$

The roots of Hill's determinant are therefore roots of the equation

$$\sin^2(\frac{1}{2}\pi i\mu) = \Delta(0) \sin^2(\frac{1}{2}\pi\sqrt{c_0}) \quad (56)$$

Although the determinant is conditionally convergent, calculating infinite determinants is numerically inefficient. Strang has devised a recursion method for calculating the determinant for the single frequency Mathieu equation [99]. The above treatment is not specific to the Hill equation since any periodic term can be recast through its Fourier transform. In any case, in Section 5.2 we present the Floquet formalism which is a more general method for solving ODEs with periodic coefficients.

5.1.2 Spectral methods

We tested various methods of solving the Hill equation and for completeness include here some comments on spectral decomposition methods. The Fourier differentiation method is an alternative to calculating determinants or continuous fractions [100]. As will be shown below, the solutions along the boundaries of the stable regions in the (a, q) plane have a period of π (or 2π). We can use this to search for the pairs (a, q) that give rise to non-trivial bounded solutions with period π (or 2π). Assuming a period of 2π , we define D to be a $N \times N$ Fourier differentiation matrix with elements given by the following formulas. For N even, $k, j = 1, \dots, N$ and $h = 2\pi/N$

$$D_{kj}^{(1)} = \begin{cases} 0 & k = j \\ \frac{1}{2}(-1)^{k-j} \cot \frac{(k-j)h}{2} & k \neq j \end{cases} \quad (57)$$

$$D_{kj}^{(2)} = \begin{cases} -\frac{\pi^2}{3h^2} - \frac{1}{6} & k = j \\ -\frac{1}{2}(-1)^{k-j} \csc^2 \frac{(k-j)h}{2} & k \neq j \end{cases}$$

where $D_{kj}^{(1)}$ and $D_{kj}^{(2)}$ correspond to the first and second derivatives respectively. Using $C = \text{diag}(\cos 2x_k)$ we can approximate Mathieu's equation as

$$(2qC - D)\mathbf{y} = a\mathbf{y} \quad (58)$$

where $\mathbf{y}$ is the vector of approximate eigenfunction values $y(x_k)$. Solutions of period π can be computed by replacing D with $4D$ and modifying C to $C = \text{diag}(\cos x_k)$ which is effectively a change of variables $x \leftrightarrow 2x$. The eigenvalue problem can now be solved and it gives N values of a for each q . Only the values of a nearest to the origin can be assumed to be accurate since they correspond to the least rapidly oscillating eigenfunctions although we have not found this to be a problem in practice, partly because we have been interested in the qualitative forms of the stability regions rather than evaluating (a, q) lines to high precision.

5.2 DIFFERENTIAL EQUATIONS WITH PERIODIC COEFFICIENTS

We have introduced the idea of a particular type of solution using the pseudopotential and Hill's method for determining the stability map of the system. The other key concept is instability produced by parametric resonance. We are mostly concerned with whether a stable solution exists and not its actual form. Thus, we only need to calculate the characteristic exponents of the solutions. We are interested in a general treatment of ODEs with periodic coefficients, such as in Eq 50. Methods for studying the stability of such systems include: Fourier series solutions that lead to determinantal equations (as discussed in Sec. 5.1), perturbation theory, spectral methods (Sec. 5.1.2) [95, 100], Lyapunov methods and integral operators [101]. An analytic solution is possible for a Hill equation where $Q(t)$ has the form of a square wave and $P(t) = 0$ (the Meissner equation). The case where $P(t)$ is constant can also be solved by making a suitable transformation which relates it to the solution of an equation with no first derivative term [102]. This is important for the systems we are interested in since the solutions with damping (friction proportional to velocity) can be found from solutions without damping.

The theory of differential equations involving periodic functions was developed towards the end of the nineteenth century by Floquet [60]. An important extension is Bloch's solution of the Schrödinger equation with a periodic potential [103] including the generalisation of Floquet's theorem to three spatial dimensions. Bloch's theorem for the form of the quantum mechanical wavefunction in a periodic system is a cornerstone of solid-state physics — it is the way to calculate the band structure of electrons in solids, hence determining whether they are metals, semiconductors or insulators. The band gaps can be explained by considering electronic wave functions in crystals as waves which are strongly scattered when their wave-

length λ fulfils the Bragg condition. This viewpoint of wave propagation (or non-propagation) in a periodic structure provides a complementary perspective on the equations.

The conceptual link to the standard material found in quantum mechanical texts may be useful to those with a physics background, however the mathematical theory of Floquet pertains for periodic functions in general (periodic in time or position). We apply the Floquet formalism to the Mathieu equation to study the parametric oscillation in mechanical systems of direct relevance to the motion of particles in a Paul trap. We also consider the Meissner equation which exhibits all the relevant features but allows for analytical calculations (see Sec. 5.4). We focus on the regions of stable behaviour and the calculation of the parameters of the system at the transition to instability. Outside the stable regions dynamical systems can undergo chaotic behaviour that is of considerable mathematical interest and has been observed in ion traps but is not considered here.

To apply the Floquet formalism we recast Eq. 50 as a system of first order equations and calculate the propagation matrix over a single period [104, 105]. Defining $y = \dot{x}$ we get:

$$\frac{d}{dt} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -Q(t) & -P(t) \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = 0 \quad (59)$$

Using two fundamental solutions with initial conditions we form the principal fundamental matrix which is equal to the identity matrix at some point in time ($t = 0$ for convenience).

$$\mathbf{X}_1(0) = (1, 0)^T \quad \text{and} \quad \mathbf{X}_2(0) = (0, 1)^T \quad (60)$$

we can write the propagation matrix as:

$$\mathbf{M} = \begin{pmatrix} x_1(T) & x_2(T) \\ \dot{x}_1(T) & \dot{x}_2(T) \end{pmatrix} \quad (61)$$

which is straightforward to calculate numerically. The characteristic equation

$$\det\{\mathbf{M} - \lambda \mathbf{I}\} = \lambda^2 - \text{tr}\{\mathbf{M}\}\lambda + \det\{\mathbf{M}\} \quad (62)$$

has eigenvalues given by

$$\lambda_{1,2} = \frac{1}{2} \left(\text{tr}\{\mathbf{M}\} \pm (\text{tr}\{\mathbf{M}\}^2 - 4 \det\{\mathbf{M}\})^{1/2} \right) \quad (63)$$

The characteristic numbers of Eq. 50, computed through the Wronskian, can be shown to satisfy:

$$\det\{\mathbf{M}\} = \lambda_1\lambda_2 = \exp\left(\int_0^T -P(\tau)d\tau\right) \quad (64)$$

First we consider the case where there is no damping term ($P(t) = 0$) hence $\det\{\mathbf{M}\} = 1$; this is a general property of symplectic matrices for undamped systems that is directly related to the Liouville theorem and expresses the perservation of phase space for a dynamic system. For an undamped system to be stable the characteristic numbers must be inside the unit circle in the complex plane $\max\{|\lambda_1|, |\lambda_2|\} \leq 1$, or equivalently $|\text{tr}\{\mathbf{M}\}| \leq 2$. The nature of the roots depends on the sign of the discriminant $\text{tr}\{\mathbf{M}\}^2 - 4$, which allows us to consider two types of regions in the parameter space:

1. where $|\text{tr}\{\mathbf{M}\}| > 2$ there are two real eigenvalues. Their product is $\lambda_1\lambda_2 = 1$ hence either $\lambda_1 > 1$ or $\lambda_2 > 1$, giving an unbounded, exponentially diverging solution.
2. where $|\text{tr}\{\mathbf{M}\}| \leq 2$ there are two imaginary eigenvalues, with $|\lambda_1| = |\lambda_2| = 1$ and $\lambda_1 = \lambda_2^*$. These can be written in the form

$$\lambda = \cos\theta \pm i\sin\theta = e^{\pm i\theta} \quad (65)$$

where $2\cos\theta = \text{tr}\{\mathbf{M}\}$. These are stable, bounded solutions.

Along the transition curves at the boundary of the above regions $\text{tr}\{\mathbf{M}\} = \pm 2$ and the discriminant is zero; thus the characteristic equation has a double root and degenerate eigenvalues $\lambda_1 = \lambda_2 = \pm 1$.

The only cases for which $P(t)$ is non-zero which we consider here (as relevant to ion trapping) are those corresponding to physical systems in which the damping of the motion is proportional to the velocity, i.e. $P(t) = 2b$ where $b > 0$ is constant [104]. The stability condition becomes

$$|\text{tr}\{\tilde{\mathbf{M}}\}| \leq 1 + e^{-2bT} \quad (66)$$

where we have written the propagation matrix as $\tilde{\mathbf{M}}$ to differentiate it with the undamped system. At first sight this equation seems counterintuitive since it appears to reduce the limit on the magnitude of $\text{tr}\{\tilde{\mathbf{M}}\}$. However, the stability region is actually enlarged since $\det\{\tilde{\mathbf{M}}\} = e^{-2bT}$ rather than unity as in the undamped case. Therefore the product of the eigenvalues in this case is bounded by a circle of radius e^{-2bT} in the complex plane. The point where one of the eigenvalues exceeds unity is $e^{2bT} + 1$ as can be seen by direct substitution in Eq. 63. The stability condition now becomes $e^{-2bT}|\text{tr}\{\tilde{\mathbf{M}}\}| \leq 1 + e^{2bT}$ which can be rearranged to Eq. 66. To compare the two cases we can assume that λ is the eigenvalue of a matrix of

the same form as for the undamped equations $\mathbf{M}$, but with $\omega^2 \rightarrow \omega^2 - (2b)^2$. This leads to the stability condition $\max\{|\lambda_1|, |\lambda_2|\} \leq e^{2bT}$. The damping term factors out when taking the trace of the propagation matrix, so that $\tilde{\mathbf{M}} = e^{2bT}\mathbf{M}$ and thus the behaviour of a system with damping can be determined straightforwardly from the related undamped system¹.

5.3 PROPERTIES OF THE MATHIEU EQUATION

The characteristic exponents of the system can be calculated numerically using Floquet theory when analytic approaches are not possible. A great deal can be learned about the stability of linear systems of ODEs, simply by examining the trace and the determinant of the coefficient matrix, without having to solve the equations since the discriminant in Eq. 63 fully characterises the system. This provides an insight into some of the ideas of Floquet theory as presented above.

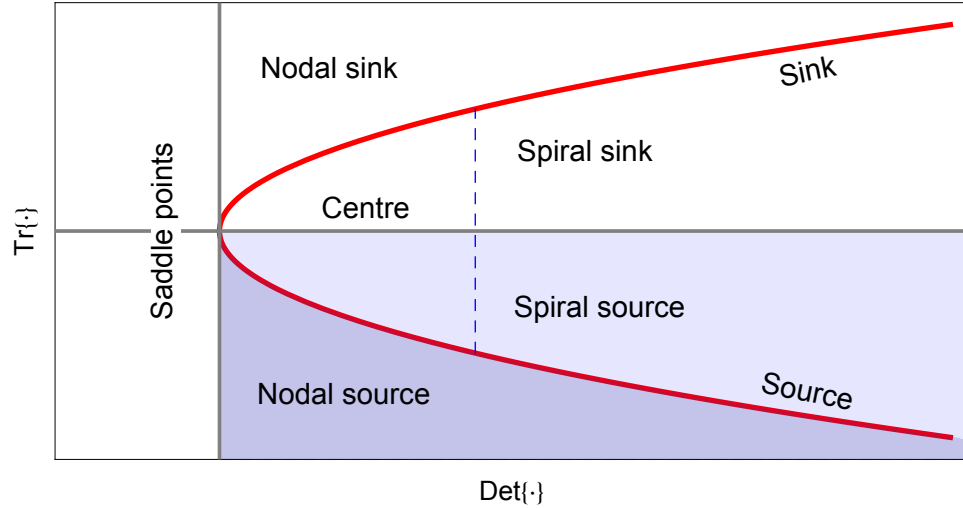


Figure 18: The trace-determinant plane is useful for classifying the nature of the equilibrium points of a linear system. The plane is divided in two regions by the parabola $\text{tr}\{\mathbf{M}\}^2 = 4\det\{\mathbf{M}\}$. On the parabola we have stable focal points (sources) and unstable (sinks). Outside the parabola the system is stable and is either spiralling towards (away from) a sink (source) or rotating around a centre. The equilibrium points of a system that conserves phase-space volume like the Mathieu equation does, lie along the $\det\{\mathbf{M}\} = 1$ dotted line.

The trace-determinant plane can be divided into two regions: where $\text{tr}\{\mathbf{M}\}^2 - 4\det\{\mathbf{M}\} > 0$ there are two distinct real eigenvalues and the system is unstable, and where $\text{tr}\{\mathbf{M}\}^2 - 4\det\{\mathbf{M}\} < 0$ the eigenvalues are complex conjugates. Along the parabola where the equality holds there is a single eigenvalue of multiplicity 2. Further classification of the system is possible by considering the real part of the eigenvalues [106]. When they are both positive the equilibrium points are sources

¹ Note: this is not the same as the system corresponding to $b = 0$.

and when negative they are sinks. The system spirals in or out of these points in phase-space and remains stable as long as $|\text{tr}\{\mathbf{M}\}| < 2$ (see Fig. 18). The stability points of the undamped Mathieu equation lie along the $\det\{\mathbf{M}\} = 1$ line and, if stable, are bounded by the parabola.

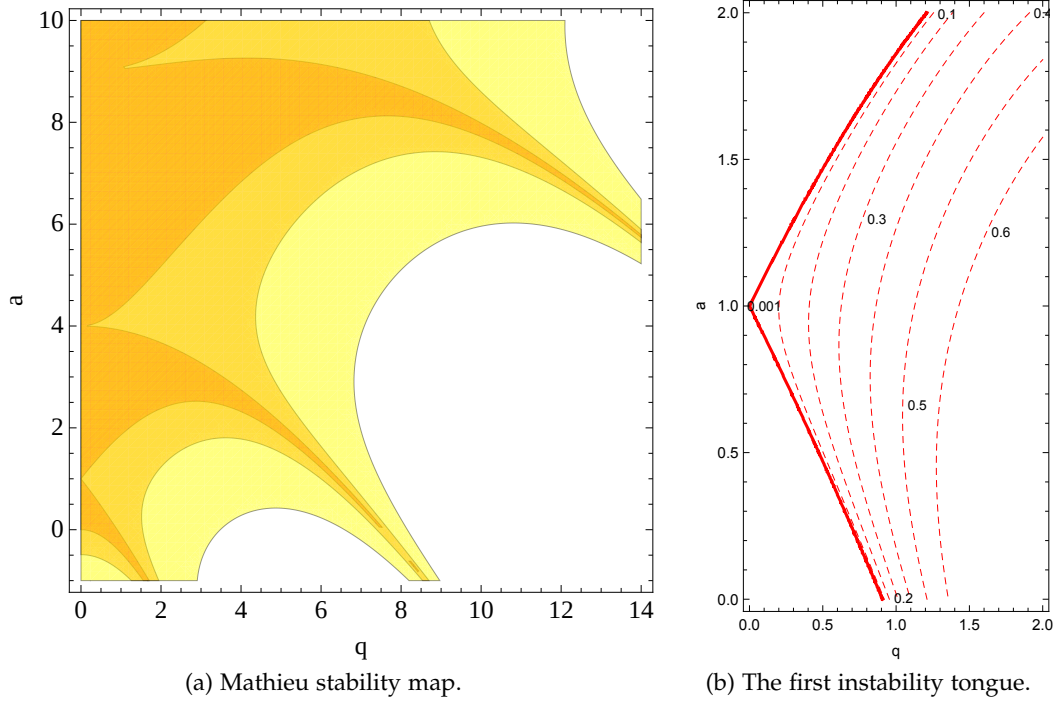


Figure 19: (a) The stability map of the Mathieu equation for different damping values and (b) a close-up of the tongue of instability centred at the first parametric resonance. As can be seen from the two variable expansion the tongues of instability lift off the a -axis even for an arbitrarily small amount of damping.

This classification is helpful for considering the stability diagram for the Mathieu equation. Although the boundaries cannot generally be calculated analytically (except for special cases such as the Meissner equation), they can be mapped out by analytic continuation of the behaviour calculated within the approximation $q \ll 1$. We have found it much simpler to approximate the propagation matrix numerically and calculate the stability region from the condition $|\text{tr}\{\mathbf{M}\}| \leq 2$. Nevertheless, the fundamental solutions to the Mathieu equation can be used for some analytic considerations; these are the Mathieu functions which are well documented in the literature of special functions. There exist two sets of eigenvalues with period π and 2π depending on the initial conditions of the Mathieu functions.

For $q \ll 1$ the eigenvalues can be expanded as a power series of q , and the width of the instability tongues is the difference of the two sets of eigenvalues [107]:

$$\lambda_n(q) - \lambda'_n(q) = \frac{2q^n}{(2^{n-1}(n-1)!)^2} (1 + \mathcal{O}(q^2)) \quad (67)$$

For $q = 0$ we recover the familiar series for the parametric resonances of the Mathieu equation $\lambda_n(0) = \lambda'_n(0) = n^2$ where n is the order of the resonance. The asymptotic behaviour of the resonance close to the $q = 0$ line indicates that an arbitrarily small value of damping is sufficient to suppress them — damping mainly affects higher order resonances (which is also true for subharmonics). The width of the instability tongues can be directly related to the damping necessary to suppress the resonances by approximating the damped Mathieu equation using q as a small parameter. Various techniques can be used, such as the Lindstedt-Poincaré method, two variable expansion, harmonic balance [108], the method of multiple scales, truncation of the determinant, etc. [109]. Let us use the Lindstedt-Poincaré method directly and apply it to the first two resonances. We write the damped Mathieu equation as:

$$\ddot{u} + 2b\dot{u} + \left(a - \sum_{m=1}^{\infty} \epsilon^m f_m(t) \right) u = 0 \quad (68)$$

where $f_m(t)$ is constant at every integration interval and q is of order $\epsilon \ll 1$. After successive approximations we find:

$$\lambda_1, \lambda'_1 = 1 \pm (\epsilon^2 - 4b^2)^{1/2} - \frac{1}{8}\epsilon^2 + \dots \quad (69)$$

$$\lambda_2, \lambda'_2 = 4 + \frac{1}{6}\epsilon^2 \pm (\frac{1}{6}\epsilon^4 - 16b^2)^{1/2} + \dots \quad (70)$$

where we have assumed that $b = \mathcal{O}(\epsilon^2)$ since if it is larger, the motion at the second parametric resonance will be completely stable. It is obvious from the shape of the instability tongues that an arbitrarily small amount of damping is enough to lift the instability from the a -axis — this is in accord with the exponential behaviour of the tongues close to the axis. The same reasoning can be applied to the two frequency case where the parametric resonances are subharmonics but their behaviour is identical.

5.4 AN ANALYTIC SOLUTION: THE MEISSNER EQUATION

The shape of the tongues of instability is of interest since it captures the fundamental behaviour of the system. It can be calculated analytically as an infinite series using the basic algebra of parametric oscillations [110]. In what follows we consolidate the mathematics introduced above in view of a series of examples that illustrate the main characteristics of the system under consideration and facilitate the connection with the two-frequency Paul trap which is introduced in Chapter 6.

The Meissner equation is a special case of a Hill equation where the periodic term is a square wave. It is presented here as an instructive example since it can be solved analytically. A square wave of angular frequency $2\pi/T$, can be related to

the usual notation used in the Mathieu equation by rescaling the time variable so that the period is π

$$\ddot{y} + [a - 2\tilde{q}\operatorname{sgn}(\cos(2t))]y = 0 \quad (71)$$

Here $2\tilde{q}$ is the amplitude of the square wave given by taking the sign (± 1) of the function $\cos(2t)$, cf. $2q\cos(2t)$ in the Mathieu equation.

5.4.1 Propagation matrices for a constant force

To explore the analytic solutions of the Meissner equation we first need to introduce the necessary propagation matrices. Consider a system with a *time-independent* force proportional to displacement:

$$\ddot{y} + c y = 0 \quad (72)$$

$$\ddot{y} = -\omega^2 y \quad (73)$$

This assumes that the constant $c = \omega^2 > 0$ acts as a restoring force. The system undergoes simple harmonic oscillation at angular frequency ω with solutions of the form $y(t) = A \cos \omega t + B \sin \omega t$. The propagation of the system from t to $t + \tau$ can be expressed as a matrix equation

$$\begin{pmatrix} y(t + \tau) \\ \dot{y}(t + \tau) \end{pmatrix} = \begin{pmatrix} \cos \omega \tau & \frac{1}{\omega} \sin \omega \tau \\ -\omega \sin \omega \tau & \cos \omega \tau \end{pmatrix} \begin{pmatrix} y(t) \\ \dot{y}(t) \end{pmatrix} \quad (74)$$

These equations for propagation from $t = 0$ to τ can be put into matrix form in terms of the vector $\mathbf{y}(t) = (y(t), \dot{y}(t))^T$ as

$$\mathbf{y}(\tau) = \mathbf{M}_\omega \mathbf{y}(0) \quad (75)$$

where the propagation matrix is

$$\mathbf{M}_\omega = \begin{pmatrix} \cos \omega \tau & \frac{1}{\omega} \sin \omega \tau \\ -\omega \sin \omega \tau & \cos \omega \tau \end{pmatrix} \quad (76)$$

and $\mathbf{y}(0)$ can be conveniently chosen to be the unit vector. Similarly for the case of $c < 0$, writing $c = -\kappa^2$ gives the propagation matrix

$$\mathbf{M}_\kappa = \begin{pmatrix} \cosh \kappa \tau & \frac{1}{\kappa} \sinh \kappa \tau \\ \kappa \sinh \kappa \tau & \cosh \kappa \tau \end{pmatrix} \quad (77)$$

It is easy to verify that $\det\{\mathbf{M}\} = 1$ for both $\mathbf{M}_\omega$ and $\mathbf{M}_\kappa$ (symplectic matrices). Note also that the limits $\omega \rightarrow 0$, or $\kappa \rightarrow 0$, give the propagation matrix for free flight.

Since $|\text{tr}\{\mathbf{M}_\omega\}| = |2\cos\omega\tau| \leq 2$ the system is always stable, but comes closest to instability when $\cos\omega\tau = \pm 1$. A system with a constant time-independent force is sensitive to perturbations that are periodic with time period $\omega T = n\pi$ with $n \in \mathbb{Z}$, or equivalently such a system is prone to become unstable if $2n\pi/T = 2\omega$. The condition for parametric amplification is that the perturbing angular frequency is twice the frequency of the system. The resonance $n = 2$ occurs at $2\pi/T = \omega$, which is the same as the (only) resonant frequency for directly driven systems.

5.4.2 Alternating periods of oscillation and exponential growth

When $2\tilde{q} \geq |a|$ the oscillatory motion of the system is described by a propagation matrix $\mathbf{M}_\omega$ containing cosine and sine functions, alternating with periods described by the matrix $\mathbf{M}_\kappa$ containing the hyperbolic equivalents. The acceleration has two possible values that in terms of the parameters in Eq. 71 can be written as

$$\begin{aligned}\omega &= \frac{\pi}{T}\sqrt{2\tilde{q}+a} \quad \text{for } t = 0 \text{ to } \tau = T/2 \\ \kappa &= \frac{\pi}{T}\sqrt{2\tilde{q}-a} \quad \text{for } t = \tau \text{ to } 2\tau = T\end{aligned}$$

This turns out to be a realistic model of a pendulum with an oscillating pivot point which captures the key features of equations with periodic terms. Integrating this uniform acceleration twice shows that the position follows a parabolic wave form, closely analogous to a cosine wave [110]. The propagation matrix for the whole time period T is the product of two matrices $\mathbf{M}_\kappa\mathbf{M}_\omega$ representing oscillation from $t = 0$ to τ and exponential behaviour for a period $\tilde{\tau}$ where $\tau + \tilde{\tau} = T$.

$$\mathbf{M} = \begin{pmatrix} \cosh\kappa\tilde{\tau}\cos\omega\tau - \frac{\omega}{\kappa}\sinh\kappa\tilde{\tau}\sin\omega\tau & M_{12} \\ M_{21} & \cosh\kappa\tilde{\tau}\cos\omega\tau + \frac{\kappa}{\omega}\sinh\kappa\tilde{\tau}\sin\omega\tau \end{pmatrix} \quad (78)$$

Hence the condition for stable solutions is

$$|2\cosh\kappa\tilde{\tau}\cos\omega\tau + \left\{\frac{\kappa}{\omega} - \frac{\omega}{\kappa}\right\}\sinh\kappa\tilde{\tau}\sin\omega\tau| \leq 2 \quad (79)$$

Note that $\omega\tau = n\pi$ always lies in an unstable region since $\cosh u > 1$ and $\sin(n\pi) = 0$. The system passes through a region of stability somewhere between each of these points as $\phi = \omega\tau$ varies, thus giving the banded structure of stability regions. Considering $\tilde{\tau} \neq \tau$ (cf. the previous example where $\tau = T/2$) allows an exact correspondence with the Kronig-Penney model of electronic band structure in solid state physics (as discussed in Appendix B) and limiting cases thereof, e.g. the Dirac comb where either $\tau \rightarrow 0$ or $\tilde{\tau} \rightarrow 0$.

