Trapped ions in a bath of ultracold atoms

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Trapped ions in a bath of ultracold atoms

Henning Alexander Fürst

2019
Trapped ions in a bath of ultracold atoms

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Henning Alexander Fürst

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Experiments on ultracold atomic systems have had a huge impact on studies and applications of quantum physics. Key breakthroughs cover the observation of complex many-body phenomena such as quantum phase transitions [1, 2, 3] and the study of quantum impurity physics [4, 5, 6]. The level of tunability and control over these systems has led to applications in emerging quantum technologies such as quantum simulation and quantum computing, where the current classical approaches could be outperformed quickly [7, 8, 9]. Also quantum metrology is in the focus of current research, where the quantum properties of the system are utilized as sensitive probes [10, 11].

Ultracold atomic experiments typically belong to one of two worlds. Historically first, ions have been trapped in electric radiofrequency (rf) traps [12, 13]. Laser cooling [14] enables the storage of individual or small clouds of ions, forming so-called Coulomb crystals, for days within the ion traps. The remarkably high degree of control of electronic and motional state at the quantum level [15, 16] led to a Nobel prize for David Wineland (shared with Serge Haroche) in 2012 [17]. Today the trapped-ion platform finds a broad range of applications within the area of atomic physics. The fields include metrology and atomic clocks [11], precision spectroscopy and tests of fundamental physics [10], quantum many-body physics [8] and quantum information processing [18, 19].

On the other side, ultracold atomic neutral gases can be created. In addition to
laser cooling, e.g., evaporative cooling is used to reach temperatures in the nanokelvin regime. For the ‘development of methods to cool and trap atoms with laser light’, a Nobel prize was awarded to Steven Chu, Claude Cohen-Tannoudji and William D. Philips in 1997 [20, 21, 22]. At such low temperatures, the atomic clouds reveal their quantum properties, leading to the formation of degenerate Fermi gases or Bose-Einstein condensates (BEC) [23]. The first observation of a BEC has been rewarded with the Nobel prize to Eric A. Cornell, Wolfgang Ketterle and Carl E. Wieman in 2001 [24, 25]. Magneto-molecular Feshbach resonances can be used to tune the interaction strength between the particles over orders of magnitude on the attractive and repulsive side [26]. Ultracold atomic clouds are used nowadays for example in precision spectroscopy and metrology applications [11], the study of quantum many-body physics [23], quantum simulations [7] and quantum chemistry [27].

In this thesis we aim to combine the two atomic systems of trapped ions and ultracold neutral atoms in a single experimental setup. Bringing together the benefits of each system, we aim to study new quantum many-body systems.

In particular, we are interested in coupling the fermionic atoms to the motion and spin of the trapped ions. In case of a single ion polarizing the atomic cloud, the system can be used to study impurity physics [28, 29]. Such an impurity interacting with a quantum bath is a nontrivial many-body model system with broad relevance to condensed matter systems. A key example is the polaron, in which an electron forms a quasiparticle by dressing with lattice phonons [5]. The full control over the ion’s quantum state will enable us to measure the coherence of the ion when interacting with the atoms. The tunability of bath-bath and ion-bath interaction strength via Feshbach resonances [26] could be utilized to tune the interaction strength over a wide range.

In the case of an ion crystal, the fermionic atoms couple to the quantized sound waves (phonons) of the crystal. This coupling is generally not present in neutral atom experiments. At the same time, the trapped-ion system does not naturally include fermionic statistics. Thus, the atom-ion system could serve as a quantum emulator of electron-phonon coupling such as in the Fröhlich model, Peierls transitions and even phonon-mediated long-range interactions [30].

Besides these prospects, we envision a number of other applications for our system. The level of control over particle numbers, electronic configuration, external fields and collision energy enables studying quantum chemistry on a single to few particle level [31]. Such studies could be used to benchmark quantum chemistry calculations. Further, we aim to use the atomic bath as a buffer gas to buffer-gas cool the trapped
ion quantum computer, where the presence of an ultracold atomic cloud could increase the quantum gate fidelities by reduced external heating effects [32]. Even atom-ion quantum gates, serving as a link between the two worlds of trapped atoms and trapped ions [33, 34] could be realized.

We are not the first group studying the interactions between ultracold atoms and ions. The first time a single trapped ion within a Bose-Einstein condensate was reported by Zipkes et al. in Prof. Michael Köhl’s group [35] and a bit later by Schmid et al. in Prof. Hecker Denschlag’s group [36]. These studies were followed by many works, investigating, e.g., quantum chemistry [37, 38, 39, 40], sympathetic cooling [41, 42, 43, 44] and ion spin dynamics [45, 46, 47]. Reviews on the experimental and theoretical progress within the field can be found in references [29, 48, 49].

Up until now, all atom-ion experiments have been performed at collision temperatures in the millikelvin regime. However, in the applications envisioned above, reaching and maintaining the so-called quantum regime is required. In this regime only the lowest partial wave of the scatterers contribute to the process, which can then be described by a single parameter, the \( s \)-wave scattering length \( a_s \). Up until now, it has proven very hard to create an atom-ion mixture that is cold enough. This is because the electric rf trapping field used for confining the ion leads to a driven motion, when the ion is not at rest (leading to so called intrinsic micromotion). Due to imperfections, typically also additional electric fields can act on the ion (leading to so called excess micromotion). Thus, energy can then be transferred from the rf field to the system when a collision between an atom and a trapped ion occurs [50], limiting attainable temperatures [51, 52, 53].