For convenience we define new variables $x = 2\tilde{q}$ and for $\tau = T/2$,

$$\begin{aligned}\omega\tau &= \frac{\pi}{2}(x+a)^{1/2} \\ \kappa\tau &= \frac{\pi}{2}(x-a)^{1/2}\end{aligned}$$

The stability condition in the quadrant $a \leq |x|$ can be written as:

$$\left| 2 \cosh\left(\frac{\pi}{2}\sqrt{x-a}\right) \cos\left(\frac{\pi}{2}\sqrt{x+a}\right) - \frac{2a}{\sqrt{x^2-a^2}} \sinh\left(\frac{\pi}{2}\sqrt{x-a}\right) \sin\left(\frac{\pi}{2}\sqrt{x+a}\right) \right| \leq 2 \quad (80)$$

For $a = 0$ (no time-independent term hence $\omega = \kappa$) the equation reduces to

$$|\text{tr}\{\mathbf{M}\}| = \left| 2 \cosh \frac{\pi\sqrt{x}}{2} \cos \frac{\pi\sqrt{x}}{2} \right| \leq 2 \quad (81)$$

The system is unstable where $x = 4n^2$, since $\cosh \alpha > 1$ for all α (e.g. at $\tilde{q} = 2$) and it is stable midway between these points where $x = (2n-1)^2$. The first stability region extends from $x = 0$ to 1.425 (or equivalently $\tilde{q} = 0.7125$). Similar numerical considerations determine how far the stability region extends along the line $a = x$. The line $a = -x$ is unstable since $\omega = 0$ on this line, and there is no restoring force below it. An important feature of this system is that if we are on the brink of instability at the point $(x, y) = (1.425, 0)$ the system becomes unstable for a small positive increment in y although the harmonic trapping is stronger. On the contrary, the system becomes more stable for negative values of y , crossing the transition curve on the other side of the stable region at $(x, a) = (1.425, -0.38)$. This can be understood in terms of parametric resonance since decreasing the overall strength of the trapping reduces the particle's oscillation frequency and so moves it away from the resonance. The values $(1.425, -0.38)$ determine the physical parameters required for a pendulum to be stable upwards (see [110] and various other textbooks).

An approximate form when $\tilde{q} \gg |a|$, or $\epsilon = a/2\tilde{q} = a/x$ is small ($|\epsilon| \ll 1$) can be found in terms of the phase $\varphi = \frac{1}{2}\pi\sqrt{2\tilde{q}}$.

$$\begin{aligned}\omega\tau &= \varphi(1+\epsilon)^{1/2} \\ \kappa\tau &= \varphi(1-\epsilon)^{1/2}\end{aligned}$$

When these quantities are small, $\varphi \ll 1$, we can expand the trigonometric functions so that the stability condition becomes

$$|\text{tr}\{\mathbf{M}\}| \simeq 2 \times \left| 1 - 2\varphi^2(\epsilon + \frac{1}{12}\varphi^2) \right| \leq 2 \quad (82)$$

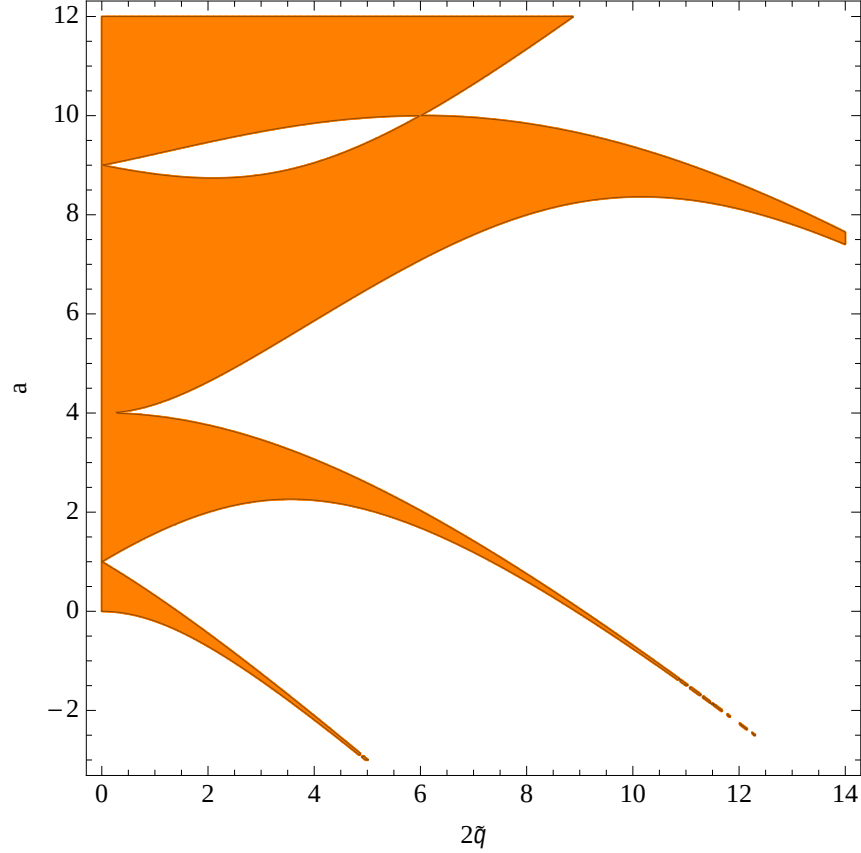


Figure 20: The region of stability (orange) for the Meissner equation. In the segment $0 < 2\tilde{q} \leq a$, the first resonance is at $(0,1)$, and the lower edge of the tongue of instability follows the curve $a = 1 - (2/\pi)\tilde{q}$, for small $\tilde{q}$. In the segment $\tilde{q} < |a|$ (region between the two lines $2\tilde{q} = \pm a$), the lower edge of the tongue of instability emanating from the first resonance passes through $(0.3, 0.6)$ and crosses the axis at $(0.7, 0)$. The lower boundary of the first stability region curves downwards from the origin following Eq. 83 for small $\tilde{q}$ and passing through $(0.7, -0.38)$.

hence $\epsilon \geq -\frac{1}{12}\phi^2$. Thus, the system is stable for small negative values of a which would be unstable for $\tilde{q} = 0$. In terms of the unscaled parameters

$$a \geq -\frac{\pi^2}{12}\tilde{q}^2 \quad (83)$$

Thus the condition $2\tilde{q} \geq |a|$ is very well fulfilled within the range of this approximate treatment. The results of this stability analysis can be summarised on a plot (Fig. 20) over the $(\tilde{q}, a)$ -plane where by symmetry only the half plane $\tilde{q} > 0$ need be considered.

The Meissner and Mathieu equations have many features in common. The general shape of their regions of stability nearest $(0,0)$ are similar which is intuitively reasonable when considering the Fourier components of a square wave, since the fundamental frequency has most influence in the stability region. Higher frequency

components of the spectrum affect the shape of instability tongues only far from the region of operation we consider. This gives strong indication that the presence of a higher frequency term in the two-frequency Paul trap does not change the nature of the lower stability region.

The parametric resonances occur at the same values for both equations since they are only determined by the periodicity. The shape of the tongues of instability for the Meissner equation for $\tilde{q} \ll 1$ are given approximately by [111]

$$\begin{aligned} \text{Case I } (n \text{ odd}) : \quad a &= n^2 \pm \frac{2}{n\pi} \tilde{q} \\ \text{Case II } (n \text{ even}) : \quad a &= n^2 \pm \frac{4}{n^2} \tilde{q}^2 \end{aligned}$$

The differences between odd and even terms arises from the different amplitudes in the Fourier series of a square wave. The width of the tongues falls off more slowly than for the Mathieu equation containing a pure cosine-wave without harmonics (width of tongues falls off as q^n). Note the resonance tongue emanating from $a = 9$ ($n = 3$) has a different shape for the Meissner equation because a square wave has a Fourier component at three times the fundamental frequency (odd terms only). The insight that can be gained about the Hill equation with two frequencies is that higher harmonics change the shape of the stability region but key features arising from parametric resonance occur whatever the form of the periodic function. Other examples for which analytic expressions for the stability conditions can be found using the matrix method include: square waves which are not symmetric, triangular and trapezoidal waveforms, and combs of Dirac δ -functions that are positive, negative, or of alternating sign [106].

THE TWO-FREQUENCY PAUL TRAP

The Paul trap, invented by Wolfgang Paul, confines ions with an oscillating electric quadrupole field [112] and has many diverse applications. The development of laser cooling techniques has had an important impact on the use of ion traps and their use as frequency standards and in quantum computing. Even charged particles without suitable optical transitions can be cooled sympathetically by exchanging energy with atomic ions amenable to laser cooling techniques. The mechanism of the Paul trap depends sensitively on the charge-to-mass ratio and this intrinsic feature of Paul traps is exploited for mass spectrometry [113]. However, this implies that when species with markedly different ratios are held in a Paul trap the more weakly confined species is pushed away from the centre due to Coulomb repulsion from the strongly trapped ion(s), resulting in phase separation of the clouds [114].

We describe a method of operating a Paul trap, with two RF driving fields, in which two species of ions experience harmonic pseudopotentials with similar spring constants even though they have *extremely different* charge-to-mass ratios. Before we present a numerical example, we describe the stability of a Hill equation with two driving terms.

6.1 STABILITY OF THE TWO-FREQUENCY TRAP

A first insight into the behaviour of the two-frequency Hill equation can be gained from looking at the Mathieu equation in the high- aq regime. To this end we introduce the concept of the critical line which separates the stability diagram in two regions with equal stable/unstable density of characteristic exponents. For the undamped Mathieu equation the critical line is simply $a = 2q$ [111, 115]. Other critical lines can be formulated when damping is included. Using the notion of kinematic similarity, the solutions of the damped Mathieu equation can be shown to be asymptotically stable when $2q < (a - b^2) \tanh \pi b$ — another estimate is given as $q - b^2 < \sqrt{ab}$ [116]. Since the usual point of operation of the Paul trap is close to the vertical axis it suffices to simply assume that all the points below the critical line are stable. The universal characteristics of the high- aq regime map directly onto the subharmonics picture.

The mathematical properties of the Mathieu equation in this regime are well studied although previously not considered relevant to ion trapping (as far as we are aware). As shown in Fig. 21 there is a critical line that runs through the centre

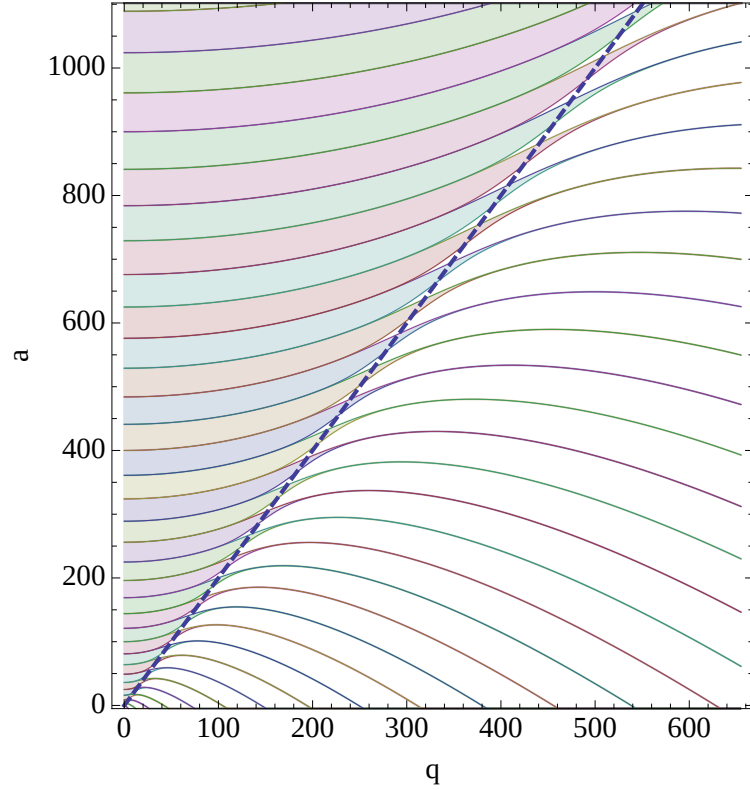


Figure 21: The dotted line $a = 2q$ is the critical line that traverses stable and unstable regions of equal density. This critical line effectively divides the map into stable (shaded) and unstable (white) regions since the width of the tongues of instability decreases exponentially for the higher harmonics

of the cusps that make up the boundary between stable and unstable regions. The widths of stable (unstable) regions decrease exponentially above (below) this line. We have observed this exponential decrease of the tongues of instabilities in our numerical simulations however we only need to reproduce their general characteristics since they will be washed away by any arbitrarily small amount of damping — in any case the assumption that experimental signals are pure cosine waves with no harmonics at the level 60 dBm is unrealistic.

Let us now define a two-frequency Hill equation:

$$\frac{d^2 y}{dt^2} + [a - 2q_1 \cos(2t) - 2q_2 \cos(2nt)] y = 0 \quad (84)$$

where n is the ratio of the two driving frequencies. A simple picture of the physical system can be formulated immediately by thinking of the $\cos(2t)$ term as inducing $n - 1$ subharmonic parametric resonances in the first stability region of a Paul trap. This, in effect, reduces the points on the diagram where the trap can be stably operated. As can be seen in Fig. 22 the width of the resonances becomes very small for large values of n . The full stability diagram has of course 3 dimensions but it is easier to just deal with a 2-dimensional projection at a time. To get a better sense

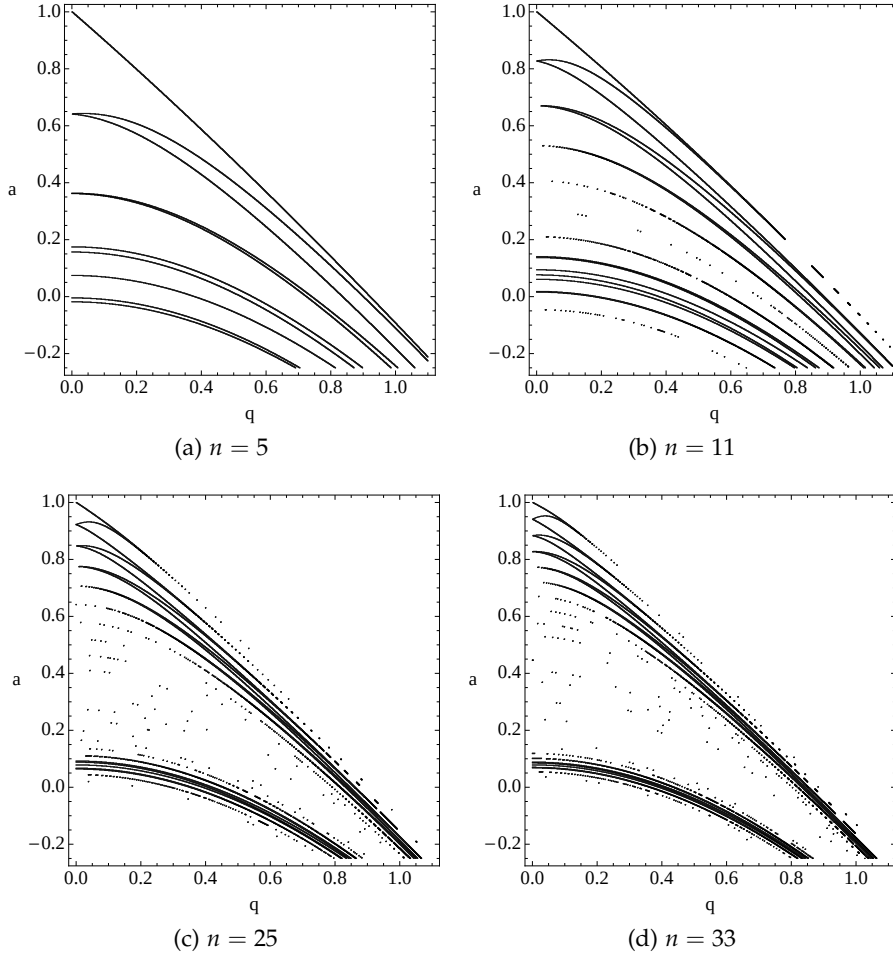


Figure 22: The first region of stability of a Paul trap with subharmonic resonances for various values of $n = 5, 11, 25, 33$ with $q = q_2$ and $q_1 = 0.04$. In every graph there are $n - 1$ resonances whose width decreases exponentially for increasing n . For a 3D trap we have to consider the stability diagrams for the other axes as well which would be identical but for a scaling and/or a reflection about the $a = 0$ axis.

of how the amplitude of the low frequency affects the stability of the system we consider the $q_1 q_2$ stability map for $a = 0$ (see Fig. 23).

We can now introduce two different regimes of operation of the trap; for small and large values of n respectively with a somewhat arbitrary transition value of $n \simeq 10$. The stability of the system in any of the two regimes is straightforward to calculate using Floquet theory by rescaling the propagation matrix to the appropriate, longer period each time. In terms of propagation matrices $\mathbf{M}^n$ has the same stability region as $\mathbf{M}$ using rescaled parameters since the frequency scaling is only different by a factor n^2 .

When $n \leq 10$ the subharmonic resonances are well defined and a stable configuration for the system can be found simply by avoiding them. Damping is less critical in this regime since the width of the resonances is rather large and in any

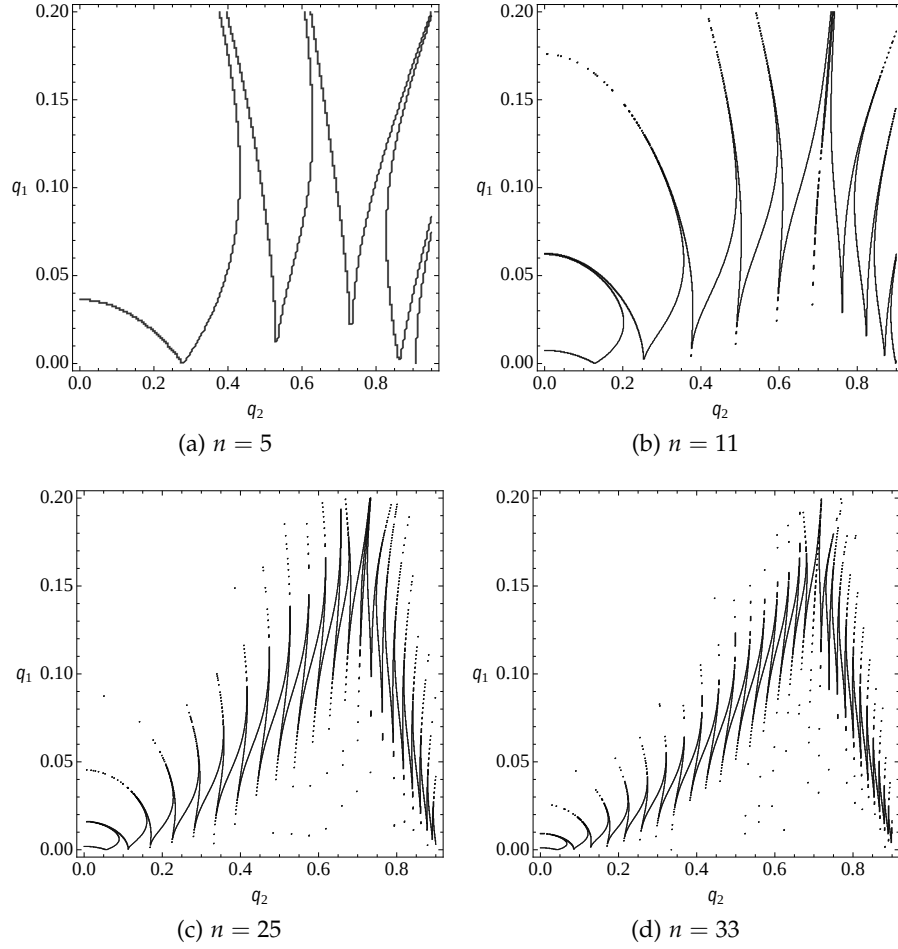


Figure 23: The region of stability as a function of the parameters q_2 and q_1 for various values of $n = \omega_2/\omega_1$: $n = 5, 11, 25, 33$. The stable region extends over the range $0 < q_2 < 0.9$ along the horizontal axis and up towards the jagged lines. In every graph there are $n - 1$ resonances whose width decreases exponentially for increasing n .

case, many stable points exist on the aq -map. For higher values of n we enter a universal regime where the density of the instability tongues in the otherwise stable region becomes so great that it is hard to avoid them. The universality of the behaviour in this regime arises because the width of most of the harmonics is exponentially small and thus any amount of damping will suppress them. We then only need to consider the position of the critical line to decide if the system is stable or not.

6.1.1 Amplitude modulation

A third frequency can be used to alter the curvature of the instability tongues and in effect the oscillation frequencies of the ions. For the most part, when away from

the resonance the oscillation frequency of the ions is given by $\omega_{ps} = \sqrt{\omega_{ps,1}^2 + \omega_{ps,2}^2}$ where $\omega_{ps,1}$ and $\omega_{ps,2}$ are the pseudopotential frequencies that arise from the respective RF driving fields. This formula breaks down when close to a parametric resonance; it is this breakdown that provides a mechanism for the oscillation frequencies and the spring constants to be adjusted.

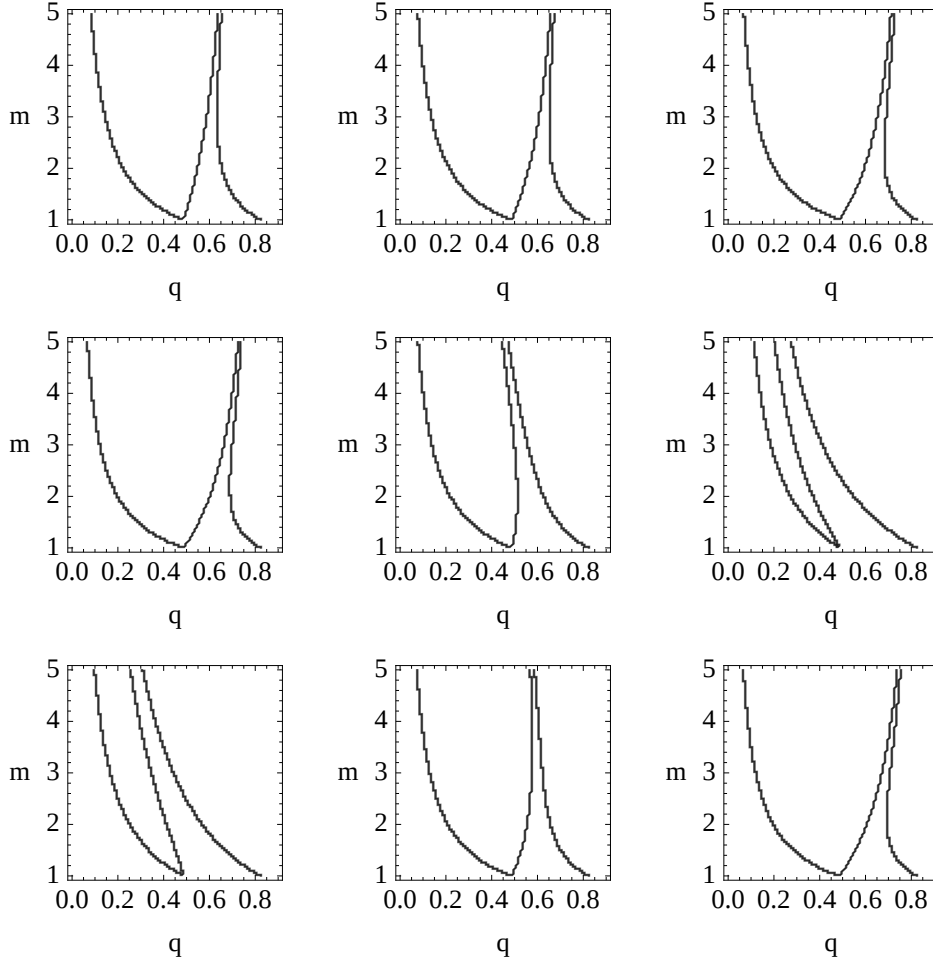


Figure 24: Change of the position of the single tongue of instability with respect to the relative phase of the amplitude modulation in Eq. 85. The relative phase θ is shifted between 0 and $3\pi/4$ in steps of $\pi/12$ from the upper left to the bottom right graph.

Fine tuning of the instability tongues can be achieved via a third frequency added in the system whose value is equal to the sum of the other two. In this way, the position of the resonances remains the same but their curvature changes depending on the relative phase. As a proof of principle of the feasibility of this scheme, Fig. 24 shows what happens to the simple Mathieu equation when the cosine term is modulated with a square wave.

$$\frac{d^2 y}{dt^2} + \left[a - \text{sgn} \left[m \sin \left(\frac{t - \theta}{2\pi} \right) \right] 2q \cos(2t) \right] y = 0 \quad (85)$$

Modulating the amplitude does not offer full freedom of choosing the phase of the the third frequency but it is nevertheless adequate for tuning the instability tongues. It is also worth noting that the system is rather robust in terms of amplitude noise since a square wave of comparable amplitude to the cosine term is required for any appreciable change of the instability tongues. This option of altering the stability characteristics of the system through amplitude modulation is not explored further, however it could readily be used in experiments to fine-tune the oscillation frequencies of the different species without changing the position of the parametric resonance induced by the subharmonics. The design of the impedance match (or resonator) can thus be fixed without limiting the tunability.

6.2 SYMPATHETIC COOLING

Sympathetic cooling of one atomic species via another has been successfully used in ion traps [92, 117] and has allowed for cooling of various species that do not have favourable atomic transitions. Additionally, quantum gate operations can be performed on one species while it is sympathetically cooled by another even if cyclic transitions exist. This approach eliminates light shifts and spontaneous scattering events which reduce the coherence of the operations. In neutral atoms it was first demonstrated in [118] and is still employed in a number of two species experiments.

6.2.1 Ions with extremely different charge-to-mass ratios

As an example, we describe the theory of two-frequency operation of an ion trap and solve the equations of motion for two species of ions with molecular mass $M_A = 138$ amu (an isotope of barium) and $M_B = 1.4 \times 10^6$ amu, e.g., a large protein or molecular complex, with charge states $+1$ and $+33$ respectively. The quadrupole electric field is created by RF radiation with angular frequencies ω_1 and ω_2 (with $\omega_2 = 100\omega_1$). Due to the very different charge-to-mass ratios, the heavy ions (molecular mass M_B) are confined most strongly by the RF field at the lower frequency ω_1 , while trapping of ions of atomic mass M_A arises from the field at ω_2 . Thus we form two almost independent Paul traps whose centres can be made coincident or moved apart. Importantly the effective spring constants can be adjusted to be the same for both species so that all the ions interact strongly. This allows efficient sympathetic cooling of the heavy ions by laser-cooled atomic ions as we demonstrate by numerical simulations for one particular example. This approach can be extended to charged particles with even more dissimilar masses.

Both species are confined tightly near the trapping centre(s) and strongly interact with each other. Atomic ions scatter laser light so that individual fluorescing ions

can be observed, thus permitting indirect detection of dark ions as “holes” in the cloud. The laser radiation can also reduce the temperature of the barium ions which in turn sympathetically cool the heavy ion. An experiment with molecular ions of mass 410 amu and barium in a single frequency trap was carried out in Schiller’s group [119] together with numerical simulations. In that work, with a linear Paul trap operating with a single RF, the more weakly trapped heavy ions migrated to the outside of the cloud of trapped ions and formed a sheath (cylindrical shell) around the $^{138}\text{Ba}^+$. More recently it has been suggested that a chain of atomic and molecular ions can act as a conveyor belt to carry the dark molecular ions into the focus of an x-ray laser (for destructive measurements) [120]. That proposal was demonstrated by experiments using Mg^+ and MgH^+ which have similar charge-to-mass ratios. Our scheme opens the way to working with much heavier ions such as those formed from biomolecules that are of great current interest for single-shot x-ray diffraction experiments. The current state of the art in mass spectrometry includes techniques for putting large biomolecules, and molecular complexes, of molecular weight of a few megadaltons (millions of amu) into vacuum, without fragmentation and surprisingly little change to their structure [121]. Paul trapping of large biomolecular ions has also been discussed for DNA (a long chain molecule), but in an aqueous solution [122] rather than the usual vacuum environment.

In our case the ions experience an AC quadrupole electric field created by RF radiation with angular frequencies ω_1 and ω_2 (with $\omega_1 \ll \omega_2$), plus a static quadrupole field. We assume familiarity with the standard theory of the Paul trapping based on the Mathieu equation [112, 91, 123]. The Newtonian equations of motion for ions in a quadrupole field generated by a voltage $V(t) = V_0 + V_1 \cos \omega_1 t + V_2 \cos \omega_2 t$ on the electrodes, with $\omega_2 = n\omega_1$ where n is an integer, can be put into the form of a Hill equation:

$$\frac{d^2 y}{dt_1^2} + \left[a_\alpha^{(1)} - 2q_{1,\alpha}^{(1)} \cos(2t_1) - 2q_{2,\alpha}^{(1)} \cos(2nt_1) \right] y = 0 \quad (86)$$

Time in Eq. 86 has been rescaled so that $\omega_1 t = 2t_1$, hence $a_\alpha^{(1)} = 4\zeta_\alpha V_0/r_0^2$, $q_{1,\alpha}^{(1)} = 2\zeta_\alpha V_1/r_0^2$ and $q_{2,\alpha}^{(1)} = 2\zeta_\alpha V_2/r_0^2$ where $\zeta_A = e/M_A\omega_1^2$ for species A and $\zeta_B = Ze/M_B\omega_1^2$ for B. The distance r_0 characterises the curvature of the potential for a given voltage and is approximately equal to the distance of the electrodes from the centre of the quadrupole field. We use this standard form of the Hill equation for the B-ions but for species A the connection with the standard theory of the Paul trap is more obvious if we rescale time such that $\omega_2 t = 2t_2$ (purely for the purpose of qualitative explanation rather than computation).

$$\frac{d^2 y}{dt_2^2} + 2b_A \frac{dy}{dt_2} + \left(a_A^{(2)} - 2q_{1,A}^{(2)} \cos\left(\frac{2t_2}{n}\right) - 2q_{2,A}^{(2)} \cos(2t_2) \right) y = 0 \quad (87)$$

M_B, ω_1	$a_B^{(1)}$	$q_{1,B}^{(1)}$	$q_{2,B}^{(1)}$
	-0.0003	0.307	10.758
M_A, ω_2	$a_A^{(2)}$	$q_{1,A}^{(2)}$	$q_{2,A}^{(2)}$
	-1.03×10^{-5}	0.009	0.318
M_A, ω_1	$a_A^{(1)}$	$q_{1,A}^{(1)}$	$q_{2,A}^{(1)}$
	-0.107	94.5	3307.4
M_B, ω_2	$a_B^{(2)}$	$q_{1,B}^{(2)}$	$q_{2,B}^{(2)}$
	-3.35×10^{-8}	2.952×10^{-5}	0.001

Table 2: There are four sets of coefficients in the two Hill equations that describe the two frequency system. The numerical values of the parameters are $\omega_1 = 2\pi \times 100$ kHz, $\omega_2 = 2\pi \times 10$ MHz, $M_A = 138$ amu and $M_B = 1.4 \times 10^6$ amu. Notice how both species effectively experience a Paul trap with $q \simeq 0.3$. The headers simply denote the pre-factors of the DC, AC driving terms since the scaling is clear from the first column of the table.

where the coefficients are scaled to ω_2 so that $a_A^{(2)} = a_A/n^2$ and $q_{i,A}^{(2)} = q_{i,A}^{(1)}/n^2$, e.g., $q_{2,A}^{(2)} = 2eV_2/(M_A\omega_2^2r_0^2)$. The damping parameter $b_A = (\omega_2\tau)^{-1}$ where τ is the velocity damping time constant (of underdamped oscillations) accounts for the laser cooling of species A (only). We seek conditions for which ions of molecular mass M_B are confined mainly by the field at ω_1 , and species A is confined by the field at ω_2 , i.e., the term proportional to $q_{1,B}^{(1)}$ dominates in Eq. 86 and $q_{2,A}^{(2)}$ dominates in Eq. 87. The secular motion of the ions resembles that of a particle in a harmonic pseudopotential with spring constant κ . This is not valid when the secular frequency $\sqrt{\kappa/M}$ is comparable with the driving frequency although there are stable solutions of the Mathieu equation for $q \leq 0.9$ when $a = 0$. We use the value $q \simeq 0.3$ since this gives robust operation of a Paul trap. A simplistic way to understand the behaviour governed by the Mathieu equation is to assume that the pseudopotential acts independently of the time-independent potential given by the parameter a . Stable solutions exist for $a < 0$ when $q \neq 0$ if trapping by the AC field is strong enough to overcome the static “anti-trapping” potential, e.g., for $q = 0.3$ there are stable solutions for $-0.045 < a < 0.085$. The existence of solutions for $a < 0$, or more precisely that $(q, a) = (0.3, 0)$ is not on the boundary of a stability region, is essential for stable operation of the Paul trap in two dimensions. There are many stability regions, however it is the one closest to $(q, a) = (0, 0)$ that is most relevant to ion trapping. Trapping in higher-order stability regions has been proposed but it is of little practical use [124, 125].

Appropriate rescaling of Eq. 86 is crucial for an intuitive understanding of the system. With two different species in the trap and two driving frequencies there are four ways of rescaling the coefficients that are summarised in Table 2.

The B -ion is mainly confined by the RF radiation at ω_1 with $q_{1,B}^{(1)} \simeq 0.3$. Although the coefficient in front of the high frequency term has a higher numerical value it does not significantly contribute to the trapping. This becomes clear if we omit the ω_1 term and rescale time to $\omega_2 t = 2t_2$. The equation of motion for the B -ion is then the Mathieu equation:

$$\frac{d^2 y_B}{dt_2^2} + \left(a_B^{(2)} - 2q_{2,B}^{(2)} \cos(2t_2) \right) y_B = 0 \quad (88)$$

with $q_{2,B}^{(2)} = 0.001$, which provides negligible trapping, i.e. the spring constant arising from this equation is $\kappa_{B,2} \ll \kappa_{B,1}$. The stability region for the B -ion is thus only slightly perturbed by the presence of the high frequency term and the trapping is predominantly due to the ω_1 term.

The effect of ω_1 on species A is more difficult to assess using Eq. 86 since ω_1 now acts as a sub-harmonic term that can excite parametric resonances. The coefficients of the oscillatory terms for the A -ion are $q_{1,A}^{(1)} = 94.5$ and $q_{2,A}^{(1)} = 3307.4$. These unusually high coefficients arise from an improper rescaling of Eq. 86 but still facilitate a connection with the high- aq regime described above. If instead we use Eq. 87 the coefficients of driving terms are $q_{1,A}^{(2)} = 0.009$ and $q_{2,A}^{(2)} = 0.32$. Trapping is mainly due to the ω_2 term while the ω_1 term introduces parametric resonances at the subharmonics, the width of which decreases rapidly with increasing n so that the higher order resonances are readily suppressed by arbitrarily weak damping. The subharmonics picture can be mapped to the high- aq regime by treating the fast oscillating term as an effective harmonic pseudopotential term a_{eff} that arises from a static quadrupole. This maps Eq. 86 to the Mathieu equation:

$$\frac{d^2 y_A}{dt_1^2} + \left(a_{eff} - 2q_{1,A}^{(1)} \cos(2t_1) \right) y_A = 0 \quad (89)$$

where for simplicity we have assumed that there is no real static field term $a = 0$ so we do not need to consider how to combine the two contributions.

The ions are confined axially by a DC voltage V_0 on the end-caps giving a harmonic potential with spring constants $\kappa_{A,z} = 2eV_0/z_0^2$ and $\kappa_{B,z} = Z\kappa_{A,z}$, since the force depends only on the charge, where z_0 characterises the distance of the end-caps from the trap centre. An ion of species B sits near the centre oscillating at $\omega_{B,z} = \sqrt{\kappa_{B,z}/M_B}$. The voltage V_0 can be adjusted so that $\omega_{A,z}$ is on resonance with ω_B , the radial frequency of species B , as illustrated in Fig. 25. As well as matching frequencies we promote transfer of energy between radial and axial modes by off-setting the axes of the quadrupole fields at ω_1 and ω_2 . This radial displacement of the potentials can be implemented by unbalancing the AC voltage (at ω_1 or ω_2) on a pair of diagonally opposite electrodes (of the 4 electrodes in a linear quadrupole) or applying a static electric field which exerts more force on $+Ze$ than singly charged

ions (or a combination of these that minimises micromotion). Additional ions of species A position themselves approximately along the z-axis and start forming a chain (since $\omega_A \gg \omega_{A,z}$).

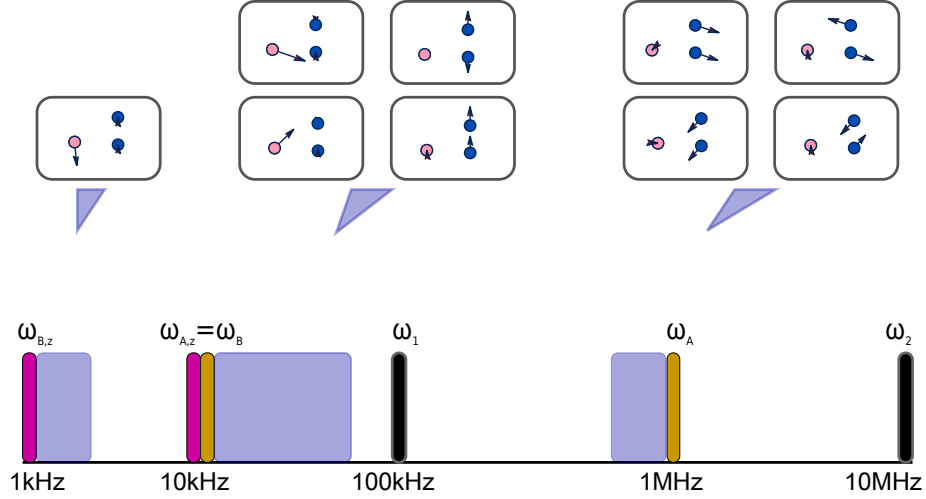


Figure 25: The important frequencies arranged on a logarithmic scale and the normal modes of a 3-ion system are shown above the relevant frequencies. For stable operation the two RF fields ω_1 and ω_2 must not parametrically excite the radial or axial secular motion of species A and B; thus the ordering of the frequencies is: $\omega_{B,z} < \omega_{A,z} \simeq \omega_B < \omega_1 < \omega_A < \omega_2$. The radial and axial frequencies ω_α , $\omega_{\alpha,z}$, where $\alpha = A, B$, correspond to the centre of mass motion for each species.

We can consider ions in a quadrupole field at each frequency ω_2 and ω_1 separately (with $V_0 = 0$).

1. The RF ω_2 gives spring constants $\kappa_A(V_2, \omega_2) = (e^2/M_A)(V_2/\omega_2)^2/(2r_0^4)$ and $\kappa_B(V_2, \omega_2) = (Z^2e^2/M_B)(V_2/\omega_2)^2/(2r_0^4)$ for ions of masses M_A and M_B when $V_1 = 0$.
2. The field at ω_1 , gives a spring constant $\kappa_B(V_1, \omega_1) = (Z^2e^2/M_B)(V_1/\omega_1)^2/(2r_0^4)$ for ions of mass M_B when $V_2 = 0$. We do not consider ions of mass M_A since they are predominantly trapped by the field at ω_2 .

In case 1 the ratio of the spring constants is $\kappa_B/\kappa_A = M_A \times Z^2/M_B$. If the two species have the same value of Z^2/M then both are strongly trapped using a single frequency. However, even when this is possible it does not allow for independent control of the secular oscillation frequencies that is vital for resonant energy transfer. Having similar spring constants for all ions is important for the following two reasons. Firstly, equal and opposite trapping forces on two ions $\kappa_A x_A = -\kappa_B x_B$ will result in similar displacements $|x_A| \approx |x_B|$. In contrast, in previous work [114] with single-frequency Paul traps the heavier ions were pushed to the outside of the trapped cloud since $\kappa_B \ll \kappa_A$. Secondly, for a cloud of ions at temperature T

both species will congregate within a similar distance from the trap centre since by equipartition of energy, $\kappa_\alpha \langle x^2 \rangle \simeq k_B T$. We can balance the spring constants by making $\kappa_A(V_2, \omega_2) = \kappa_B(V_1, \omega_1)$. This assumes that $\kappa_B(V_2, \omega_2) < \kappa_B(V_1, \omega_1)$ and indeed the field at ω_1 can have the dominant influence on species B even if $V_1 \ll V_2$. This corresponds to case 1 for species A, as in typical experiments with atomic ions, whilst the spring constant for species B is close to that in case 2. The secular frequency (in the pseudopotential approximation) is $q/2\sqrt{2}$ times the radio-frequency hence for $q = 0.3$ we have $\omega_B \simeq 0.1\omega_1$ and $\omega_A \simeq 0.1\omega_2$ resulting in the hierarchy of frequencies: $\omega_B < \omega_1 < \omega_A < \omega_2$ (see Fig. 25). The field at ω_2 has negligible effect on species B and acts to increase trapping in any case; thus for these ions two-frequency operation gives a pseudopotential very similar to a standard single-frequency Paul trap (for typical operating parameters). The quadrupole field at ω_1 leads to parametric resonances at frequencies given by $m\omega_1 = 2\omega_A$ where $m \in \mathbb{Z}$ is the order of the resonance. The width of these resonances decreases rapidly with increasing order making them very sensitive to damping which may be experimentally realised through laser cooling. In the numerical calculations we chose $\omega_A/2\pi = 1$ MHz as a reasonable experimental value hence $\{\omega_B, \omega_1, \omega_A, \omega_2\}/2\pi = 0.01, 0.1, 1, 10$ MHz, as illustrated in Fig. 25. The potential of a linear Paul trap has cylindrical symmetry and secular frequencies in the x and y -directions are referred to as the radial frequency.

Figure 26 shows the stability diagram as a function of $q_{2,A}^{(2)}$ and $q_{1,A}^{(2)}$ (with $n = 100$) for ions of mass M_A . The solid line that forms the top border of the shaded band is the critical line¹ that traverses equal distances in the stable and unstable regions [115, 126]. All calculations have been performed under the assumption of a pure sinusoidal oscillation, though harmonics might be important in practice. Parametric excitation of M_A by $V_1 \cos(\omega_1 t)$ produces tongues of instability which get wider as the amplitude V_1 increases. Figure 26 has been calculated without including any damping which would in any case only suppress the instabilities [127, 102]. The instabilities should in theory reach all the way to the horizontal axis but the resonances are too fine for the numeric calculations to capture them. In this sense, the granularity of the numerics acts as an effective damping parameter.

We have investigated the dynamics of the system of ions mainly after its transition to a Coulomb-crystal phase. Cooling down to this stage can be achieved by means of a conventional single-frequency operation of a linear Paul trap [114] and then the second frequency can be turned on adiabatically.

Our numerical simulations (discussed further in Ch. 7) show that a typical megadalton biomolecular ion can be sympathetically cooled by atomic barium ions. The

¹ Numerical calculations over a wider range of parameters show that the critical curve has a maximum around $\tilde{q}_A = 0.71$ and on either side of it is approximated by the curves $q_A/n^2 = 0.23\tilde{q}_A^2$ for $0 < \tilde{q}_A < 0.71$ and $q_A/n^2 = 0.57(0.91 - \tilde{q}_A)$ for $0.71 < \tilde{q}_A < 0.91$. The stability region extends up to $\tilde{q}_A = 0.91$ as expected from the Mathieu equation.

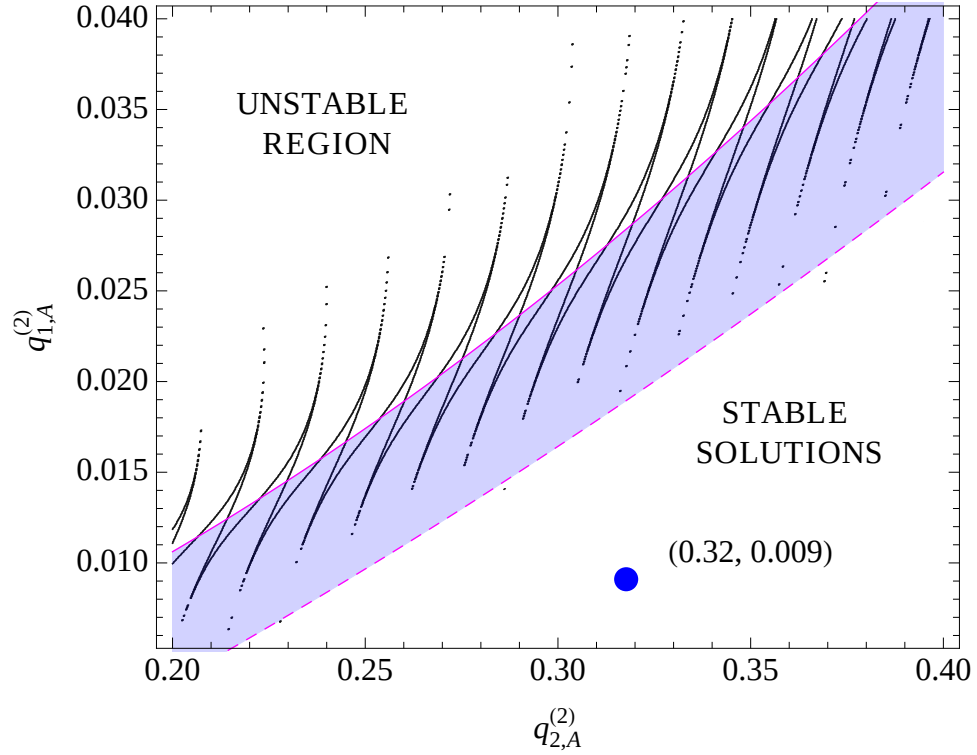


Figure 26: An expanded view of the stability plot for $n = 100$ showing the point $(0.32, 0.009)$ used in further calculations. The solid zig-zagging line is the transition curve between the region of stability (underneath) and instability (above). The critical curve passing through stable and unstable regions of equal width is shown as a solid line at the top of the shaded band. The tongues of instability become narrower below the critical line and asymptotically their width decreases exponentially (and similarly for the stability regions going upwards).

heavy ion settles to the centre of the trap and the presence of this non-fluorescing (dark) ion can be deduced from its large effect on the positions of the observable atomic ions. An intrinsic part of mass spectrometry is fragmentation: observing the breaking apart of a large biological complex bit by bit, whilst retaining the largest fragments in the trap to determine their charge-to-mass, would allow the investigation of single biomolecular complexes without ensemble averaging. For large charged particles there may be coupling between their rotational degrees of freedom and the translational motion of the atomic ions in the trap giving information about the moments of inertia (and hence shape). Another direction in which this two-frequency Paul trap could be developed is cooling of mesoscopic objects to their quantum ground state and adapting the sophisticated techniques developed for quantum information processing with trapping ions (e.g. quantum gates) to investigate quantum properties such as entanglement. Furthermore, a large ion in a sea of lighter ones furnishes a highly controllable system in which to investigate decoherence and (non-)Markovian dynamics. We have presented an example of how to solve the problem of confining ions of widely different charge-to-mass

ratios with the same effective spring constant. Many interesting possibilities follow from this extension of laser techniques for sympathetic cooling by laser-cooled atomic ions. We have chosen a comfortably large mass ratio to demonstrate the two-frequency operation but it also works for lower mass ratios. A further interesting application of the two-frequency Paul trap is the sympathetic cooling of positrons by Be^+ ions which has been demonstrated experimentally in a Penning trap [128] — this cooling of the light particles by a heavier ion represents a role reversal as compared to the above.

6.2.2 Ions with similar charge-to-mass ratio

The limitation of the method as applied to arbitrarily large differences of charge-to-mass ratios comes from the fact that the axial frequencies become very small as the difference increases (although there are ways to overcome this, e.g., by using 3 driving frequencies). The operation of the two-frequency trap gets somewhat more complicated to understand when the two driving frequencies are of similar order of magnitude and the picture of two independent traps is no longer valid. Nevertheless, the two-frequency trap can still be used for sympathetic cooling of ions with similar masses. In the literature concerned mainly with atomic ions [129] the mass ratios of sympathetically cooled ions do not exceed $\mu \simeq 3$ which is regarded as a practical limit in single frequency Paul traps. Cooling is inefficient for larger ratios because the secular oscillation frequencies scale as $1/\mu$. More recently this has been extended to much heavier (but multiply charged) ions [114, 130, 117]. Here we confine ourselves to the atomic regime and show that the two-frequency method can still be applied. This regime differs from the presentation of the previous section in two main regards: the number of ions is deliberately kept small and they are all positioned on the [RF](#) null line since any micromotion heating will quickly force the system to decohere.

We consider only atomic ions with charge 1e.

As an example, we discuss the case of cooling an $^{199}\text{Hg}^+$ ion using a $^9\text{Be}^+$ ion with a mass ratio $\mu \simeq 22$. The $^9\text{Be}^+$ is stably trapped using $\omega_1 = 60\text{ MHz}$ and $q = 0.39$. The secular oscillation frequencies for $^9\text{Be}^+$ are (8.6, 7.7, 0.9) MHz where an anisotropy of 0.9 is assumed in the radial direction. The axial oscillation frequency is deliberately kept low so it does not affect the stability of the $^{199}\text{Hg}^+$ ion. The secular frequencies for $^{199}\text{Hg}^+$ are (0.35, 0.31, 0.16) MHz. This leaves enough room between the oscillation frequencies to add a second [RF](#) field so that $n = \omega_2/\omega_1 = 10$. The effect of this field is to pull the oscillation frequencies of the two ions towards it hence effectively reducing the gap between them. The energy transfer seems to take place through a beating of ω_2 with the low lying frequencies. The above parameters are not necessarily optimised but already show

significantly better coupling between the ions with the final temperature as well as the cooling rate of $^{199}\text{Hg}^+$ being about 3 times higher as found in MD simulations.

This result is not necessarily applicable to quantum logic schemes, since, in order to improve the efficiency of the sympathetic cooling, the axial trapping frequency had to be greatly reduced. This limits the speed at which quantum gates can be performed. We envisage the method to be applicable in quantum simulation of condensed matter Hamiltonians using mixed-species ion chains [131, 132].

6.3 MASS SPECTROMETRY

The two-frequency trap can be used in mass spectrometry applications where no sympathetic cooling is necessary. By adjusting the spring constants, the heavy, weakly trapped ion can be pulled in towards the RF null line. A cloud of lighter ions can be used as a probe for the existence of the (non-fluorescing) heavy one, simply by looking at the column density deformations.

Although ions in a trap are normally characterised by an oscillation frequency we find it useful to use the spring constant $\kappa_\alpha = M_\alpha \omega_i^2$ in this context. The great novelty of the two-frequency trap is that it makes it possible for the two species to have the same spring constants $\kappa_A = \kappa_B$, hence similar displacements from the centre of the trapping potential. In previous experiments [114, 119] low Q_α/M_α particles were pushed to the outside of a cloud of atomic ions with much higher charge-to-mass ratio. The two frequency operation of the trap solves this problem.

The trap can be designed such that $\kappa_B \simeq \kappa_B^{(1)}$ and $\kappa_A \simeq \kappa_A^{(2)}$ which means that the dominant contribution for the heavy ion M_B comes from the lower frequency ω_1 , and the higher frequency $\omega_2 > \omega_1$ mostly affects the lighter ion $M_A \ll M_B$. The required ratio of the dominant spring constants is

$$\frac{\kappa_A^{(2)}}{\kappa_B^{(1)}} = \frac{(V_2/\omega_2)^2 \times (Q_A^2/M_A)}{(V_1/\omega_1)^2 \times (Q_B^2/M_B)} \simeq 1 \quad (90)$$

This could be achieved in a single-frequency trap only if the ions have the same Q_α^2/M_α , however this quantity generally decreases for heavy ions, as illustrated for the particular example of singly charged atomic $^{138}\text{Ba}^+$ ions and large biomolecular ions. Note that developing a technique to put the heavier ions into a higher charge state might not balance the spring constants because of the discretisation of charge. Adjusting the values of V_i/ω_i , for $i = 1, 2$ in Eq. 90 we can achieve a precise balance of the spring constants for the two species. It follows that $\kappa_B^{(2)}/\kappa_B^{(1)} \ll 1$, hence justifying the approximation $\kappa_B \simeq \kappa_B^{(1)}$. The justification that $\kappa_A \simeq \kappa_A^{(2)}$ is slightly different and can be traced to the fact that the variation of the trapping potential at ω_1 is slow enough to be adiabatic with respect to ω_2 .

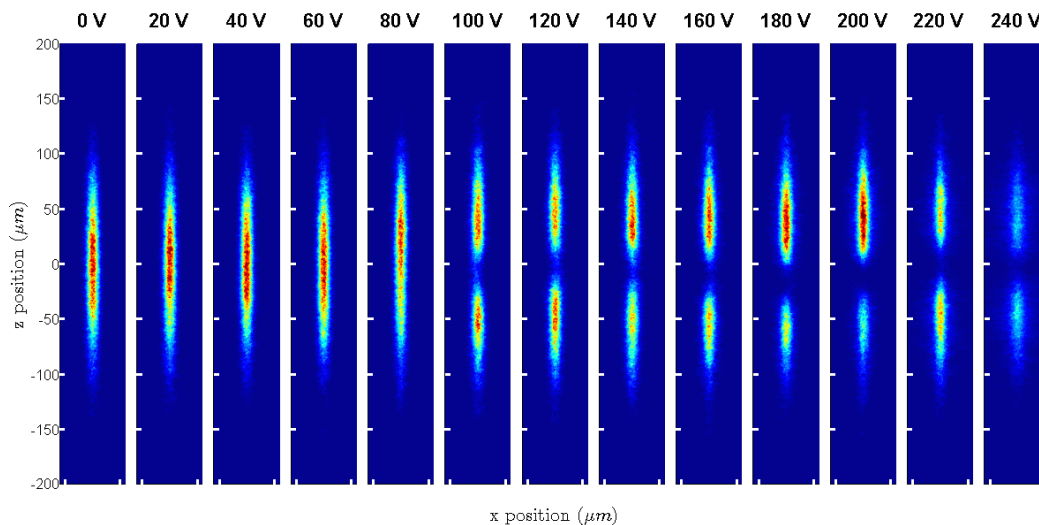


Figure 27: A linear Paul trap confines a cloud of $^{138}\text{Ba}^+$ ions and the large biomolecule of the previous Section. For single frequency operation the weakly confined biomolecule, repelled by the $^{138}\text{Ba}^+$ ions, inhabits a volume away from the trap centre. Application of a second slower RF tightens the biomolecule's spring constant and at sufficient amplitude it can exceed that of the $^{138}\text{Ba}^+$ ions (determined predominantly by the faster RF) and displace them from the trap centre. The data for this figure were generated using LAMMPS (see Appendix C).

The above considerations arose mainly from experimental practice, e.g. the range of mass spectrometers can be extended to lower charge-to-mass ratios (characteristic of higher masses such as mega-Dalton protein complexes) by reducing the frequency of the guiding field of the two-dimensional Paul trap along whose axis the ions travel. Two species of different masses can be trapped almost independently by using different frequencies, but in principle the idea of nested traps can be extended to three, or more, species with widely spaced masses. The coupling of multiple RF signals to the electrodes of the trap becomes easier the more widely spaced the frequencies are since the matching networks can work almost independently from each other.

One approach to the design process is to start from conditions suitable for trapping $^{138}\text{Ba}^+$ and a convenient frequency for experiments, e.g. $\omega_2 = 2\pi \times 10\text{ MHz}$. These are readily achievable values, and traps have been operated with considerably higher frequencies. The minimum frequency ratio sets the minimum mass ratio, thus for $\omega_1 < \omega_2 \times \sqrt{M_A/M_B}$ we can find values V_1 and ω_1 which give the same spring constant for species A and B, for physically realistic values of the charge Q_B .

6.4 CONCLUSION

We have shown how the two-frequency operation of an ion trap gives tight confinement with similar spring constants for two species of charged particles with widely different Q/M and explored the range of the ratios of Q/M for which this method can work. The example we have presented falls well within this range with a ratio of Q/M of the order of 10^5 . We spent considerable time exploring whether the idea could be demonstrated in an existing experimental apparatus, e.g. experiments with $^{40}\text{Ca}^+$ and $^{131}\text{Xe}^+$, or $^{40}\text{Ca}^+$ and $^1\text{H}^+$. Regions of stable operation could be found for only a few ions of each species which we deemed to be not practical for measurements.

Dehmelt suggested the two-frequency operation of an ion trap [133] as a way of trapping positrons (or electrons) simultaneously with antiprotons (where Q/M differs by $M_p/M_e = 1836$), however, to our knowledge no treatment of the parametric excitation has been given. We briefly numerically investigated schemes where a particle of very high Q/M , e.g., positrons/electrons, is co-trapped with atomic ions but it seems difficult to achieve a stable configuration for these systems because of the intrinsic heating from micromotion [134]. This seems to be the reason why Penning traps were used for trapping leptons, which led to many of the great successes of early work on ion trapping by Dehmelt's group including Wineland and others. The restriction due to micromotion heating can be understood through a simple numeric argument. If the upper frequency is around 1 GHz and the maximum damping rate is restricted to a few MHz (although it is likely to be even less because of inefficient coupling of modes) then the heating needs to be very small over 1000s of RF cycles which is very hard to achieve (even numerical calculations need to start with the leptons at low initial energy which would greatly restrict the usefulness). Note however that we did not undertake a detailed study of all cooling mechanisms that might be relevant, such as emission of radiation from the oscillating charge or damping through currents induced in the electrodes as in the original Penning trap work [135, 136]. Another case where sympathetic cooling by the more massive species (with lower Q/M) might become important is for negative ions. There are very few if any negative atomic ions with stable excited levels that can be laser cooled, thus there are strong constraints in the application of sympathetic cooling. There are proposals to trap and cool $^{192}\text{Os}^-$ [137] or La^- [138] and the two-frequency method could be used to sympathetically cool other ions arising from low mass elements such as hydrogen.

NORMAL MODES AND MOLECULAR DYNAMICS

We consider the normal modes of oscillation of ionic Coulomb crystals, that represent the minimum energy state in Paul traps under certain conditions. We define a Coulomb molecule as consisting of N atomic ions and a single biomolecular ion with a much smaller charge-to-mass ratio, co-trapped in a two-frequency ion trap. The translational motion of the atomic ions is damped by laser-cooling while the molecular ion is sympathetically cooled. We find an optimal configuration of the system parameters that maximises the coupling between the modes and leads to maximum cooling efficiency for the molecular ion. The parameters are the same as in Section 6.2.1.

The application of laser cooling techniques to clouds of trapped ions allowed experiments to reach the regime where Coulomb crystals are formed, i.e., low temperatures where the ions form regular arrays. Unlike in a solid-state crystal however, the confining potential in a Paul trap is time dependent. Thus the ions in a Coulomb crystal will be undergoing micromotion, except in especially simple cases such as a single row of ions lying along the axis of a linear Paul trap. Nevertheless, the mathematical description of the general case has a close analogy with the usual treatment for finding the normal modes of a set of coupled oscillators, e.g. phonons. The properties of the Coulomb molecule, such as its stability, can be determined by linearising the equations of motion about the dynamical solution (the potential minimum for the dynamical problem) taking into account the periodic motion of the equilibrium positions of the ions [139]. The effect of micromotion is shown to be significant for Coulomb molecules where the ions are displaced from the RF null line. Configurations similar to Coulomb molecules are referred to in the literature as crystals with a mass defect.

The general theory for normal modes in undamped vibrating linear systems was developed by Lagrange around 1762, a few years after Bernoulli had introduced the idea of superposition. More than a century later, Lord Rayleigh extended the theory to classically damped systems by introducing the concept of a dissipation function.

The dissipation function of a classically damped system is proportional to the mass and the Hessian of the system.

7.1 COULOMB CRYSTALS IN LINEAR ION TRAPS

Let us consider a chain of N ions in a linear Paul trap [140]. The interaction potential can be written as:

$$\begin{aligned}
 V(\vec{x}) = & \frac{1}{2} \sum_{i=1}^N m_i (\omega_{x,i}^2 x_i^2 + \omega_{y,i}^2 y_i^2 + \omega_{z,i}^2 z_i^2) + \\
 & + \sum_{i=1}^N Z_i e \vec{E} \cdot \vec{x}_i + \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^N \frac{e^2}{4\pi\epsilon_0} \frac{Z_i Z_j}{|\vec{x}_j - \vec{x}_i|}
 \end{aligned} \tag{91}$$

where all the symbols have their usual meaning. An electric field interaction term is included in the potential for adjusting the displacement of the ions from the RF null line. The ions are displaced by different amounts since they have a different charge and are subject to different radial trapping strength. Application of the electric field leads to non-axial crystals and promotes coupling between the radial and axial modes of oscillation. In the pseudopotential approximation the equilibrium positions of the ions can simply be found by minimising the potential:

$$\left(\frac{\partial V}{\partial \vec{x}_i} \right)_{\vec{x}_i = \vec{x}_i^{(0)}} = 0 \tag{92}$$

The equilibrium positions along the symmetry axis of the trap can be shown to follow the simple relationship [141]:

$$z_{min}(N) = \left(\frac{Z^2 e^2}{4\pi\epsilon_0 m \omega^2} \right)^{1/3} \frac{2.018}{N^{0.559}} \tag{93}$$

which is valid for ions of the same species. Allowing for ions with different mass and charge will obviously modify that but we can always use single species chains as consistency checks. The system can be effectively described as a system of coupled oscillators with the restoring forces for each particle arising through the competition between the trapping potential and the Coulomb repulsion of the ions. The equations of motion can be written in matrix form (we ignore damping for now):

$$\mathbf{M} \ddot{\vec{x}}(t) + \mathbf{K} \vec{x}(t) = \mathbf{0} \tag{94}$$

where $\vec{x}(t)$ is a column vector of the dependent variables, $\mathbf{M}$ is a diagonal matrix whose elements are the masses of the ions (not to be confused with the propagation matrix in the previous Chapters) and $\mathbf{K}$ is the Hessian of the system. The Hessian

matrix is effectively the Jacobian of the gradient of the potential function and its elements can be calculated simply as:

$$K_{ij} = \frac{\partial^2 V}{\partial x_i \partial x_j} \quad (95)$$

In practice, it is easier to calculate the Hessian directly as the numerical derivative of the forces since these are normally known in a typical MD simulation (see Section 7.4). All matrices are $3N \times 3N$ for a 3-dimensional system and they must be symmetric for any physically realisable isolated system. They are also positive definite or at least non-negative. Looking for normal modes solutions of Eq. 94 we arrive at:

$$(\mathbf{M}\omega^2 + \mathbf{K})\vec{x}(t) = \mathbf{0} \quad (96)$$

In order for the system above to have a solution the determinant of the coefficients needs to vanish $\det\{\mathbf{M}\omega^2 + \mathbf{K}\} = 0$. For the modes to be normal, $\mathbf{M}$ needs to be a scalar multiple of the identity matrix. If this is not the case we need to weight the modes by the masses. From Eq. 94:

$$\begin{aligned} \mathbf{M}^{1/2}\mathbf{M}^{1/2}\ddot{\vec{x}}(t) + \mathbf{K}\mathbf{M}^{-1/2}\mathbf{M}^{1/2}\vec{x}(t) &= \mathbf{0} \\ \mathbf{I}\ddot{\vec{y}}(t) + \mathbf{M}^{-1/2}\mathbf{K}\mathbf{M}^{-1/2}\vec{y}(t) &= \mathbf{0} \end{aligned} \quad (97)$$

where $y(t) = \mathbf{M}^{1/2}\vec{x}(t)$ are the mass weighted coordinates. The condition for the solution of the system now becomes an eigenvalue equation for the mass weighted Hessian. Rotating the Hessian with the eigenvectors matrix uncouples the equations of motion since the mass matrix is already diagonal. One point we could make here concerns eigenvalues with multiplicity $m > 1$. The m eigenvectors associated with them might not be orthogonal so we do not have an orthonormal basis to describe the system. Nevertheless, it is possible to show that since the Hessian is positive definite and symmetric, Gram-Schmidt orthogonalisation will always lead to a proper basis.

Assuming a single laser cooled species in the trap, the damping is classical and we can directly form the mass weighted Hessian and solve the eigensystem. The damping of each eigenmode is read out of the rotated damping matrix. With non-classical damping we use Foss' method as discussed in the next Section. This leads to complex root pairs only (no overdamping) and linearly independent eigenvectors with information on both the position and velocity of the eigenmodes. Foss' method also works with classical damping of course and gives identical results to the straightforward eigensystem solution.

7.2 DAMPED SYSTEMS

Following the same line of thought as above, we arrive at the following condition for the existence of solutions in a damped system.

$$\det \{\mathbf{M}\omega^2 + \mathbf{G}\omega + \mathbf{K}\} = 0 \quad (98)$$

where $\mathbf{G}$ is the damping matrix. This cannot be cast as an eigenvalue equation but is in principle easy to solve. In practice though, it suffers a great deal from numerical roundoff errors since the systems we are studying have parameters of significantly different scales. Assuming the elements of the Hessian matrix roughly fall into two different orders of magnitude n_1, n_2 , the coefficients of the characteristic polynomial will scale as $\propto N \times O(n_1 - n_2)$. This quickly leads to very stiff system that suffers from roundoff numerical errors. Qualitatively though we see that the equation must have $3N$ complex roots whose imaginary part is the frequency of the mode and the real part corresponds to damping. For the system to be stable the real part of all the modes must be negative.

To obtain the solution of the system we need to make the distinction between classical and non-classical damping [142, 143]. Assuming $\mathbf{Q}$ is a matrix containing the eigenvectors of the Hessian, we will refer to $\mathbf{G}$ as classical if $\mathbf{Q}^T \mathbf{G} \mathbf{Q}$ is diagonal. The equations of motion are then uncoupled. It is straightforward to show that this is the case if $\mathbf{G} = \alpha \mathbf{M} + \beta \mathbf{K}$ (a more general condition has been shown by Caughey [143]). In this case it is easy to get the solution from the eigenvalue equation (Eq. 97) and then rotate the damping matrix with the eigenvectors and read off the damping values from it. In this way we avoid solving the damped determinant.

To treat more generalised (non-classical) damping we follow the method developed by K. A. Foss, whereby the problem of solving the determinant equation is transformed into an eigenvalue problem in the $2 \times 3N$ space. From an engineer's perspective this is equivalent to a state-space model of the system. We start by introducing the generalised state-space vector $\vec{z} = \{\{\dot{\vec{x}}\}, \{\vec{x}\}\}^T$. After a few simple calculations we can recast the equations of motion as:

$$(\mathbf{I}\omega^{-1} + \mathbf{U})\vec{\phi}(t) = \mathbf{0} \quad (99)$$

where $\vec{z} = \exp(\omega t)\vec{\phi}$ a $2N \times 1$ vector and $\mathbf{U}$ is the following block matrix:

$$\mathbf{U} = \begin{bmatrix} \mathbf{0} & \mathbf{I} \\ -\mathbf{K}^{-1}\mathbf{M} & -\mathbf{K}^{-1}\mathbf{G} \end{bmatrix} \quad (100)$$

Foss' method is based on the assumption that the $\vec{\phi}$ vectors form a complete set. This is not always the case though and the method will fail to give a solution in

*Assuming that the
size of the Hessian is
 $3N \times 3N$.*

these cases. The damped mode frequencies for systems with normal eigenmodes can be shown to be always equal or less than the undamped ones. The solution for mode i oscillates at a frequency $\omega_{ii} = (k_{ii}/m_{ii} - (c_{ii}/2m_{ii})^2)^{1/2}$, where the matrix elements refer to the corresponding diagonalised matrices.

Overdamped systems might have real roots which lead to problems with root multiplicity since $\mathbf{U}$ is not symmetric. For this reason we only consider complex conjugate root pairs.

7.3 SYMMETRIC COULOMB MOLECULES WITH THREE IONS

Sympathetic cooling of ions has been studied extensively — see, for example [144, 129, 145]. The main motivation in these articles is performing quantum logic gates or clock measurements, whereas one species has a convenient cooling transition and can be used as a bath while the other one has a small linewidth (clock) transition. The theoretical treatment in these papers concerns a single frequency trap and aims at identifying mode gaps that can provide isolation between “hot” and “cold” modes. The main characteristic that defines the dynamics of these systems is that the oscillation frequencies of the ions scale as $1/\mu$ where μ is the mass ratio. In a two-frequency trap (as shown in Chapter 6) the oscillation frequencies can be made to scale roughly as $1/\sqrt{\mu}$ which inevitably brings the modes closer and promotes sympathetic cooling.

We continue with the example of Sec 6.2.1 and discuss the behaviour of normal modes in the two-frequency trap. The ions’ radial and axial oscillation frequencies are taken to be 11.4 kHz and 0.7 kHz respectively. For species A we have $\omega_{A,z} = 11.4$ kHz and $\omega_A = 1$ MHz so that $\omega_{A,z} = \omega_B$. The A-B-A configuration can be continuously transformed from a linear chain (cf., CO₂) to a two-dimensional crystal (cf., H₂O) by the application of an external electric field (see Fig. 28). The position of the ions is a smooth function of the electric field and there is no clear threshold value for the transition to a two-dimensional crystal as observed when changing the ω_z/ω_r ratio. For the purposes of this example we define the threshold value as the value that the ions form an equilateral triangle.

Because of the high charge (+33e) of the heavy ion we are only concerned with values of the electric field up to 500 V/m. This is close to the noise level for some traps. On one hand then, the highly charged ion is more susceptible to noise but at the same time the increased magnitude of the Coulomb interaction means that the system can crystallise at much higher temperatures. This can be easily shown by the application of a Lindemann type criterion, where the phase transition from a gas to a crystal takes place roughly at the temperature where the fluctuations of the ions is less than half their spacing.

The normal modes for the A-B-A configuration are shown as a function of the applied electric field in Fig. 29. They are normalised to the fundamental frequency $\omega_0 = 2\pi \times 11.4$ kHz which is taken to be the common value of the axial frequency of the heavy ion and the radial frequency of the light ion. As expected, their values

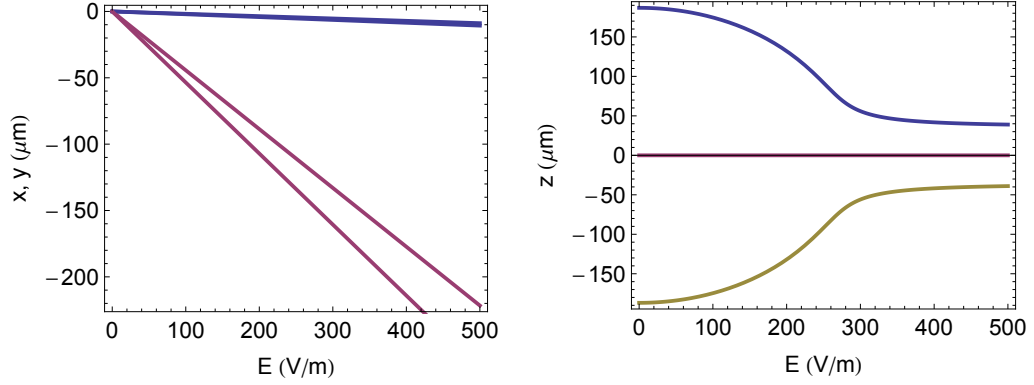


Figure 28: Position of the three ions in the A-B-A configuration for a given radial electric field along the diagonal axis of the trap. The blue and green lines correspond to the light A ions (overlapping completely for the x and y axes) and the magenta ones to the B ion. The radial trapping frequencies are $\omega_y = 0.9\omega_x$ so that the azimuthal symmetry is broken. The threshold value for the electric field is about 240 V/m.

remain the same until the electric field gets close to the threshold value. Significant mixing is then observed which leads to much faster cooling times. The fact that the coupling between all the modes is stronger at the threshold value of the electric field becomes apparent in Fig. 30 which depicts the damping time of all the normal modes of the system.

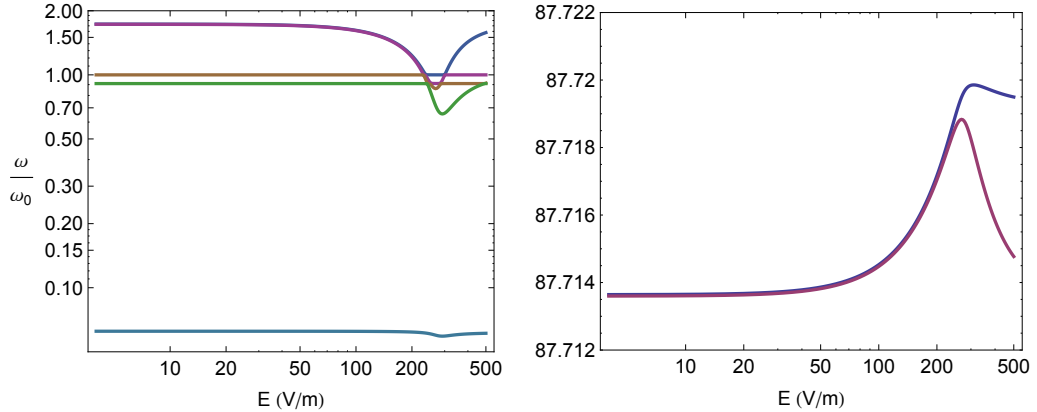


Figure 29: Normal modes spectrum for a symmetric Coulomb molecule comprised of three atoms. The normal modes can be grouped to high frequency modes (RHS) with values very close to the secular radial frequency of the light ions at 1 MHz and low frequency modes (LHS) at 0.7 kHz to 20 kHz. Sympathetic cooling is most efficient at the threshold value of the electric field where the mode mixing is maximal.

Assuming the characteristic damping time of the light ions is about $60\mu\text{s}$ we find modes of the system that take up to a few hundred ms to thermalise. The value of the characteristic damping time of the light ions has been chosen to be the

theoretical Doppler damping time for $^{138}\text{Ba}^+$. This needs not be the case for the strong coupling regime where much faster cooling rates can be achieved [146]. The choice of damping time affects how accurate must the frequencies be matched for efficient energy transfer between the ions. If the system is over-damped the Q of the resonator is decreased and frequency matching becomes less crucial.

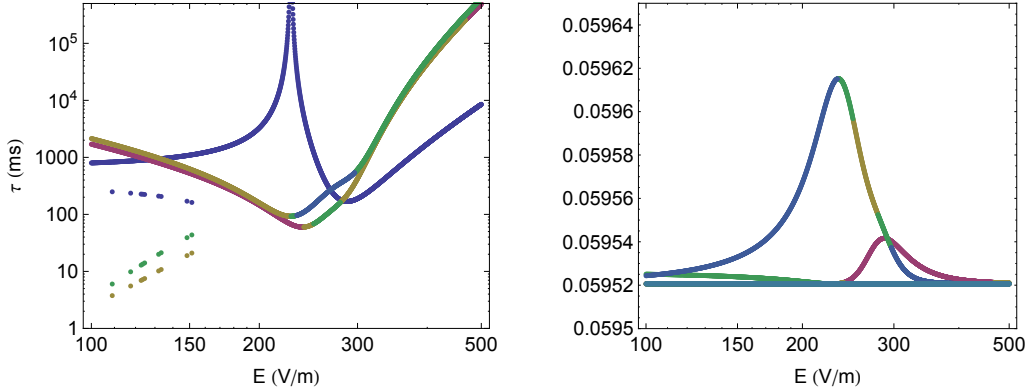


Figure 30: Damping times of the high (RHS) and low frequency normal modes (LHS). The light ions are being damped at a characteristic time $\tau = 60 \mu\text{s}$. Some of the normal modes involve a large amplitude motion of the heavy ion and are not being damped as fast. However, the damping time for these modes is still only of the order of hundreds of ms. The scattered points on the LHS are due to the minimisation algorithm failing. Some mode mixing is observed but a slow mode always remains.

The spatial symmetries of the system categorically affect the energy transfer between the two species. The efficiency of the sympathetic cooling increases as the various symmetries of the crystal are broken. A linear molecule has a C_2 axis of rotation in addition to C_∞ . There are also infinite numbers of σ_∞ planes parallel to the C_∞ as well as a σ_h plane along the vertical axis. These symmetries, along with the centre of inversion along the primary axis mean that the molecule is classified in the $D_{\infty h}$ point group. The C_∞ and σ_∞ symmetries can be broken by the application of a radial electric field. That leaves us with only a C_2 rotation axis and two planes of symmetry (cf., H_2O), thus the molecule belongs to the C_{2v} group. An extra symmetry plane can be broken by choosing non symmetric Coulomb molecules, e.g., $\text{A}_2\text{-B-A}$. This molecule will cool faster as shown in Table 3, but this improvement cannot be ascribed solely to the symmetry break since there is the addition of one more coolant ion in the system. Lastly, since the Coulomb molecules are constrained to a trap, we need to make sure that $\omega_x \neq \omega_y$ so that there is no azimuthal symmetry. A difference of 10% in trapping frequencies is typical in ion traps and we have assumed this is the case in the calculations in this Section. There is also the possibility of applying a DC electric field on split endcaps to tilt the principal axis

Anharmonicity shifts can also be included [147].

of the crystal [148, 132] which is not considered here since it involves a somewhat more specialised apparatus.

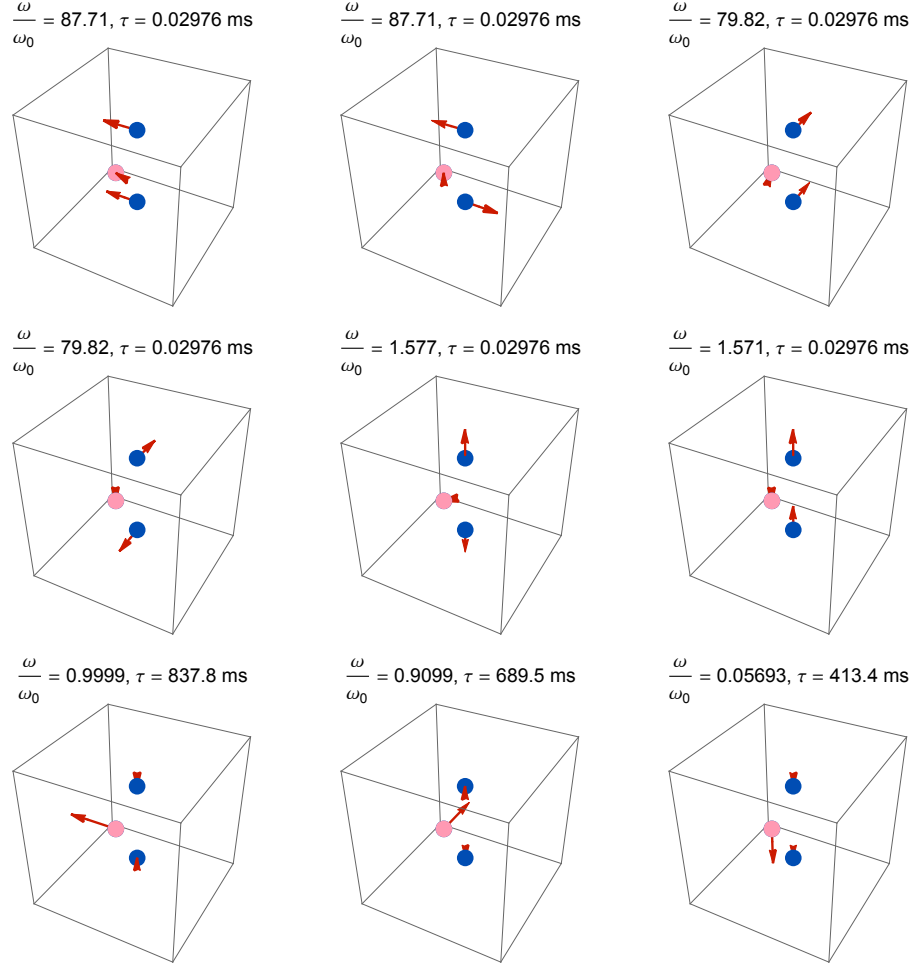


Figure 31: Amplitudes of motion of for the $3N$ normal modes of the Coulomb molecule. The frequency of the mode (referenced to ω_0) as well as the characteristic energy damping time of each mode are shown as headers in each plot. A few “swinging” modes involve a large amplitude for the heavy ion but much smaller amplitudes for the light ones and hence are damped at a slower rate (these are in the third row).

The peak in the damping time at the threshold value in Fig. 30 can be easily interpreted via a symmetry picture since an equilateral triangle introduces yet another symmetry on the system. Immediately above the threshold value, the crystal “melts” and the damping times are much faster. In a realistic experimental sequence we envisage the heavy ion being pulled in towards the centre of the trap by adjusting the amplitude of the slower RF field. In effect, this assumes the role of an applied electric field and the system is going to explore all of the spatial configurations allowed. The net damping time thus, is going to be some weighted average of all the configurations.

The modes that are not begin cooled as fast involve a relatively large amplitude of motion of the heavy ion. Fig. 31 depicts all $3N$ modes for the A-B-A configuration. The cooling efficiency is not optimal for this molecule since we only have $N - 1$ ions scattering photons. This difference becomes less important as the Coulomb molecules become larger. In any case, we identify three “swinging” modes that are being damped at a slower rate and the amplitude of motion of the heavy ion is much larger than that of the light ones. Nevertheless, the damping time of these modes is still around 1 sec which is experimentally reasonable. The slowest mode sets the minimum temperature that can be achieved as well as the rethermalisation time in case the system is knocked out of equilibrium. Both these considerations are not overly important in chemistry experiments involving ultra cold ions.

7.3.1 Limits due to micromotion

The pseudopotential approximation has been assumed in the previous example. Although this works well when the ions are on the RF null line the influence of the micromotion becomes more important for two-dimensional molecules. A more detailed analysis including micromotion effects [149, 150] shows various frequency shifts of the normal modes spectrum of “peculiar” crystals. This is not too much of a concern in our case since the Q of the system is very low and in any case the parameters of the trap can always be adjusted to arrange for a resonance condition. The real limit on the system is imposed from micromotion induced heating which increases linearly with the applied electric field. Although, some heating can be tolerated due to the higher crystallisation temperature of the system, it turns out it is not possible to use the optimal value of the electric field (right above the threshold value) since micromotion heating dominates the dynamics completely. A more conservative value of the electric field of about 100 V/m has to be chosen to satisfy both opposing constraints. The damping times quoted in Fig. 31 correspond to this value for the electric field.

7.4 MOLECULAR DYNAMICS

The normal mode analysis is important for understanding the system and it shows how to optimise the transfer of energy by matching the frequencies and breaking the symmetries of the system by an applied electric field. However in Paul traps there is parametric heating, or micromotion heating, even for single ions and it is therefore important to numerically simulate the whole system. The micromotion occurs at a much higher frequency than the secular motion of the ions which leads to very stiff systems, i.e. there is a large range of time scales and the time step

n	m=1	m=2	m=3	m=4	m=5
1	796, 623				
2	182, 30	429, 190			
3	257, 39	102, 37	320, 53		
4	118, 48	140, 38	75, 43	272, 27	
5	166, 59	140, 43	92, 38	66, 40	261, 18

Table 3: Values for the characteristic energy damping time for various configurations of ions in the trap: A_n -B- A_m . The two numbers at the n^{th} row of the m^{th} column are the energy damping times (in milliseconds) for the radial and axial motions respectively of the ion of species B in these Coulomb molecules. Systems with a small asymmetry show efficient transfer of energy that promotes sympathetic cooling — see text for details.

of any numerical integration must be small compared to the inverse of the fastest frequency.

MD simulations are extensively used to extract macroscopic physical quantities of multi-particle systems via simulation of the equations of motion of the individual particles. For N particles, the number of particle-particle interactions that need to be computed scales as N^2 , and so direct integration of the equations of motion quickly becomes computationally expensive. An efficient way to perform such simulations is by using the highly optimised LAMMPS code (see Appendix C). Alternative simulation methods include Direct Simulation Monte-Carlo (DSMC) as developed by Bird [151].

Table 3 shows the results of our numerical calculations for a single ion of species B. We show results for symmetric and asymmetric Coulomb molecules of the form A_n -B- A_m , with the B-ion deliberately displaced in the radial direction. For example, A-B-A has a configuration resembling that of an H_2O molecule with A-ions at coordinates $(r, z) = (17.1, \pm 57.9)$ relative to the centre of mass of the system which coincides very closely with the massive B-ion. Similarly, configurations with more ions are not linear, by design, in our simulations. Using a damping time $\tau = 60 \mu\text{s}$ for species A (close to the theoretical optimum for $^{138}\text{Ba}^+$) we get damping times of the order of 100 ms for species B. Table 3 shows that the damping rate depends strongly on the size and degree of asymmetry of the Coulomb molecule although highly asymmetric molecules do not seem to lead to much faster damping rates. We find that frequency matching is easily achieved especially when the number of ions is large and hence the system has a larger number of normal modes.

The axial modes of such a chain, or linear Coulomb crystal, have higher frequency than the centre-of-mass mode whereas higher-order radial modes have lower frequency. Thus, adding more ions tends to close the gap in the frequency spectrum of normal modes where we have placed ω_1 (to avoid parametric exci-

tation of these modes). This limits the number of ions of species A that can be accommodated in the same potential well.

7.5 CONCLUSION

Initial estimates based on normal modes analysis suggested using large electric fields to change the geometry of the Coulomb molecule but the [LAMMPS](#) simulations showed that this would lead to significant heating so a compromise was found.

We found that the sympathetic cooling works sufficiently well in a linear quadrupole trap with a small applied radial electric field however there are simple ways to improve the cooling rate which can be investigated in future work. It might be beneficial to increase the axial frequency of the massive ions, $\omega_{B,z} = 0.7 \text{ kHz}$, to be the same as that of the radial frequency ω_B . An octupole static potential along the z-axis of the trap (also with a radial electric field) rather than the purely quadratic of a quadrupole could be used instead. The latter has a constant curvature whereas the second derivative of a potential proportional to z^4 is zero at the centre and increases with z . With the additional electric field (linear potential) the highly charged ion can be positioned at a finite distance, e.g. $z = 70 \mu\text{m}$ with a chain of atomic ions extending to lower displacements. In this way we would hope to both increase the secular frequency for the massive ion and also make the axial and radial secular oscillations have almost the same frequency. This near degeneracy would mean that it is only necessary to apply a small perturbation to mix the motion in these (orthogonal) degrees of freedom, i.e., the electric field along the diagonal would be less than that required to mix modes at around 1 and 10 kHz respectively. This scheme seems realistic when considering the normal mode of the system but a detailed numerical analysis has not been performed yet. A practical scheme for making Paul traps with an octupole along the z-axis has been worked out in the Oxford ion trapping group [[152](#)]. Electrodynamical traps whose behaviour is dominated by an octupole field in the radial direction are commonly used for trapping and guiding molecules, and recently an interesting scheme which combines octupole and quadrupole fields has been proposed where the [RF](#) is zero along 3 parallel lines [[153](#)] thus effectively creating 3 parallel linear quadrupole traps (for ions that are cold enough so that they stay in the region around these lines).

Part III

APPENDIX

RF IMPEDANCE MATCHING

When dealing with practical implementations of RF circuitry, there is always the need to match the impedances of interconnected blocks to achieve maximum power transfer between the source and the load [154]. Off-the-shelf components conform to the $50\ \Omega$ standard but special care needs to be taken when connecting any other component.

At high enough frequencies spurious components and parasitics become important so theoretical calculations and simulations often fail and in-situ measurements have to be made to determine the values of the components. To this end we acquired the excellent Bode-100 from Omicron Lab which is an inexpensive, feature-rich vector network analyser. Its frequency range is from 1 Hz to 40 MHz which covers the whole range of interest for our ^{87}Rb experiment (except for microwave components). Its low frequency operation means it can be used to improve the matching of the 7 kHz field currently used to drive the TOP coils, although matching at such low acoustic frequencies is much less involved and normally requires simply a transformer.

The second necessary tool for impedance matching is the Smith chart which can be used to guide the impedance matching process without any computation required. The Smith chart is a conformal mapping of the complex impedance cartesian plane to a circle and it was originally developed by Phillip Smith in 1940 [155].

A.1 TRANSMISSION LINES AND THE SMITH CHART

The literature on transmission lines, transfer functions and RF matching networks is vast and we will not attempt to cover all these concepts here. For an excellent review on “Why play the matchmaker” see [154, 156]. The only two relevant quantities we will use is the reflection coefficient Γ and the Voltage Standing-Wave Ratio (VSWR) which are defined as:

$$\Gamma = \frac{Z_L - 50}{Z_L + 50} \quad \text{and} \quad \text{VSWR} = \frac{1 + |\Gamma|}{1 - |\Gamma|} \quad (101)$$

A matching network inserted between the source and the load aims at making the load impedance $Z_L = 50\ \Omega$ and thus $\Gamma = 0$. The VSWR is a measure of how accurate this transformation must be and for typical RF electronics is about 1.5:1 and as much as 4:1 for high power sources. The matching network topology involves

T, L and Π networks (or combinations of them) that can be used to match a load starting at any arbitrary position on the Smith chart. The geometry of the matching network needs to allow for maximum current $I = \sqrt{P/50}$ (rather than power) going through the RF trap coils. In practice we prefer using a two-capacitor L network since the parasitics are smaller, it does not introduce a resistive component like wound inductors do, and can match any load from the upper right quadrant of the Smith chart. A counterargument for this would be that the frequency spread is asymmetric but it makes little practical difference in our case.

The use of Smith chart is satisfyingly easy. The centre of the chart corresponds to the matched point for a chart normalised at $50\ \Omega$. The leftmost (rightmost) point along the real axis corresponds to open (short) circuits. The upper (lower) semi-circle can be thought as inductive (capacitive). This makes it straightforward to identify the self-resonance of a coil as the point where it crosses over to the lower semicircle. Moreover, the only transformations possible are the following:

- Series (shunt) capacitors rotate the load towards the lower semicircle along circles of constant impedance (admittance).
- Accordingly, series (shunt) inductors rotate the load towards the upper semicircle along circles of constant impedance (admittance).
- Series (shunt) resistors move the load's impedance (admittance) along lines where the imaginary part of the impedance is constant.
- A transmission line rotates the whole chart by an amount proportional to its length. Equivalently a stub parallel line — open or shorted — rotates the chart by the same amount but the load needs to be mirrored about the centre first so we consider its admittance value.

To illustrate its use let us consider two examples. The first is a single frequency, very high-Q matching network and the second is a wideband, lossy one.

A.1.1.1 *Single-frequency matching*

The RF trap in the ^{87}Rb experiment was redesigned with new coils having a self-resonance of about 7 MHz, cf. to 1.6 MHz before. Allowing for higher frequencies is desirable for reaching a 2D regime in the shell trap [157]. The old coils were not matched and they had to be driven with 28 W amplifiers to get adequate current through them. Before taking them out we decided to impedance match them and were able to achieve twice the current using only 1 W amplifiers! The new coils were matched at 2 MHz using an L capacitor network (see Fig. 32). The first capacitor (looking from the load) rotates the load onto the 20 mS admittance circle. The second one follows that circle to the centre of the chart, thus matching the load. The

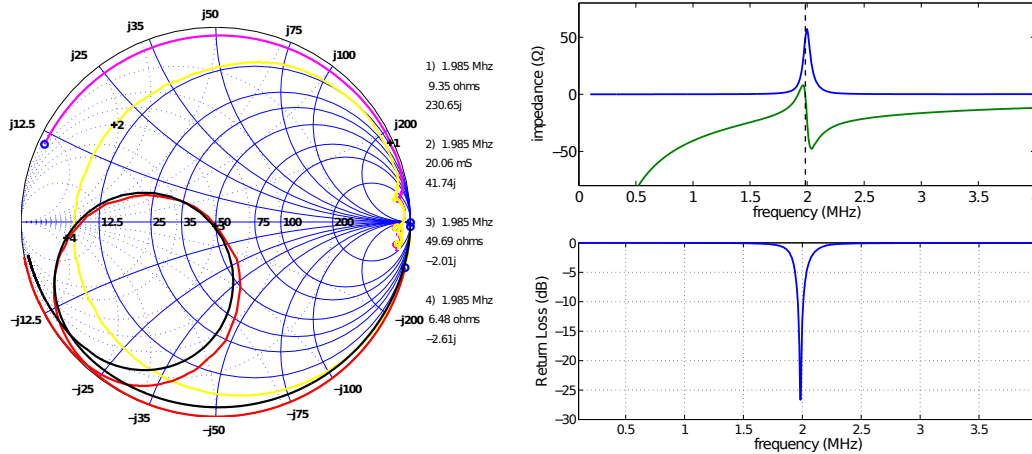


Figure 32: The load impedance can be seen on the Smith chart. The impedance of the bare coil (magenta) is rotated twice by the L network. The final result (red) matches the measured one (black) very closely. When matched, the network behaves as a real $50\ \Omega$ load. The S_{11} parameter shows a very sharp resonance with minimal return losses.

length of the cable connecting the load to the amplifiers is irrelevant when the load is matched. The S_{11} parameter of the two-port scattering matrix shows a $-25\ \text{dBm}$ return loss.

A.1.2 Wideband matching

Resistive components or multi-stage networks are normally used to achieve a large bandwidth network. We avoid the resistive components because of the associated drop in current. The multi-stage networks cannot realistically have more than 3-4 stages since parasitics pile up, which was indeed the case with the various Chebyshev filters we tried. In theory, smaller steps on the Smith chart can be used to contain the load inside constants lines of low Q so the bandwidth is increased. This becomes increasingly cumbersome though, when the load is matched close to the self-resonance and almost impossible when starting from a very high- Q load. Hence, this technique is normally reserved for transforming resistive loads where the Q of the transformation can be selected at will.

More elaborate matching network geometries can be designed using series and parallel stub tuning. The necessary frequency spread can be achieved without resorting to lossy components. Stub tuning is used mainly in microwave frequencies since the length of the stubs has to be of the order of the wavelength. For microwave frequencies this translates to a few micrometers, cf. to tens of meters for RF. Nevertheless, a wideband impedance match can still be achieved using stubs in the RF regime with reasonable cable lengths along with a combination of series

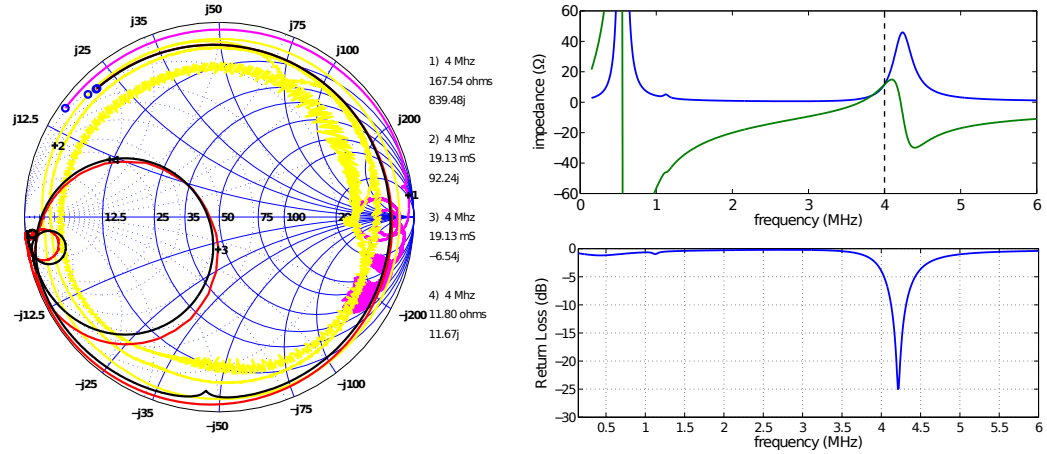


Figure 33: The impedance of the load is spread out (yellow) using a long coaxial cable. A shunt capacitor brings the 4 MHz point close to the centre of the Smith chart (red). The black curve is the measured reflection power which closely matches the expected one. The impedance of the load is almost 50Ω at 4 MHz with some structure observed in the very low frequencies. The S_{11} parameter shows a 3 dB bandwidth of about 1 MHz at $f_0 = 4$ MHz.

and parallel passive components. The main problem with this approach is that the smallest reposition of the stub leads to resonance drifts due to capacitive coupling. A much more robust approach was found, which takes advantage of the natural dispersion of an RG58 cable as seen in Fig. 33. A single 14 m coaxial cable is used in series with the load to spread the frequencies out. A shunt capacitor then transforms the load to 50Ω . We were able to achieve a bandwidth of about 1 MHz which is more than enough for the experiments described in Chapter 3. This value is even more impressive if recast in terms of fractional bandwidth $\Delta_{3dB}/f_0 \simeq 25\%$.

THE KRONIG-PENNEY MODEL

Kronig and Penney used a simple “toy model” to investigate the propagation of wave functions in periodic potentials. They considered a potential $V(x)$ that is square waveform, i.e., a regularly spaced square wells of finite depth. The usual treatment found in many quantum mechanics textbooks [158] involves a considerable amount of algebra. The main principles can be illustrated much more concisely by considering a potential of the form of regularly spaced delta functions (aka a Dirac comb). Indeed, the results we shall derive for a comb of delta-functions correspond to those found by Kronig and Penney in the appropriate limits: a negative comb if the width of the square wells tends to zero (and their depth tends to infinity), and a positive comb if barriers become delta-functions. Although none these potentials is very realistic, they manifest the characteristic features of the solutions of the Schrödinger equation in a periodic potential.

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V(x)\psi = E\psi \quad (102)$$

where $V(x + X) = V(x)$. Before considering the Dirac comb, it is useful to recall the results for a single δ -function. It is dimensionally convenient to express the potential as

$$V(x) = \frac{\hbar^2\beta}{2m}\delta(x) \quad (103)$$

where the parameter β has dimensions of length^{-1} , and characterises the strength of the δ -function potential. Note that the potential must be negative $V(x) < 0$ for there to be bound states, i.e., $\beta < 0$. Integrating over a small range from $-\epsilon$ to ϵ gives

$$\left[\frac{d\psi}{dx} \right]_{-\epsilon}^{\epsilon} = -\beta\psi(0) \quad (104)$$

since

$$\int_{-\epsilon}^{\epsilon} E\psi dx \approx 2\epsilon E\psi(0) \rightarrow 0 \text{ as } \epsilon \rightarrow 0 \quad (105)$$

A wave function with $E < 0$, has the form $Ae^{\kappa x}$ for $x < 0$ and $Be^{-\kappa x}$ for $x > 0$. Continuity at $x = 0$ requires that $\psi(0_-) = \psi(0_+)$ hence $A = B$. Combined with the discontinuity requirement for the derivatives it leads to $\kappa = -\beta/2$ (with $\beta < 0$ for bounded solutions). This system has one (and only one) bound state of energy:

$$E = -\frac{\hbar^2}{2m}\kappa^2 = -\frac{\hbar^2}{2m} \frac{\beta^2}{4} \quad (106)$$

We now apply the same approach to the Dirac comb with spacing a between δ -functions.

$$V(x) = -\frac{\hbar^2}{2m} \sum_{n=-\infty}^{\infty} \delta(x - na) \quad (107)$$

The conditions for continuity of ψ and its derivative ψ' at each δ -function are

$$\begin{aligned} \psi(na_+) &= \psi(na_-) \\ \psi'(na_+) - \psi'(na_-) &= -\beta\psi(na_-) \end{aligned}$$

These can be expressed as a matrix equation

$$\begin{pmatrix} \psi(na_+) \\ \psi'(na_+) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ -\beta & 1 \end{pmatrix} \begin{pmatrix} \psi(na_-) \\ \psi'(na_-) \end{pmatrix} \quad (108)$$

The same matrix describes the effect of a δ -function potential on a particle with positive energy $E > 0$. In this case the equation for the derivatives implies that $2ik = \beta$, which can be satisfied for both positive and negative values of β .

Now we shall consider the propagation of the wave function between the δ -functions, e.g., from $x = 0_+$ to a_- . This is the same as for the interval from na_+ to $(n+1)a_-$. Using the shorthand notation $\psi_0 = \psi(0_+)$ and $\psi'_0 = \psi'(0_+)$ we can write:

$$\begin{aligned} \psi_0 &= A + B \\ \psi'_0 &= ik(A - B) \end{aligned}$$

Hence

$$\begin{aligned} 2A &= \psi_0 + \frac{1}{ik}\psi'_0 \\ 2B &= \psi_0 - \frac{1}{ik}\psi'_0 \end{aligned}$$

After propagation over the interval 0 to a the wave function and its derivative are

$$\begin{aligned} \psi(a_-) &= Ae^{ika} + Be^{-ika} \\ \psi'(a_-) &= ik(Ae^{ika} - Be^{-ika}) \end{aligned}$$

Hence

$$\psi(a_-) = \frac{1}{2} \left\{ \left(\psi_0 + \frac{1}{ik}\psi'_0 \right) e^{ika} + \left(\psi_0 - \frac{1}{ik}\psi'_0 \right) e^{-ika} \right\} = \cos(ka)\psi_0 + \frac{1}{k} \sin(ka)\psi'_0 \quad (109)$$

Similarly $\psi'(a_-)$ can be found, and the resulting two equations can be written in matrix form as

$$\begin{pmatrix} \psi(a_-) \\ \psi'(a_-) \end{pmatrix} = \begin{pmatrix} \cos(ka) & \frac{1}{k} \sin(ka) \\ -k \sin(ka) & \cos(ka) \end{pmatrix} \begin{pmatrix} \psi(0_+) \\ \psi'(0_-) \end{pmatrix} \quad (110)$$

The determinant of the matrix is unity, as is that of the matrix for the δ -function potential. This is a general property of propagation matrices since they are symplectic. It follows that the matrix product

$$\mathbf{M} = \begin{pmatrix} \cos(ka) & \frac{1}{k} \sin(ka) \\ -k \sin(ka) & \cos(ka) \end{pmatrix} \begin{pmatrix} 1 & 0 \\ -\beta & 1 \end{pmatrix} \quad (111)$$

has $\det\{\mathbf{M}\} = 1$. The diagonal elements are $M_{11} = \cos(ka) - \frac{\beta}{k} \sin(ka)$, and $M_{22} = \cos(ka)$. Hence

$$\text{tr}\{\mathbf{M}\} = M_{11} + M_{22} = 2 \cos(ka) - \frac{\beta}{k} \sin(ka) \quad (112)$$

We want to know about the eigenvalues λ in the equation

$$\begin{pmatrix} \psi(x+na) \\ \psi'(x+na) \end{pmatrix} = \mathbf{M}^n \begin{pmatrix} \psi(x) \\ \psi'(x) \end{pmatrix} = \lambda^n \begin{pmatrix} \psi(x) \\ \psi'(x) \end{pmatrix} \quad (113)$$

The condition for stable solutions is $|\lambda| \leq 1$, which gives

$$\left| \frac{1}{2} \text{tr}\{\mathbf{M}\} \right| = \left| \cos(ka) - \frac{1}{2} \beta a \frac{\sin(ka)}{ka} \right| \leq 1 \quad (114)$$

In the theory of electronic band structure in solids, the ranges of energy $E = \hbar^2 k^2 / 2m$, for which this condition is not satisfied are called band gaps — these particles do not propagate through the periodic structure. This equation can be solved graphically however the key point is the existence of gaps in the eigenenergies of the Schrödinger equation with a periodic potential where the solutions are not stable.

To pursue the analogy even further we can write the above condition as:

$$\cos(\tilde{k}a) = \cos(ka) - \frac{1}{2} \beta a \frac{\sin(ka)}{ka} \quad (115)$$

where $\tilde{k}$ is a quantity with the same dimensions as momentum which is known as quasi- or crystal momentum ($\tilde{k} \rightarrow k$ as $\beta \rightarrow 0$). For allowed energies, i.e., those lying

within the bands, the eigenvalues of the propagation matrix are $\lambda = \cos(\tilde{k}a) \pm i \sin(\tilde{k}a) = e^{\pm i\tilde{k}a}$ and

$$\psi(x+a) = e^{\pm i\tilde{k}a} \psi(x) \quad (116)$$

This implies that

$$\psi(x) = e^{\pm i\tilde{k}x} u(x) \quad (117)$$

where $u(x+a) = u(x)$ is a periodic function — this is Bloch's theorem. Note that rather than stating this theorem at the outset, as in many treatments of the band structure, we have shown that the wave function must have this form in a periodic potential. The transition between stability regions occurs when $ka = n\pi$ or $ka = n\pi - \beta a/n\pi$ corresponding to $\cos n\pi = (-1)^n$ and $\sin n\pi = 0$. There are no stable solutions for wave vectors k in the range $(n\pi - \delta)/a$ to $n\pi/a$, where $\delta/a = -\beta/(n\pi)$ has the opposite sign to β . This is readily seen by graphing the function and/or considering the sign of the trigonometric functions around $n\pi$. This case corresponds to the nearly-free-electron model (when β is small) where a band gap opens up at $k = n\pi/a$.

We present a Matlab wrapper, LIon, that allows a user to write, run and analyse ion trap simulations. The actual MD simulation is performed in another program, LAMMPS, to take advantage of its proven efficiency. LAMMPS is a classical MD code, the current version of which has been in active development since 2004. The project's longevity and highly active use (the original 1995 paper [159] was cited 1,127 times (!) in 2013) has resulted in an optimised and reliable program.

Many of the efficiency and scaling problems that present themselves when simulating ion clouds have already been solved in biomolecular MD simulations which normally deal with much larger particle numbers. A noticeable difference is that dominant force fields in biomolecular MD are short range (e.g. the van der Waals potential), though implementations of longer range interactions are often included in these software packages. Nonetheless, many of the techniques used remain relevant: the use of spatial decomposition of the simulation region to balance processor load, optimised long-range interaction calculations using the GPU and implementation of OpenMP and MPI for deployment to HPC resources.

LAMMPS, although traditionally used in the context of short-range forces, is perfectly capable of efficient and reliable simulation of ion traps, a problem dominated by the long range Coulomb interaction. Our wrapper offers multiple methods for initialising the system, evaluating the dynamics and post-processing the results. The use of validation scripts to test the results are consistent with theory ensures data produced using LIon is reliable. Moreover, it draws on the rich features of LAMMPS to offer the user features not seen in other ion trap simulation packages. These features are not presented here, but include the capability of simulating protein structures in aqueous Paul traps [122], treating collections of ions as rigid bodies and simulating collisions between ions and a buffer gas described by ion-neutral potentials.

C.1 IMPLEMENTATION OF LION

MD simulations are configured by calling functions of a LAMMPSimulation object in Matlab (see Fig. 34). Once the input file is setup the simulation is executed and the file is parsed by a child instance of LAMMPS. This instance simulates evolution of the system and generates output for analysis. An asynchronous update loop in Matlab monitors the progress of this process, allowing error interception and diagnostic

updates. Upon completion of the simulation the [LAMMPS](#) process is terminated and control reverts to Matlab for analysis of the generated data.

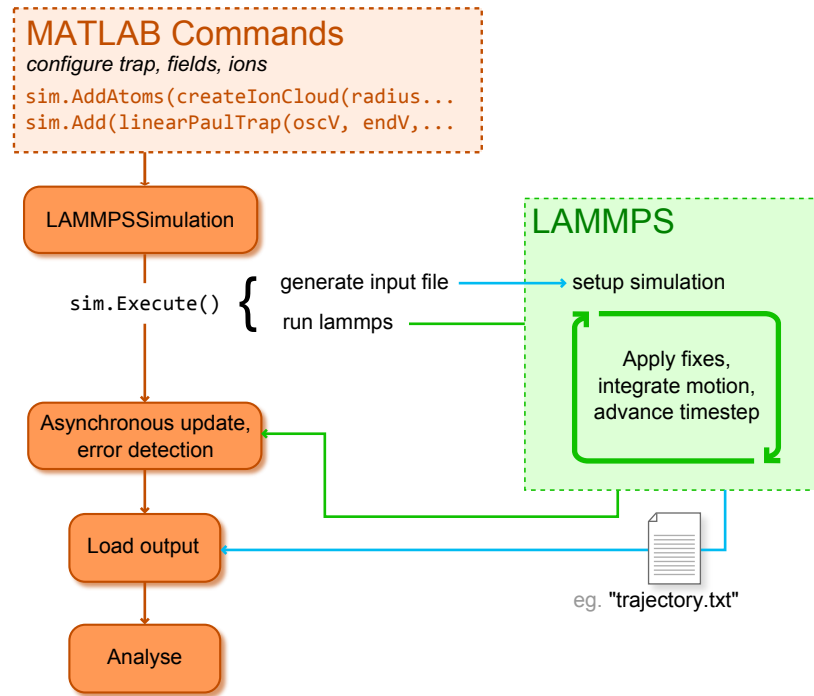


Figure 34: Flow diagram depicting configuration and execution of a LAMMPS simulation using Llon. Once the trap and ion cloud parameters are configured, control is handed to [LAMMPS](#) for the simulation while the Matlab command line is updated through an asynchronous loop. The output of the simulation is then loaded in Matlab for post-processing.

C.1.1 Writing the Input File

Simulations in [LAMMPS](#) are configured through a series of commands, input either via a console or read from an input file. To run the configured simulation, Llon first creates an input file comprised of the various facets of the simulation, then invokes an instance of [LAMMPS](#) with this file as input.

First, simulation level properties such as the definition of pairwise interactions are written to the input file. The simulation domain is fixed, atoms are placed and their properties defined (mass, charge, rigid body collections, etc.). If the simulation time step has not been explicitly set by the user, Llon chooses the largest timestep that resolves the highest characteristic frequency of the trapping fields — the [RF](#) field for full dynamics simulations or the trap frequency when the pseudopotential approximation is used.

Next, an enumeration is made through a cell array of `PrioritisedCfgObject`, whose elements individually define aspects of the simulation such as trap fields,

Name	Description
LAMPSSimulation	A simulation in Llon. See section C.1.2.
cfgObject	Base class for “elements” that comprise the input file to LAMMPS. See section C.1.1
PrioritisedCfgObject	Elements that are order specific within the LAMMPS input file.
LAMPSPFix	Elements representing fixes, e.g. electric fields, damping forces, Langevin baths.
LAMPSPRunCommand	Simulation commands, e.g. run, minimise.
LAMPSPDump	Implements a LAMMPS command that configures data output.
LAMPSPVariable	Quantities that may be output from LAMMPS via the dump command, which generates a LAMMPS-Dump object. See User Guide for detail.

Table 4: Overview and description of classes in Llon.

laser cooling forces, Langevin baths and were added to the LAMPSSimulation object during the configuration stage. The `cfgFileHandle` ordered method is invoked for each `PrioritisedCfgObject` and a portion of text is returned, written as a series of LAMMPS commands (see Table 5), which is added to the input file.

C.1.2 LAMPSSimulation Object

A simulation in LAMMPS is represented in Matlab by the LAMPSSimulation class. The implementation has made use of Matlab’s support for classes via `classdef` such that behaviour may be encapsulated, to expose public access only for those methods intended for the end-user. An overview of the different classes contained in the package is given in Table 4.

The LAMPSSimulation object’s function is to collate properties relating to the simulation, either directly (for example, the size of the simulation domain) or through collections of modular elements that define individual facets of the simulation. Examples of such elements include applied electric fields (a subset of *fixes* in the language of LAMMPS) and initial locations of atoms.

At the start of each Llon simulation, an object of this type should be created by invoking the `LAMPSSimulation()` constructor. In the following, when referring to a LAMPSSimulation object in both examples and text we will frequently use the shorthand `sim`:

```
sim = LAMPSSimulation();
```

LAMMPSFix	linearPaulTrap, sphericalPaulTrapPseudopotential, sphericalPaulTrap, linearPaulTrapPseudopotential, langevinBath, efield, cylindricalSH0, SH0, laserCool, fixNVEIntegrator
LAMMPSRunCommand	thermalVelocities, runCommand, placeAtoms, minimize, dump, defineSimulationBox, custom, createIonCloud

Table 5: Overview of commands for configuring simulation. See each individual command’s documentation for further detail or the worked example (Section C.4).

It is recommended that each `sim` be executed only once. Script files should be written with the creation of `sim` at the start of a section and `sim.Execute()` at the end. After this the user should avoid modifying `sim` (warnings are given should the user attempt to) in order that the `sim` object remain a faithful reflection to when the [LAMMPS](#) input file was written and executed and it can be linked to any subsequent simulation data output.

C.2 INSTALLATION & USER GUIDE

To use Llon the relevant files must first be added to the Matlab path variable. Included with the wrapper is the script `SetPaths.m`, located in the root directory, which performs this operation on execution. Changes made to path by this script are temporary — it should be run once at the start of each new Matlab session.

First time installation requires that the location of the [LAMMPS](#) executable is configured. This location should be stored in a file in ANSI format and saved at `LAMMPS Wrapper\Lammps.cfg`, and must include the executable explicitly. For example `C:\lammps\lmp_win_no-mpi.exe` is valid content for this file. Should a user attempt to execute a simulation without having performed this step an error will be thrown explaining the above.

This allows the user to use multiple versions of [LAMMPS](#) that have been built with different features, such as GPU acceleration through CUDA or openCL¹. The Llon user guide is distributed in the form of a Matlab html help package. Further information, including detailed descriptions of more examples and a complete documentation of all functions, may be found in it.

¹ On Windows operating systems use of the GPU accelerated packages requires the user to compile source code themselves. This may be done through cygwin, see tutorial on building [LAMMPS](#) under Windows.

C.3 VALIDATION SCRIPTS

To ensure data generated by [LAMMPS](#) is correct a number of verification programs have been written (see Table 6). The validation scripts provide a quick and easy way to ensure an extension does not render the wrapper unreliable. When modifying the wrapper a user should re-run these validations and ensure the output of each complies with the theoretical predictions — this ensures the integrity of the wrapper is maintained during further development.

Script	Assists with Verification of:
SecularFreqPseudoLinearPT	linear trap, pseudopotential
SecularFreqRFLinearPT	linear trap, full RF
SecularFreqPseudoSphericalPT	spherical trap, pseudopotential
SecularFreqRFSphericalPT	spherical trap, full RF
AxialSeparation	axial force of linear trap ion-ion repulsion
NormalModePseudoLinearPT	pseudopotential, linear trap, ion-ion repulsion
NormalModeRFLinearPT	RF linear trap, ion-ion repulsion
NormalModePseudoSphericalPT	pseudopotential, spherical trap, ion-ion repulsion
NormalModeRFSphericalPT	RF spherical trap, ion-ion repulsion

Table 6: Overview of validation scripts supplied with LIon.

C.3.1 *Single-Ion Validation*

The validation scripts `SecularFreqPseudoLinearPT` and `SecularFreqRFLinearPT`, each perform a series of simulations in [LAMMPS](#), the first using a pseudopotential approximation, which replaces the oscillating electric field with an appropriate harmonic trap of frequency ω_i , and the second using the exact electric field. The measured secular frequency of a simulation in [LAMMPS](#) is determined by the Fourier component of the single ion trajectory along each axis, that has the largest amplitude. This is plotted against theoretical predictions to verify the confinement potential is correct. Single-ion validations help verify the implementation of trap fields in LIon but offer no validation with regards to Coulomb-coulomb interactions between separate ions.

C.3.2 *Equilibrium Separation*

Linear Coulomb crystals are arrangements of ions along the axis of a linear Paul trap. They occur for tight radial trapping, where the highest-frequency axial normal modes of the crystal are a lower frequency than the lowest radial normal modes, such that the most energetically favourable configuration is a string of ions along the trap axis. Since the potential is mass dependent, the separation between ions depends on the number of ions in the linear Coulomb crystal.

Execution of the `AxialSeparation` script simulates a short dynamical evolution for small numbers of ions (2-10) which are quickly damped by a Langevin bath to cool them into their lowest energy configuration. The graph produced by the simulation compares these lowest energy configurations to theoretical predictions. While only applicable to a small numbers of ions, this validation is quick to run and assists with verifying that the correct Coulomb repulsion force is applied. Correct separations prove the Coulomb force extends over the entire crystal, and is not truncated by neighbour binning or the pair cutoff variable in `LAMMPS` (see for example http://lammmps.sandia.gov/doc/pair_coul.html).

C.3.3 *Normal Modes*

A more rigorous verification of the ion-ion repulsion forces, that can be applied to large numbers of ions and trap geometries other than linear, is to examine the normal mode spectra of ions. In the pseudopotential approximation, confinement along each axis can be considered harmonic in the limit of low a , q . To calculate the normal mode spectra we form the mass-weighted Hessian matrix of the atomic coordinates, for the lowest energy configuration of ions in the harmonic well. The eigenvalues of this matrix are the frequencies of each normal mode (given by the corresponding eigenvectors).

To validate the normal mode spectra of `LIon` we start with a number of ions in a trap. The energy of these ions is minimised — either the pseudopotential approximation of the trap or a heavily damped evolution in the full `RF` may be used. The final minimised position is taken to be the lowest energy configuration of the ions from which the mass-weighted Hessian is constructed. Once minimised, the undamped system is evolved for a large number of time steps and periodic kicks are given to the system by randomising atomic velocities. This ensures all normal modes of the system undergo some excitation and will be present in the final spectra. Positions are output twice every `RF` cycle. Limitations set by Nyquist's theorem make the micromotion not observable but the frequency of the normal modes of the system is necessarily much less than the `RF`.

Finally, atomic positions are loaded from the output file. Each atomic coordinate's Fourier transform is overlaid on the same axis, and theoretical normal mode frequencies are overlaid as red lines. For the pseudopotential approximation to the Paul trap, there should be perfect agreement between theoretical spectra and results from [LAMMPS](#). For the full [RF](#) electric fields slight deviation is expected [139, 160]. This validation of the ion-ion repulsion force may take a long time for large atom numbers. Several variants exist: `NormalModePseudoLinearPT`, `NormalModeRFLinearPT`, `NormalModePseudoSphericalPT` and `NormalModeRFSphericalPT`. All these scripts also ensure the correct trap forces are used in `Llon`, as an incorrect strength of confinement will result in erroneous spectra — however to verify this behaviour the method of Section [C.3.1](#) is much faster.

C.4 SIMULATION EXAMPLE

Here we demonstrate use of the `Llon` wrapper to configure an example simulation. In this simulation we create the electric field of an ion trap, confine a small cloud of ions and cool them by application of a Langevin bath. The positions of atoms are output every 10 timesteps, and a secular velocity is also calculated for each atom by averaging the instantaneous velocities over an [RF](#) cycle. The relevant script may be found in `Examples/SimpleExample.m` of the `Llon` distribution, along with more detailed examples.

First, we create a new `LAMPSSimulation` object by invoking the constructor for this class:

```
sim = LAMPSSimulation();
```

Next, we configure the simulation domain for the ions. This defines the minimum lower limit to the spatial region which will be simulated. The simulation box may expand beyond these initial limits, but all atoms must be initially placed within this region or an error will be thrown by [LAMMPS](#). More information may be found in the documentation for the [LAMMPS](#) `boundary` and `box` commands. A guideline for optimisation is to ensure the simulation domain fits the enclosed atoms tightly. This ensures that when the domain is spatially partitioned there are an approximately equal number of atoms per processor. When reducing the simulation box, the following error may be observed:

```
Cannot use neighbor bins - box size << cutoff
```

As discussed in the documentation on the `neighbour` command a solution is to use the `nsq` style to build neighbour lists. However, this comes with a caveat of worse scaling (proportional to number of atoms per processor squared). Alternatively, the neighbour “skin” size or the Coulomb repulsion cutoff may be reduced, but this

action may result in ion-ion repulsion not spanning the full length of the Coulomb crystal. It is advisable to re-run the verification of normal modes (see Section C.3.3) for a similar sized Coulomb crystal if these are changed. To set the initial simulation domain:

```
sim.SetSimulationDomain(1e-3, 1e-3, 1e-3);
```

Next we need to add some atoms. First we define a new atom type, specifying the charge and mass of the ion. Then we place three atoms along the z-axis of the trap at distances of $0, \pm 1 \mu\text{m}$ from the origin.

```
charge = -1;
mass = 30;
ions = sim.AddAtomType(charge, mass);
sim.AddAtoms(placeAtoms(ions, [0 0 0]', [0 0 0]', [-1 0 1]'*1e-6));
```

Then we add an oscillating electric field corresponding to a linear Paul trap geometry (following the notation in Berkeland et al. [161]). The trap below has an oscillating and endcap voltage of 300V and 1V respectively, $z_0 = 5.5 \text{ mm}$, $r_0 = 7 \text{ mm}$, geometric constant $\kappa = 0.244$ and $\text{RF } \Omega = 3.85 \text{ MHz}$. See `linearPaulTrap`'s documentation for more information:

```
RF = 3.85e6;
sim.Add(linearPaulTrap(300, 1, 5.5e-3, 7e-3, 0.244, RF));
```

To cool the translational motion of the ions, we attach a Langevin bath to the system. The bath specified here exponentially lowers the temperature of the ensemble to 3 mK by applying a viscous damping force with a relaxation time of $10 \mu\text{s}$ and a random “kick” each timestep.

```
sim.Add(langevinBath(3e-3, 1e-5));
```

Alternatively we could specify a more realistic model of laser cooling by applying the viscous damping force to only one axis of motion, so that only atoms propagating parallel a cooling laser beam are slowed, and discriminate between atom types, so that only one species is cooled. This allows simulations of sympathetic cooling rates similar to the methods of Zhang et. al. [130]. To add a laser cooling term:

```
sim.Add(laserCool(ions, [1e-5 0 0]));
```

where we have specified laser cooling along the x-axis only. We configure the simulation to output data by adding a dump to the `sim` object. In this example we output atomic positions every 10 steps and RF -averaged secular velocities every RF cycle.

```
sim.Add(dump('positions.txt', {'id', 'x', 'y', 'z'}, 10));
sim.Add(dump('secV.txt', {'id', timeAvg({'vx', 'vy', 'vz'}, 1/RF)}));
```


The `runCommand` is used to declare evolution for a number of timesteps:

```
sim.Add(runCommand(10000));
```

Having configured a simulation, we invoke execution. This writes the input file to [LAMMPS](#), launches a [LAMMPS](#) process and runs the simulation.

```
sim.Execute();
```

To finish the example, we read the atomic trajectories generated by the simulation (stored in `positions.txt`) and plot a 3D graph of the data:

```
[timestep, ~, x,y,z] = readDump('positions.txt');  
plot3(x',y',z');
```

Lion aspires to be a all-in-one solution for simulating the equations of motion of trapped charged particles. The language traditionally used in biochemistry has been translated using physical concepts and presented in a transparent way to the user.

PRECISE SHAPING OF LASER LIGHT BY AN ACOUSTO-OPTIC DEFLECTOR

We present a laser beam shaping method using acousto-optic deflection of light and discuss its application to dipole trapping of ultracold atoms. By driving the acousto-optic deflector with multiple frequencies, we generate an array of overlapping diffraction-limited beams that combine to form an arbitrary-shaped smooth and continuous trapping potential. Confinement of atoms in a flat-bottomed potential formed by a laser beam with uniform intensity over its central region confers numerous advantages over the harmonic confinement intrinsic to Gaussian beam dipole traps and many other trapping schemes. We demonstrate the versatility of this beam shaping method by generating potentials with large flat-topped regions as well as intensity patterns compensating for residual external potentials to create a uniform background to which the trapping potential of experimental interest can be added.

D.1 INTRODUCTION

Precise shaping of laser beams is crucial to their application as confining potentials for ultracold atoms. Notable among the applications for such trapped cold atomic systems is the quantum simulation of many-particle condensed matter systems in periodic potentials [162]. Beam shaping is increasingly important too in the creation, as well as subsequent manipulation, of a Bose-Einstein condensate (BEC). Following the initial demonstration of crossing the BEC transition by purely optical means [163], increasingly precise schemes have been developed by which to optically cool and compress an atomic cloud, including a proposed scheme whereby dynamic beam shaping techniques transform the potential between a sequence of power-laws [164]. Minimising perturbative effects in any such experiment requires the potential experienced by the atoms to smoothly and accurately conform to a target intensity. However, accurate beam shaping becomes more challenging the greater the deviation from the diffraction-limited Laguerre-Gaussian or Hermite-Gaussian propagation modes. Additional considerations include restricting the formation of interference fringes, caused either by rapid phase variations across the beam profile or high beam coherence in an imperfect optical system. Further constraints on optical potentials are imposed by the characteristics of the surrounding

experiment: stringent requirements on the form of a trapping potential may be at odds with the nature of any additional confinement.

A prominent starting point for many quantum simulation experiments is the experimental realisation of the Bose-Hubbard Hamiltonian achieved by loading quantum degenerate bosonic atoms into an optical lattice [2]:

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} a_i^\dagger a_j + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) + \sum_i \epsilon_i \hat{n}_i \quad (118)$$

This provides an experimental framework within which to simulate the electron gas in solids, with the freedom to tune interparticle interactions by manipulating lattice parameters. Investigations may be performed into the effects of disorder, and within the Mott Insulator regime whereby atoms are localised onto individual lattice sites into topological states in the fractional quantum Hall effect, or even as a starting point for a quantum register [165, 3, 166, 167]. However, the validity of the cold atom system as a quantum simulator strongly depends on the form of the trapping potential. The last term in equation 118 denotes an energy offset on individual lattice sites arising from a typically harmonic external atomic confinement. The spatial dependence of the system density arising from the external potential [2] associated with alternating superfluid and Mott-insulating regions is colloquially referred to as the ‘wedding-cake’ structure. The resultant blurring of phase transitions makes comparison with theory less direct; eliminating this effect would allow answers to open questions such as the phase diagram of the fermionic Hubbard model [168]. Precise control of the intensity distribution and elimination of external effects would be beneficial too in many other experimental situations including the observation of wave dynamics and quantum chaos using Bose-Einstein condensation confined in an optical corral-type potential [169].

Compensation for the harmonic trapping term can be achieved either by providing a uniform compensatory intensity canvas on which to form optical lattices produced using standard techniques such as standing wave interference, or by directly modifying the trapping potential of experimental interest. Flat-topped beams hold particular appeal in this regard, used either as a square well potential or to directly form standing wave optical lattices without a Gaussian envelope profile. Whatever the precise form of the chosen potential, an accurate and smoothly-varying beam profile is imperative to confining, manipulating and probing the trapped atoms.

The freedom to meet the constraints imposed on the optical potential by experimental applications is granted by relaxing restrictions on the trapping plane phase. Optical trapping of ultracold atoms is facilitated by the dipole force, associated with a potential $U_{dip}(\vec{r}) \propto \frac{I(\vec{r})}{\delta}$ with $I(\vec{r})$ the spatially dependent laser intensity and δ the detuning of laser light from resonance. The dipole force therefore depends on the intensity gradient of the laser light. Any phase gradient affects only the scatter-

ing force, negligible under detuning far from the atomic resonance due to its I/δ^2 dependence in comparison to the I/δ dependence of the dipole force.

Diffraction optical elements can be used to provide the necessary beam shaping precision and versatility. Using these techniques, we can obtain both continuous arbitrary intensity distributions and exotic lattice configurations inaccessible with standing wave interference alone such as circular distributions corresponding to an infinite 1D lattice [170, 171]. Our approach centres upon diffracting an incident laser beam using an acousto-optic deflector (AOD). The diffractive standing wave pattern established in the AOD crystal is determined by a multiplexed input acoustic frequency signal generated using an arbitrary waveform synthesiser (AWS). The relative amplitudes within the multiplexed input determine the proportion of the total light diverted into the first diffracted order corresponding to the appropriate frequency, such that the total intensity pattern corresponds to the sum of the constituent diffracted beams. We thereby achieve precise control over both the position and amplitude of each diffracted beam. The application to discrete lattice patterns is evident, but by calculating the effect of neighbouring beam sites on each other, this approach can be easily extended to produce arbitrary composite continuous patterns including flat-topped beams. Alternatively, rather than the superposition of static frequencies, rapid deflection of a single beam such that trapped atoms experience a time-averaged potential has been successfully demonstrated with minimal heating of trapped atoms [172]. A combination of time-averaging and the composite beam approach presented here could yield a smoothly dynamically-varying potential, additionally enhancing the scalability of both methods.

A popular alternative approach to generating arbitrary and dynamic potentials is to use a computer-generated hologram imposed on an incident laser beam using a spatial light modulator (SLM), an array of either liquid crystal or micro-mirror pixels programmatically altering the beam phase. Improved versatility in the range of accessible potentials is granted the higher the phase resolution of each pixel, though this increases the complexity of the required numerical phase profile calculation. Iterative Fourier transform algorithms (IFTAs), of which multiple variants exist [173], are extensively used to perform these high-resolution phase calculations. Pixel switching frequency is an important consideration if dynamic manipulation of trapped atoms is an experimental goal. The Texas Instruments digital micro-mirror device (DMD) SLM has a switching frequency on the order of 50 kHz, and a Boulder Nonlinear Systems ferroelectric liquid crystal SLM around 1 kHz. However, these are both binary devices; with a phase resolution of $2\pi/256$, a Boulder Nonlinear Systems nematic liquid crystal SLM is capable of a far more versatile range of truly arbitrary potentials, but the switching frequency of hundreds of Hz could limit their applicability to dynamic manipulation of optical trapping potentials. An AOD update frequency on the order of 10 MHz, allowing the successful

low-noise dipole trap painting in reference [172], allows almost seamless switching between dynamic frames, thus combining the versatility and switching rate necessary for an arbitrary dynamic manipulation sequence.

In experimental situations without restrictions on the image plane phase, a significant advantage of using an AOD to form large continuous patterns is that the resultant potential is composed of multiple beams of different frequencies, the precise frequency separation dependent on the desired beam location and the details of the optical system. This frequency difference circumvents interference effects associated with a highly coherent single sculpted beam. Furthermore, despite power losses associated with diffraction into the zeroth and higher orders, these unwanted beams are easily eliminated from the trapping plane intensity distribution. In contrast, achieving the highest accuracy reproduction of large continuous arbitrary targets using spatial light modulation requires introduction of limited amplitude freedom in the trapping plane [173], resulting in a significant noise accumulation near the trapping potential which could detrimentally perturb the experimental system.

We illustrate below the accuracy and versatility of the composite beam method for a range of continuous trapping potentials, and demonstrate a process by which an external potential can be compensated to produce a trapping potential tailored to specific experimental requirements. The first example compensates a harmonic term in a square well target potential; the applicability of the AOD beam shaping method to arbitrary continuous potentials is then illustrated, indicating the power of the method in both creating and compensating arbitrary continuous potentials as required by the experimental conditions. Details of the experimental methods follow these examples.

D.2 BEAM SHAPING USING AN ACOUSTO-OPTIC DEFLECTOR

D.2.1 *Compensation potential*

The effect of the additional harmonic confinement term is perhaps most immediately obvious with regard to flat-topped target potentials, although the compensation principle is identical irrespective of the target. As discussed above, such flat-topped beams are experimentally applicable both in their own right and as a canvas on which to produce other arbitrary potentials.

To create a flat-topped beam using the superposition of diffracted beams, we initially consider the Sparrow resolution criterion [174, 175]. This refinement of the Rayleigh criterion is a popular criterion in astronomy, stating that multiple beams are indistinguishable, i.e. their composite intensity distribution perfectly flat, if the

second derivative of this distribution is zero. The spacing a between adjacent beams to achieve a flat-topped composite potential is therefore chosen according to:

$$\frac{d}{dx}\{f(x) + f(x+a)\} = 0 \quad \text{and} \quad \frac{d^2}{dx^2}\{f(x) + f(x+a)\} = 0 \quad (119)$$

In two dimensions, the intensity distribution $f(x, y)$ is the sum of the N constituent Gaussian beams, with $1/e^2$ waist w , and relative amplitudes A_n and positions (x_n, y_n) :

$$f(x, y) = \sum_n^N A_n e^{-2((x-x_n)^2 + (y-y_n)^2)/w^2} \quad (120)$$

The accuracy of this approach diminishes with an increasing number of constituent beams, so the beam spacings calculated using the Sparrow criterion are used as a starting point for a feedback process that iteratively optimises beam spacings and relative amplitudes based on the intensity variations measured across the composite beam profile.

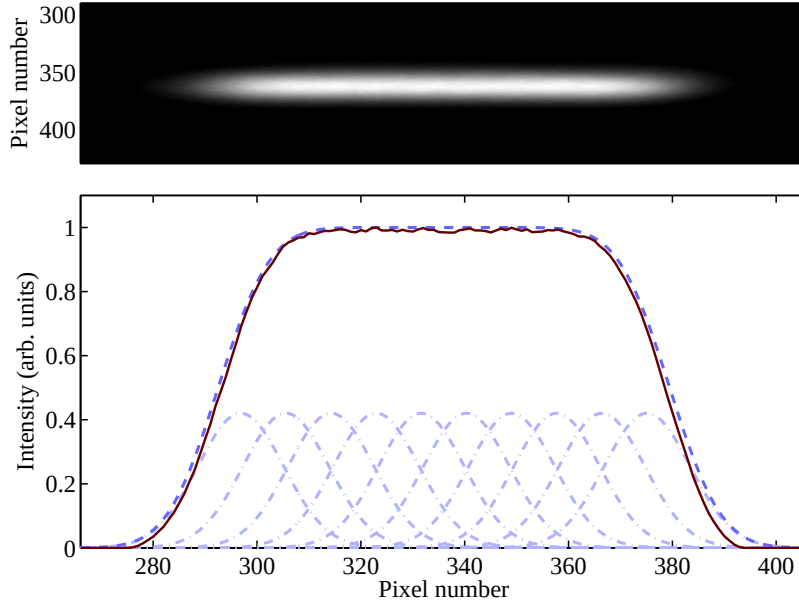


Figure 35: Intensity distribution measured using a CCD camera (top) for a flat-topped beam comprising ten individual Gaussians of identical amplitude, with a line profile (bottom, solid line). Superposition of the dash-dot Gaussians yields the calculated target intensity distribution (dashed line).

Figure 35 shows the experimental realisation of a flat-topped intensity profile comprising 10 deflected beam components. In this case, the Sparrow criterion suggests a separation between adjacent beams of $a = 0.527w$, with w the beam waist. After optimisation, the experimental error is 1.4% over the flat region of the intensity profile and 2.3% over the full distribution. In this and subsequent figures, the

corrugations visible on the compensation potential arise from dust specks on the imaging camera rather than being features of the potential itself.

Using a sequence of equal-amplitude constituent beams, the composite potential has a power-law dependence scaling approximately with the number of beams used:

$$I(x) = \sum_n A_n x^n \quad (121)$$

The beam shown in figure 35 is therefore associated with a potential proportional to x^{10} . Whilst the example shown is for a single row of Gaussians, this principle can be readily extended to constructing arbitrary-shaped two-dimensional potentials by deflecting the beam in both x - and y -directions with separations calculated as above (see the Experimental Techniques section in the appendix for discussion of the dual-axis AOD). The only subtlety arising from additional rows of beams is that if the frequency spacing is equal in both x - and y -directions, then beams lying along diagonal lines have the same frequency and thus interfere. Such undesirable interference is easily avoided by using different frequency spacings and elliptical spots to maintain the Sparrow criterion; elliptical distributions occur anyway in the focal plane of an optical system with a high numerical aperture and linearly polarised light [176]. This extension is simple in comparison to a similar extension of the target output of a computer-generated hologram. With an IFTA used to improve the range and versatility of accessible patterns, hologram calculation becomes more complicated for large continuous potentials due to the appearance of optical vortices in the calculation process [177]. However, with an appropriate Sparrow separation calculation, the superposition of deflected AOD spots is identical in both directions. Furthermore, limited by a finite pixel array, spatial light modulators find it difficult to realise a sharp edge to a flat-topped beam due to the high Fourier-space frequencies required. A super-Lorentzian target array is therefore often used, the order of which is a compromise between flatness and calculation accuracy. The AOD composite beam approach, however, has an intensity falloff limited only by the beam waist. For example, using a composite flat-top consisting of 10 beams as in figure 35, the intensity falls from 95% of its maximum value to 5% over $1.6w$, whereas an eighth-order super-Lorentzian as demonstrated in [178], of identical width, has the same intensity falloff over $2.0w$. The accuracy of exotic patterns calculated using an IFTA can be improved by incorporating Helmholtz propagation into the hologram calculation process [179]. However, this does not as yet match the approximately 1% RMS error setting the current accuracy limit on a flat-top generated by spatial light modulation [178], albeit generated using a binary device that limits the complexity of possible target patterns. This SLM accuracy limit is slightly higher than the accuracy obtained using the AOD com-

posite beams above. However, this small difference in accuracy is compensated by the edge definition and greater intensity distribution complexity possible with the AOD as opposed to a binary SLM.

However, these flat-topped beams are unlikely to be used in isolation. Typically harmonic, the external potential of a magnetic trap or additional dipole trapping beam will dominate over higher-order power-law terms unless compensated. The flexibility of the composite beam AOD approach allows such compensation to be implemented straightforwardly, with a potential cancelling out the dominant low-order terms of the power-law Taylor expansion created by manipulating the light field parameters.

A harmonic potential along the x-axis can be expressed as a Taylor series up to the order we want to cancel:

$$V_{tot}(x) = \sum_{n=0}^N \frac{V_{tot}^{(n)}(x_0)}{n!} (x - x_0)^n + \mathcal{O}(N+1) \quad (122)$$

Along the same axis the AOD-generated composite potential has the form:

$$V_{dip}(x) = \sum_{n=1}^N a_i V_{beam}(x - s_i) \quad (123)$$

where N is the number of beams used, a_i the amplitude of each beam, s_i the displacement along the x-axis, and $V_{beam}(x)$ the Gaussian function produced by each constituent deflected beam. The optimal set of parameters a_i, s_i to cancel the external potential are determined using an optimisation routine.

Figure 36 illustrates the use of 6 blue-detuned beams to cancel an $\mathcal{O}(2)$ term, with matching performed using the Taylor expansion of the potentials. For this example, the experimental error over the entire pattern is 1.8%.

Smoothing the nonuniform density distribution of an ultracold gas cloud trapped in an optical box has been experimentally demonstrated using repulsive spots of laser light positioned using an acousto-optic modulator at points along the axis of the cloud [180]. This illustrates the viability of the compensation method in correcting small-scale or rapidly-varying beam imperfections that can fragment the cloud. However, the current approach and potential generated in figure 36 focusses primarily on offering compensation for large-scale external or residual continuous harmonic potentials perturbing the overall form of the trapping potential. As in reference [180], these may be superimposed onto a dipole potential to smooth out the residual confinement terms and provide a uniform intensity canvas, but the combination of this compensation with continuous beam shaping also allows the trapping laser beams to be directly modified.

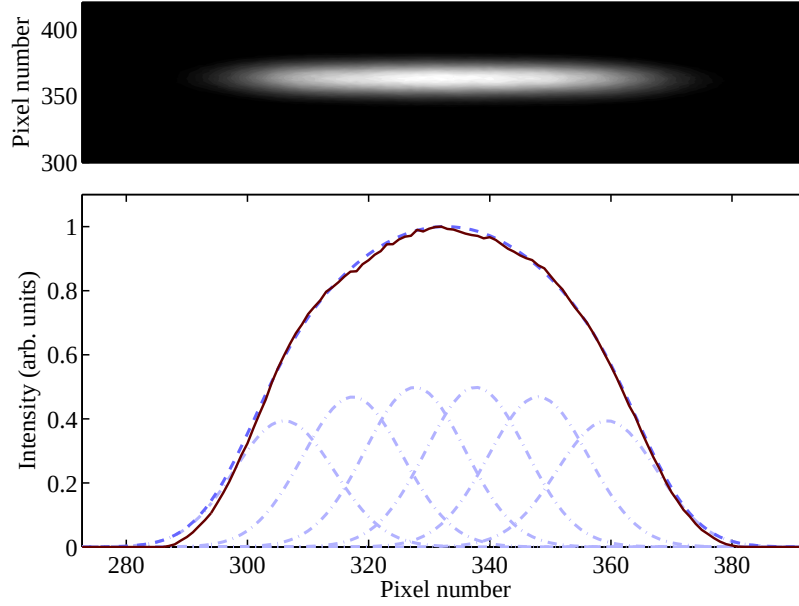


Figure 36: Intensity distribution measured using a CCD camera (top) and the corresponding line profile (bottom, solid line) for a harmonic compensation potential, with the target intensity distribution (dashed line) the sum of the dash-dot Gaussians.

D.2.2 Arbitrary continuous potentials

As indicated by the ability to modify the target to incorporate a compensation term, this beam sculpting approach can be applied to generating arbitrary discrete or continuous trapping potentials. The example illustrated in figure 37 extends the flat-topped beam of figure 35 by the addition of a spatially separated single Gaussian, to form a potential analogous to a single well connected to a reservoir of variable size. This type of potential has been used for theoretical studies of tunneling and decoherence [181] and our method is well-suited to realising this in practice.

The flat-topped reservoir of figure 37 consists of 9 deflected beams, optimised from the starting point of equal amplitude and a Sparrow separation of $0.616w$. The well depth is controlled by a low-amplitude Gaussian midway between the reservoir and a spatially separated single well. The parameters defining the potential and the interplay between reservoir and single well are sufficiently flexible that the intensity distribution can be easily and precisely modified, allowing dynamic real-time manipulation of trapped atoms. The illustrated experimental realisation has an error of 2.1% over the entire pattern region.

This example illustrates the utility of this method in generating both arbitrary, non-symmetric continuous potentials, and single diffraction-limited points that could be arranged in a discrete lattice structure. Although this method is most suit-

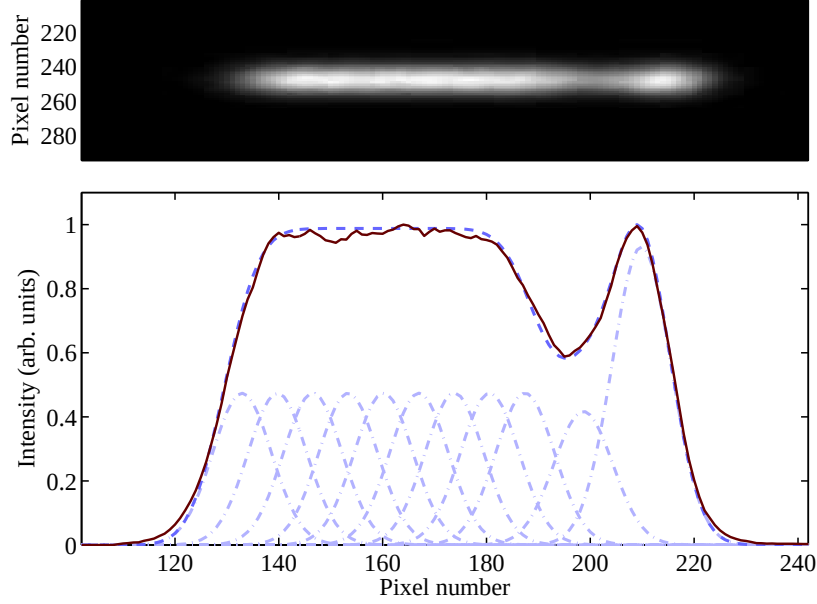


Figure 37: Intensity distribution measured using a CCD camera (top) and corresponding line profile (bottom, solid line) for an extension of the flat-topped beam creating a broad reservoir connected to a single well, with applications to studying decoherence in quantum systems. The target intensity (dashed line) is the sum of the dash-dot Gaussians.

able for shapes that can be expressed as sums of Gaussians, this is not a significant limitation: numerous arbitrary intensity distributions can be generated with a high level of accuracy. The reproduction accuracy of all patterns could be significantly improved with further optimisation.

D.3 CONCLUSION

The power of the composite beam method lies in its simplicity. With rudimentary optimisation based on feedback from the external system used to inform choice of the applied field, large continuous potentials, or indeed discrete patterns, may be reproduced without loss of accuracy resulting from interference or increased numerical calculation complexity. Arbitrary patterns, particularly flat-topped beams, can be produced with an error of around 2%, comparing favourably to results demonstrated using SLM techniques, and without compromise on either versatility or frame update rate. Systematic optimisation would further enhance this accuracy. Although approached from the opposite direction, superposition of constant frequencies is comparable to the rapid painting of a single beam presented in [172] in terms of the access to arbitrary continuous potentials with high reproduction accuracy; furthermore, the scalability of each of these methods could be enhanced by their combination.

Alongside other examples, the versatility of the approach has been utilised in producing a blue-detuned compensation potential, which could be used either to directly shape a target potential, or as a compensatory canvas on which to construct additional potentials. This could significantly improve the relation of quantum simulation experiments to theoretical calculations, allowing phase transitions to be investigated with greater clarity. The compensation process could also be applied in SLM-based experiments, although measures would have to be employed to restrict vortex formation in large continuous distributions. Whilst this investigation focussed upon flat-topped and compensatory potentials, and a uniform continuous potential for decoherence investigations, the precise shaping inherent in the composite beam approach holds universal appeal in accurately shaping arbitrary discrete and continuous trapping potentials for a wide range of processes.

D.4 EXPERIMENTAL TECHNIQUES

Beam shaping is performed using a dual-axis AOD (Isomet LSA110A-830XY). Aligned to a central frequency of 45 MHz, angular deviations in either the x- or y-directions are determined according to

$$\Delta\theta = \frac{\Delta f \lambda}{u_s} \quad (124)$$

where $u_s \approx 610 \text{ ms}^{-1}$ is the measured speed of sound in the AOD TiO_2 crystal, Δf the frequency deviation and λ the wavelength of light used: 780 nm in section D.2.1 and 830 nm in section D.2.2. The resultant linear separation of spots corresponding to different diffraction angles is fixed by a lens placed at a focal length from the AOD, serving to focus the spatially separated beam components onto a CCD camera (Unibrain Fire-i 521b) as well as ensuring parallel propagation to this point. For imaging purposes, this focussing lens was of focal length $f = 40 \text{ cm}$ in section D.2.1 and $f = 50 \text{ cm}$ in section D.2.2, yielding diffraction-limited beam sizes of $162 \text{ }\mu\text{m}$ and $203 \text{ }\mu\text{m}$ respectively. To apply this technique to dipole force traps requires significantly smaller diffraction-limited beam sizes; for example, an objective lens with a focal length of 4 cm and corresponding diffraction-limited beam size of $1.6 \text{ }\mu\text{m}$ would feasibly produce a trapping frequency of a few kHz. This is well below the hundreds of kHz acoustic deflection frequency difference between constituent beams of the composite potential such that any beating between neighbouring spots will have no influence on trapped atoms.

Relative amplitudes A_n and image-plane positions (x_n, y_n) of the multiple spots comprising the sculpted beam are computationally determined by fitting a function corresponding to equation 120, a sum of Gaussian beams, to a target intensity array with the Sparrow criterion providing a useful starting point for flat-topped beams. A small amount of manual optimisation is performed on the experimental output,

although the results are likely to benefit from an automated optimisation routine as has been demonstrated in conjunction with an IFTA for holographic beam shaping [182]. The frequencies corresponding to the necessary relative separations are calculated, and then imposed upon the AOD using an arbitrary waveform synthesiser (AWS) (Hewlett Packard 8770A). Granting independent control of the relative amplitudes a_i of its constituent frequency components f_i , the AWS output resembles a multiplexed signal of the form:

$$f_{out} = \sum_{i=1}^N a_i f_i \quad (125)$$

With a maximum output of 1 dBm, the AWS signal is first amplified using a 1.6 W amplifier (Motorola CA2832C). The calculated frequencies are transmitted to the AWS internal memory using a Labview GPIB interface; the frequency is incorporated in the expression for the output signal via the input value n according to the 125 MHz internal clock frequency:

$$f = \frac{n}{\text{number of elements}} 125 \text{ MHz} \quad (126)$$

A series of spatially separated spots requires an output signal consisting of all appropriate frequencies at the correct relative amplitudes to create the multiplexed standing wave diffraction pattern in the AOD. The GPIB signal takes the form:

$$S_{in} = \sum_i a_i \sin\left(\frac{2\pi n_i}{L}\right) \quad (127)$$

Where a_i is the amplitude associated with each frequency f_i , with the total amplitude less than 2048, and L the total packet length. The packet length is the number of total number of points per period multiplied by the total number of periods in each wave segment, and must be less than 5320. The number of points per period is a compromise between being a multiple of 8 and a multiple of the time period associated with the lowest beating frequency in the signal as a fraction of the internal clock period. This latter condition minimises flicker at the start of each wave segment loop. The number of deflecting frequencies output through the AWS at a single time can limit the complexity of the composite intensity profile. However, the examples illustrated above demonstrate that even a restricted number of deflected beams can be used to accurately reproduce a range of potentials.

DESIGN OF A MILLIMETRE-SCALE MAGNETIC SURFACE TRAP FOR COLD ATOMS

We study a novel millimetre-scale magnetic trap for ultracold atoms, in which the current carrying conductors can be situated outside the vacuum region, a few mm away from the atoms. This design generates a magnetic field gradient in excess of 1000 G/cm at a distance of 2 mm from the conductors. We perform electromagnetic and thermo-mechanical characterisation using Finite Element Methods (FEM). The predicted behaviour has been verified by electrical and thermal measurements on a prototype, but has not been implemented on an apparatus with cold atoms. Operating this trap at the highest gradient allows rapid evaporative cooling comparable to that achieved by atom chips.

E.1 INTRODUCTION

The confinement of atoms by magnetic fields is widely used to hold clouds of atoms in a region of high vacuum where they are well insulated from the environment. This enables atoms to be cooled by evaporation, and if the density is sufficiently high, quantum degeneracy can be achieved in dilute atomic vapour. Bose-Einstein condensation was first observed using a Time-Orbiting Potential (TOP) trap based on a quadrupole magnetic field with an additional rotating bias field [183], and soon after in a Ioffe-Pritchard with static fields [184, 185]. There are numerous other trapping configurations including a combination of magnetic fields and repulsive dipole forces from a laser beam (plugged quadrupole) and dressed-atom adiabatic potentials [185, 12], both of which can be used to form ring-shaped clouds as well as simply connected geometries. Instead of classifying traps by their principle of operation, they can be categorised by their method of construction.

The first generation of traps were wound with water-cooled copper wire, outside the vacuum chamber in most cases, so that the current carrying conductors were at least a few centimetres from the atoms – we call these cm-scale traps. Later, so-called atom chips were developed using microfabricated wires on the surface of a substrate inside the high vacuum only tens of micrometres away from the atoms [186, 187, 188, 189, 190, 191, 192]. The advantage of having the atoms in close proximity to the wires can readily be seen by differentiating the expression obtained from the Biot-Savart law; the force on the atoms is proportional to the gradient of the magnetic field which is $B' = (\mu_0/2\pi) I/r^2$ at a distance r from a wire carrying

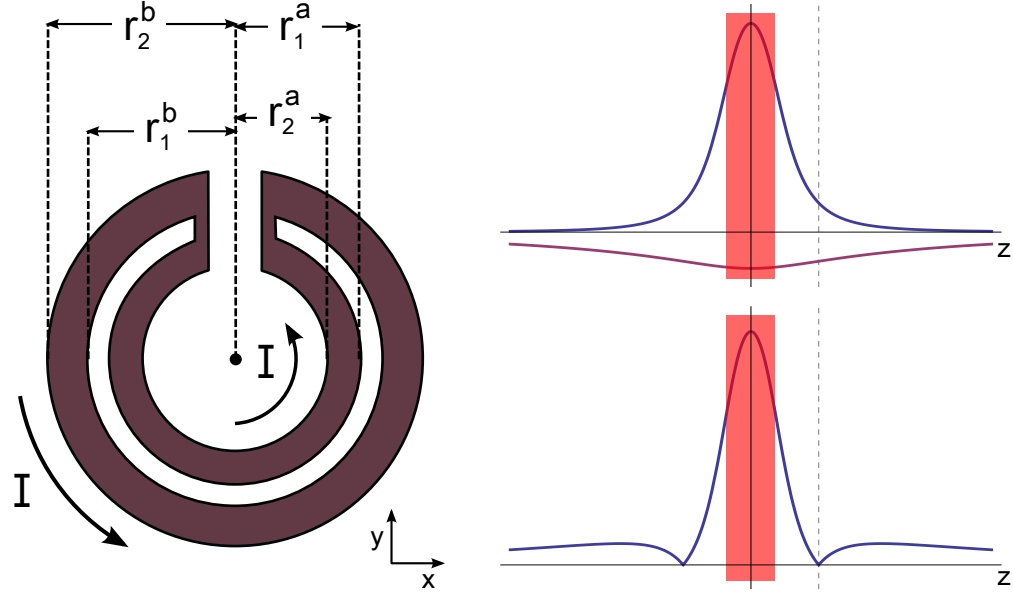


Figure 38: Current flows counterclockwise in the inner ring and in the opposite sense in the outer one. The inner, outer radii are 1 mm, 2 mm, and 3 mm, 24 mm for the inner and outer ring respectively. The plots on the right hand side show the field from each ring (upper) and the total field of the configuration (lower). The field is zero at a point about 2 mm from the surface of the conductors. The extent of the 2 mm thick conductor is shown in red block shading.

current I , e.g. a distance $r = 10 \mu\text{m}$ and $I = 1 \text{ A}$ gives $B' = 2 \times 10^5 \text{ G/cm}$. In many atom chips the conductors lie in the same plane; the use of a surface trap to give a Ioffe field was described by Weinstein and Libbrecht [193] which resembles the design presented here. However, shortcomings of atom chips include the restriction of optical access when there is a surface close to the atoms. Also the region of space over which the trapping field extends is relatively small and an auxiliary trap is required to load atoms into the small capture volume. A key advantage of the small scale traps is their much lower power dissipation, e.g., to reach gradients of 1000 G/cm a typical cm-scale trap will dissipate electrical power of several kW which is somewhat cumbersome although readily manageable in a laboratory environment with suitable electrical power supplies and cooling.

There has been some work with conductors of intermediate size, which we call mm-scale traps, notably [194, 195, 196, 197], and we give details of a new trap of this type in this paper. The design goals were to achieve the required magnetic field gradient with current conductors outside the vacuum region, using only a moderate electrical power of about 1 kW. We assume that the atoms are 2 mm from the current carrying conductors, i.e. the vacuum windows are thin ($< 1 \text{ mm}$). Moreover the design allows for a 1 mm diameter hole through which a laser beam can be directed along the symmetry axis of the trap, thus making it compatible

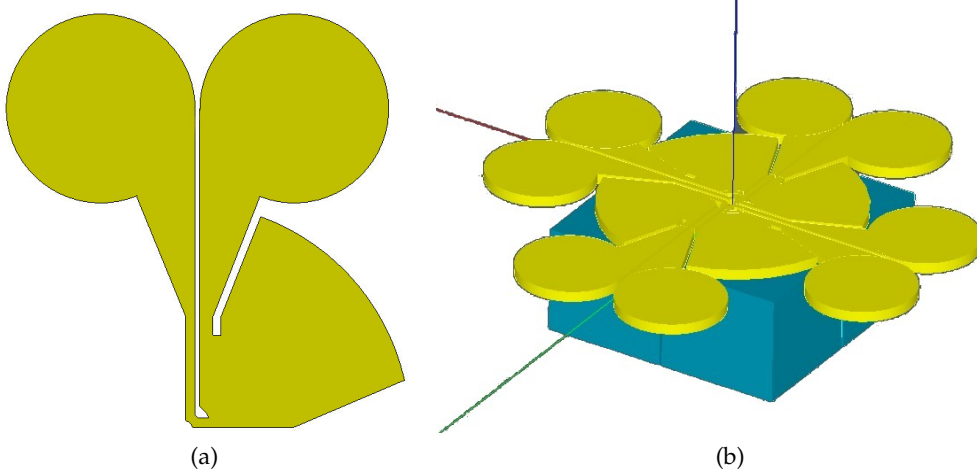


Figure 39: Design of the patterned planar conductor. (a) The trap comprises of four identical slices with electrical connections made at the large disks around the outer circumference. The various cuts in the conducting slices force the current flow to be clockwise on the outer ring and anticlockwise on the inner one as it flows between the two electrical connections. The radii of the rings are the same as in Fig. 38. (b) A schematic of the assembled trap mounted on a cooling block. The block is divided into four electrically isolated pieces in order to avoid unwanted eddy currents.

with optical lattice experiments. In such experiments the beams forming the lattice typically have a waist size of $100\mu\text{m}$ to $300\mu\text{m}$ to facilitate overlap and give a long Rayleigh range. In this paper we report on the design and preliminary testing of the thermal loading and field measurements, but not actual trapping of atoms. However confinement of cold atoms is possible by various approaches using a magnetic quadrupole field and a suitable ultra-high vacuum apparatus.

E.1.1 Principle of operation

Quadrupole traps are often formed by using two coaxial coils of equal dimensions that are not on the same plane, with current flowing in opposite directions. In contrast, this design generates a quadrupole field using two concentric rings of different radius (lying on the same plane) [198] as illustrated in figure 38. The coils are connected in series so that the current flowing through them is equal. We calculate the magnetic field using the Biot-Savart law. Integrating the contributions to the field over the radial and angular coordinates of a current carrying loop gives the field along the symmetry axis as follows:

$$B = \mu_0 \sqrt{\frac{P\lambda}{r_1\rho}} G_z \quad (128)$$

where P is the total power dissipated in the conductor, λ is a numerical factor which accounts for the non-uniform distribution of current in the conductor, ρ is the resistivity of the conductor, r_1 is the inner radius of the conductor, and

$$G_z = g \left((\gamma + \beta) \log \frac{\alpha + \sqrt{\alpha^2 + (\gamma + \beta)^2}}{1 + \sqrt{1 + (\gamma + \beta)^2}} - (\gamma - \beta) \log \frac{\alpha + \sqrt{\alpha^2 + (\gamma - \beta)^2}}{1 + \sqrt{1 + (\gamma - \beta)^2}} \right) \quad (129)$$

This unitless geometric factor depends on $\alpha = r_2/r_1$ which is the ratio of the outer radius of the conductor r_2 to the inner radius r_1 , $\beta = l/2r_2$ which is the ratio of the thickness of the conductor l to the outer radius and $\gamma = (z_2 + z_1)/2r_1$, a rescaled coordinate with z_1, z_2 being the distance to the point where the magnetic field is measured on axis from the close and the far surface of the conductor respectively and $g = [8\pi\beta(\alpha^2 - 1)]^{-1/2}$. In our configuration, the total field produced is simply calculated as the sum of two rings with opposite currents and different sizes.

The non-uniform current density distribution in the actual trap leads to a reduction in the magnetic field as compared to the field produced by two ring conductors with uniform current density. Fitting the data from the finite element analysis with Eq. 128 we find $\lambda = 0.39$. The atoms are trapped near the zero of the magnetic field where the field contributions from the two rings with opposite currents cancel each other. We simulated the behaviour of this current distribution using the software package RADIA from the European Synchrotron Radiation Facility [199]. As can be seen in figure 38, both rings give magnetic fields that have a maximum at the centre but the field from the smaller ring falls off more rapidly with distance than that of the larger ring. The position where the two fields cancel depends on the geometry of the conductors and the current flow.

Cold atoms in a magnetic trap follow the field adiabatically so that the trapping potential only depends on the magnitude of the field. Atoms are only trapped in weak-field seeking states because a static magnetic field cannot have local maxima in free space. Since such states are not the minimum energy states, atoms may be ejected from the trap by inelastic collisions and can be lost from the trap through Majorana transitions when they pass near a point where the field is zero [200]. One way to plug the leakage of atoms through Majorana spin flips is by creating a TOP trap [183]. This can be implemented by modulating the current of each quadrant of this trap or by the addition of a rotating bias field generated using external coils. The inductance of the trap is of the order of a few nH which means it cannot be measured easily. The eddy currents are thus not expected to be significant and can be further reduced by reducing the surface of the trap if necessary.

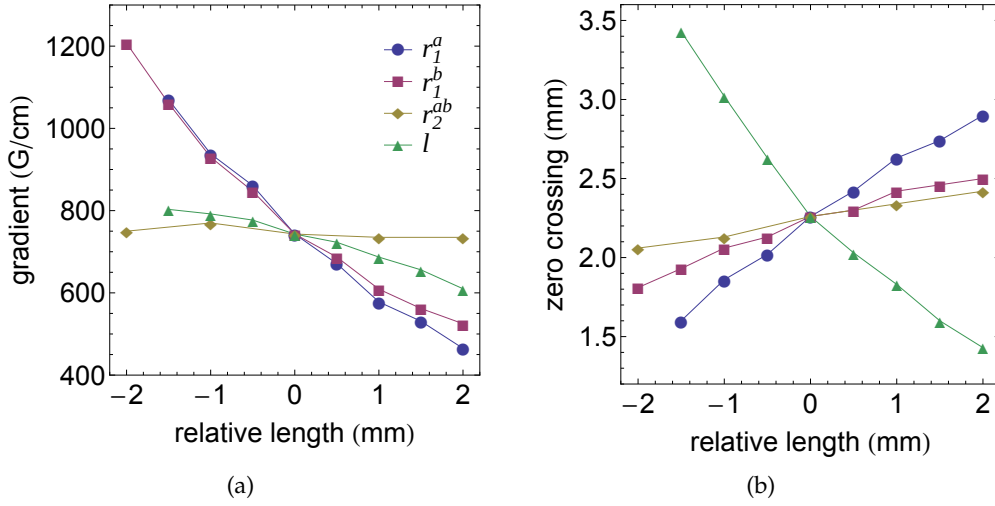


Figure 40: Effect of varying the relevant dimensions of the trap on (a) the magnetic field gradient and (b) the point where the magnetic field is zero measured from the surface of the trap. The dimensions are referenced to the initial conditions that were chosen to be the dimensions of the two concentric rings (see Fig. 38). The lines are a guide to the eye.

E.2 DESIGN OF THE PATTERNED PLANAR CONDUCTOR

Based on the above considerations we designed a trap capable of producing high magnetic field gradients while still mounted outside the vacuum apparatus. In each of the four identical pieces shown in figure 39, current flows in through one contact point (disk) and out through the adjacent disk. We designed the trap using freely available finite element software included in the CAELinux distribution ¹. Our optimised design generates a quadrupole magnetic field with a gradient in excess of 1000 G/cm centred at a distance of 2 mm from the top surface of the conductors.

We used the approximation of two current-carrying rings (as in figure 38) to determine the initial values for the dimensions of the trap. Although numerical optimisation techniques can be used [201], simply varying the parameters relative to the initial values is adequate for observing the trends shown in figure 40. The position where the field is zero increases with increasing radii. Decreasing the thickness has the same effect albeit much more pronounced. The gradient increases when decreasing any of the dimensions, with the thickness of the trap and the dimensions of the outer ring contributing the most. With these trends in mind we

¹ The Computer Aided Engineering Linux distribution <http://www.caelinux.com/CMS/> is based on Ubuntu and includes a plethora of open-source software. The SALOME project <http://www.salome-platform.org/> aims to develop an open-source CAD-to-FEA link based on Open CASCADE. Elmer <http://www.csc.fi/english/pages/elmer> is an open-source multiphysical simulation software that uses the Finite Element Method to solve the partial differential equations describing a physical system.

chose the three innermost radii to be as small as possible and scaled r_2^b to increase the distance from the front surface of the conductor where the field is zero. We also try to keep l as small as realistically possible. The dimensions of the final trap are $r_1^a = 1$ mm, $r_2^a = 2$ mm, $r_1^b = 3$ mm, $r_2^b = 24$ mm and $l = 2$ mm. These values optimise the gradient for a given current at a fixed distance from the surface of the conductors.

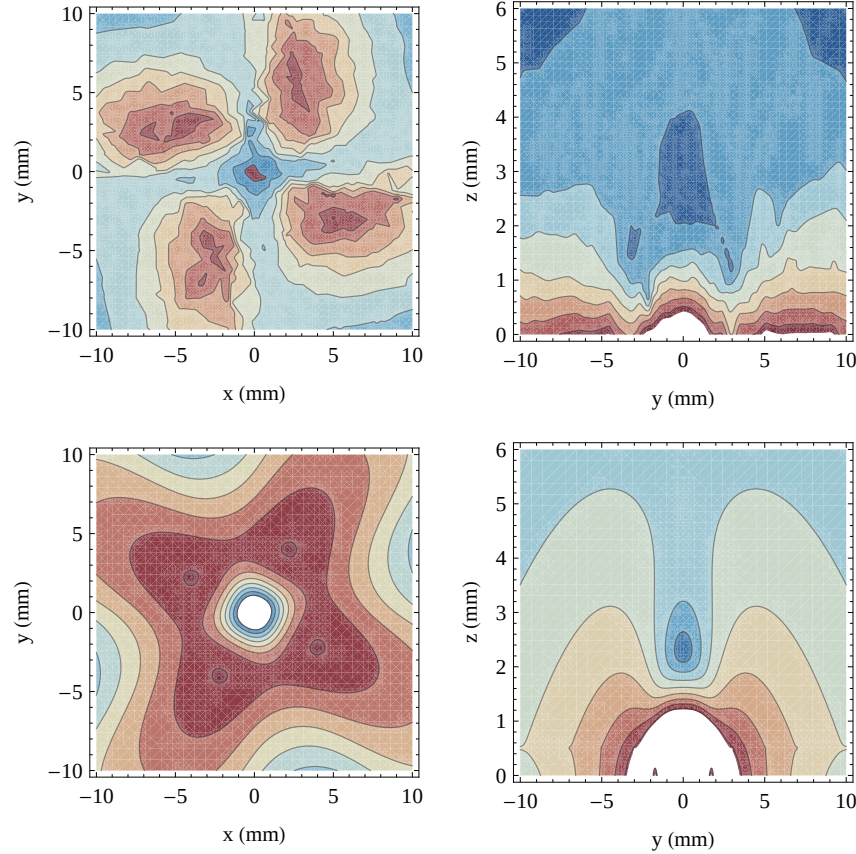


Figure 41: Contour plots of the magnetic field amplitude along the xy -plane for $z=2.5$ mm where the field is zero (first column) and yz -plane (second column). The top row figures show the FEM output while the bottom ones the idealised results from the Radia software. The effect of the non-uniform current density can be clearly seen on the xy -plane. A grid of size $\delta x = \delta y = 65 \mu\text{m}$ and $\delta z = 40 \mu\text{m}$ was used for the FEM simulations, leading to simulation times of a few hours.

The magnetic field of the optimised trap is shown in figure 41. The Finite Element Method (FEM) shows the true distribution taking into account the steady-state non-uniform current density within the conductors, including the effect of their shape and temperature variations with position. For comparison we also plot the idealised magnetic field distribution. It is interesting to note in figure 41 that there is an apparent rotation of the field on the xy -plane. This is due to the profile of the current distribution (figure 42a) which is dictated by the shape of the trap. The

current density increases significantly at the conical entry point and this manifests as an apparent rotation of the magnetic field.

The trap behaves like a surface trap albeit at a much larger scale. Its fourfold symmetry does not give rise to multipole orders of the field higher than the quadrupole. The depth of the trap is determined by the difference in the amplitude of the field between the zero point about 2 mm above the conductor and the secondary maximum about 4 mm above where the field is 200 gauss (for 400 A). This corresponds to a trap depth of 6.7 mK. This is over an order of magnitude higher than the temperatures than can be achieved by laser cooling of atoms, e.g., the Doppler cooling limit for atomic rubidium is 140 μ K. Thus, loading of the trap is expected to be straightforward by directly capturing the laser-cooled atoms without the use of an additional compressing trap.

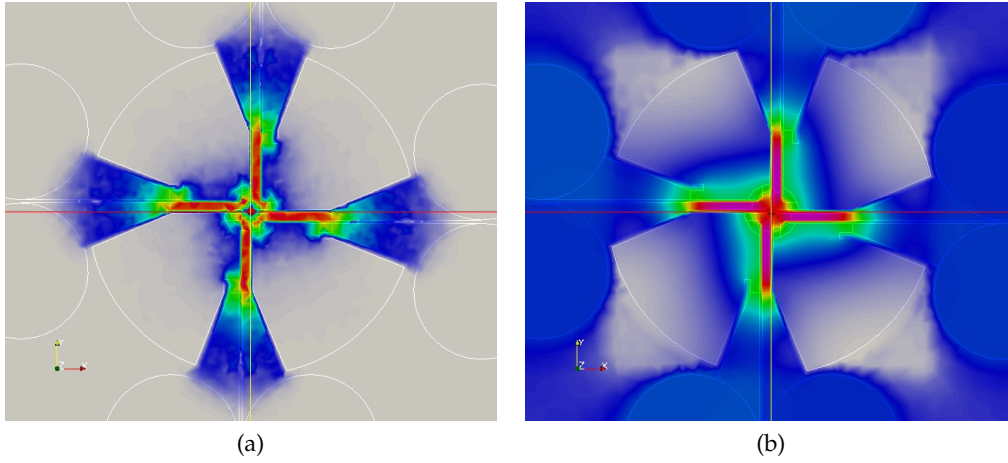


Figure 42: (a) The current density distribution and (b) the temperature distribution are closely related. The maxima of both (red regions) correspond to the narrow parts of the conductors of cross section $2\text{ mm} \times 2\text{ mm}$. According to the FEM simulations, the maximum temperature should not exceed 50°C with the cooling block at 12°C .

E.2.1 Construction of the trap

The trap is precision machined from a 2 mm thick copper plate in four identical slices using Wire Electrical Discharge Machining. Dielectric is placed between the cuts to keep the slices isolated. The width of the cuts has been optimised to balance the conflicting demands of low local temperature and strong, uniform and symmetric magnetic field. The conductors are fixed onto a cooling block which also serves as a mechanical mounting. The current carrying cables are attached to the trap symmetrically to minimise field distortions. Additional shim coils are used to counter external bias fields.

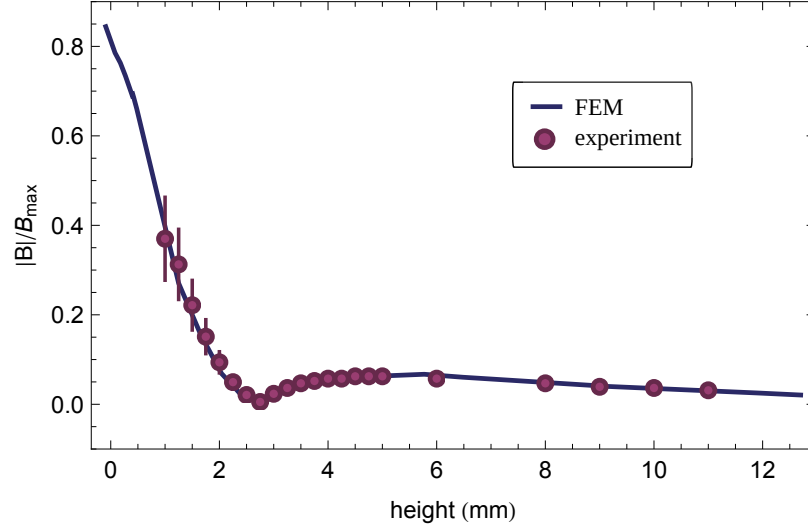


Figure 43: A comparison of the measured magnetic field amplitude (data points) against the numerically calculated profile (line). All data are normalised to the maximum magnetic field at the centre of the trap. The active area of the Hall sensor is taken to be at 1.5 mm from its surface. For this reason no data were taken at distances smaller than 1.5 mm. The height is measured from the centre of the trap. The agreement of the experimental data with the theory is excellent. Uncertainties arise mainly from the probe resolution and are roughly proportional to the magnitude of the field.

The trap can be cooled very efficiently using a cooling block with chilled water running through it attached on one side of the trap. The cooling block is surrounded by an insulating material which serves as a mounting point for the trap. The trap is securely attached to it using countersunk screws (not shown) and some epoxy resin (Araldite 2011) at points where thermal conductance is not critical. The cooling block is modelled in FEM as a block of copper with water flowing through it at a pressure of 4 bar and temperature of 12 °C. There is a large thermal conductance because of the large surface area, leading to efficient cooling. FEM simulations show that the trap stays at less than 50 °C with 400 A running through it. More importantly, cooling should be uniform across the volume of the trap although some warmer spots are generated where the current density is high, i.e. where the aspect ratio is close to unity. Nevertheless, these are symmetric and therefore do not distort the field. A significant advantage over using two separate coils is that any fluctuations coming from non-laminar water flow or uneven heat extraction are common mode, which increases the trap stability. Numerical simulations of the magnetic field show that distortions of the field due to corrugations on the surface of the trap are negligible. The natural length scale of the trap is a few millimetres, much larger than features arising from surface roughness.

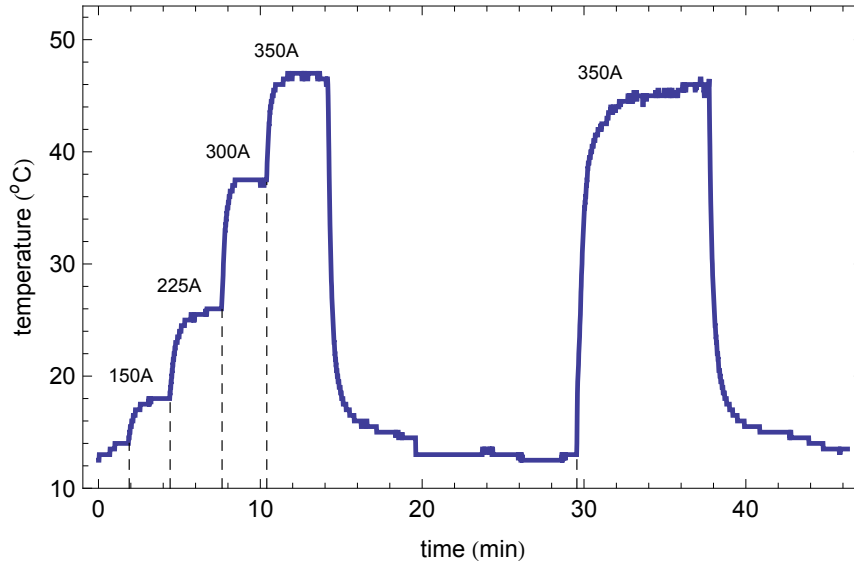


Figure 44: Measurement of the temperature of the water-cooled trap for various values of the applied current. The temperature is measured at the hottest point of the trap (see Fig. 42b). In the first cycle the temperature is left to stabilise for the shown current values. The second cycle represents a more realistic operation of the trap where the maximum current is applied instantly. The dashed lines correspond to the time the current changes value. The temperature falls off exponentially after switch-off with a characteristic time of 18 s.

E.3 MEASUREMENTS

The magnetic field was measured using a Hall sensor (634ss2 from Honeywell in a 4-pin Dual In-Line (DIP) package). This sensor was chosen due to its sensitivity and small size. Although the height of the DIP package is about 2.2 mm we were able to measure sub-millimetre field changes with it since the active area of the sensor is much smaller and located at about 1.5 mm from its surface.

The measurement of the magnetic field was using with a phase sensitive detection scheme with a current of 1.8 A switched at 20 Hz. The output of the Hall probe was amplified by an active low pass filter with $\tau = 1$ ms. After accounting for the tolerances of the passive elements and the losses of the phase analyser, the sensitivity of the measurement was found to be $(8 \pm 2) \times 10^5 \text{ mV/T}$. As shown in figure 43 the measured values agree extremely well with the expected ones.

We measured the temperature distribution using a standard type K temperature probe. Since the thinnest parts of the trap present the highest resistance they tend to get hotter (as can be seen in figure 42b). The trap is water-cooled directly using water at 14°C and 10 L/min flow. The trap was connected to the high current leads using 7 cm long copper flats to ensure a good electrical connection and also distance it from the current leads since it was found that heat from the leads was increasing the steady state temperature of the trap. First, we increased the current

in steps of 75 A up to a maximum of 350 A and let the temperature stabilise at each step. After switching the current off and waiting for the temperature to stabilise again the maximum current was run through the trap and the cycle repeated. One period of this cycle can be seen in figure 44. The maximum temperature of about 48 °C was reached at a lower current than expected from the numerical simulations, 350 A cf. 400 A. This is mainly due to the thermal conductance being smaller than in the FEM simulations where it was assumed to be effectively perfect. Therefore, a system where water in direct contact with the surface of the copper conductors was used to cool the trap and achieve design specifications. We note that this is the maximum steady state temperature that is attained after about 10 min of operation of the trap at maximum current. In practice we expect the trap to be operated only for a few ten seconds per experimental run so its maximum working temperature will be even lower.

E.4 CONCLUSION

We have demonstrated a new concept for a mm-scale surface trap that incorporates good aspects of the two main trap categories, micro- and macroscopic. It can be situated outside the vacuum region since the trap centre is at 2 mm from its surface and its power consumption is modest (~ 1 kW). Although there is scope for further improvements of this design in future iterations, it is already capable of producing very high gradients (> 1000 G/cm) and can be water-cooled very efficiently because of its small size and large surface area. Cold atoms applications where compactness is important could greatly benefit from this approach.

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