Cetina et al. [54] theorized that the combination of a light atom and a heavy ion can overcome this heating effect and reach the quantum regime within an ion trap. Therefore, we employ the combination with the highest mass ratio of all species that allow for straightforward laser cooling, \( m_i/m_a \approx 24–29 \), given by Yb\(^{+}\)/Li. As we will show, this combination should allow to reach \( s \)-wave collision energies despite the presence of an rf trap. Although we did not reach the quantum regime yet within this thesis, we obtained a number of encouraging results that point the way towards reaching it in the near future and give rise to study even atom-ion Feshbach resonances [55, 56, 57, 58] which have been predicted for our system [59] and should allow for tuning the atom-ion interaction strength.
1. Introduction

1.1. Scope of this thesis

In this thesis we describe an experimental setup designed for preparing an ultracold sample of $^6$Li atoms and overlap it with Yb$^+$ ions that are trapped in a radiofrequency trap. Within this thesis, we focus on answering the following main research questions.

- Can our system reach the quantum regime of interacting atoms and ions?
- Is the ionic spin conserved when colliding with a spin-polarized atomic gas such that it can be used as a buffer-gas cooled qubit?
- Can we expect to tune the atom-ion interaction in the ultracold regime by using Feshbach resonances?

This thesis is organized as follows:

Chapter 2 introduces the theoretical framework of classical atom-ion interactions within an rf ion trap and the mathematical model of ion trapping, including all types of micromotion that typically lead to collision-induced heating of the ion. Based on these classical interactions, we present a numerical framework that is used to simulate and analyze collisions between $^6$Li atoms and trapped $^{171}$Yb$^+$ ions. We investigate whether we can reach the quantum regime using realistic parameters that are accessible in our experiment, taking into account experimental imperfections. We give a limit on the remaining number of motional quanta that can be expected for the trapped ions and calculate the cooling rate. We find that the quantum regime in the Yb$^+/^6$Li system should be within reach after modest improvements of our ion trapping setup. In addition, we study the collisional cooling dynamics of multiple trapped ions in linear Coulomb-crystals, as their combination with cold atoms was proposed as a solid-state emulator [30]. We find that the dynamics is essentially the same as for the one ion case, which is beneficial for the study of fermion-phonon coupling in atom-ion systems. For a 2D Coulomb-crystal instead, micromotion-induced heating is unavoidable when overlapped completely with the atomic cloud. We find that immersing only one of the ions in the atomic bath still leads to cooling of around half of the oscillator modes of the ion crystal. This result shows, that efficient ultracold buffer-gas cooling may be achieved even for ion crystals that are much larger than the extent of the buffer gas.

In chapter 3 we present the experimental setup which was partially designed and built up by me. We describe the combined atom-ion vacuum system and the four pairs of
magnetic field coils used to trap and cool the $^6\text{Li}$ atoms. We introduce all relevant laser systems, their stabilization mechanisms and their beam paths into the vacuum chamber for cooling and imaging of both atoms and ions. Further, we present the microwave setup used to manipulate the hyperfine ground state qubit in $^{171}\text{Yb}^+$ and our realizations of fast current switches to switch off the coils or their polarity, which is required to take absorption images of the atoms and to produce large magnetic fields for evaporative cooling of $^6\text{Li}$.

Having described all relevant parts of the experiment, we present ion trapping tools, techniques and measurements that are required for studying atom-ion interactions in chapter 4. We characterize the ion trap including the trapping potentials, state detection, so-called excess micromotion and heating rate. Note that we used these experimentally obtained parameters in the numerical simulations performed in chapter 2. Further, we utilize the ion to measure magnetic fields and the local vacuum quality.

As a second ingredient for the creation of an ultracold mixture, we present and characterize the atom trapping in chapter 5, including all steps necessary to create and image an optically trapped ultracold cloud of $^6\text{Li}$ atoms at the position of the trapped ion within our experimental setup. We present results on forced evaporative cooling to temperatures below 1 $\mu$K which is far below the $s$-wave limit of the $^6\text{Li}/\text{Yb}^+$ system.

In chapter 6 we analyze the spin-exchange and spin-relaxation behavior within the ground states of $^{171}\text{Yb}^+$ and $^{174}\text{Yb}^+$ when colliding with spin polarized $^6\text{Li}$ in the stretched spin state. We find large spin-exchange probabilities between 0.44(11) to 1.03(12) per Langevin collision, depending on the isotope. Further, we find slow spin-relaxation rates that do not conserve the total spin of the colliding atom-ion pair. The rates found represent an upper limit, as the spin polarization of the atomic cloud is not pure. We model the system using \textit{ab initio} quantum scattering calculations and find that the large spin-exchange rates can be obtained when the difference of singlet and triplet scattering lengths is large. Surprisingly, even for temperatures far above the $s$-wave regime, the predicted spin-exchange rates depend strongly on this difference. Similar effects have been observed in Refs. [60, 61]. The result points towards the existence of broad Feshbach resonances at low collision energies [26]. Additionally, we find that the spin-relaxation in our system should be around an order of magnitude slower than in the Rb/Yb$^+$ system [45, 46], in agreement with our measurements. Thus, we conclude that the $^6\text{Li}/\text{Yb}^+$ system is a promising candidate for the exploration of atom-ion Feshbach resonances that enable tuning of the interaction strength. The
low spin-relaxation rates may be beneficial for the use of Yb\(^+\) as a buffer-gas cooled qubit.

In chapter 7 we perform spectroscopic measurements on the 329 nm \(2S_{1/2} \rightarrow 2P_{3/2}\) transition in all accessible isotopes of Yb\(^+\), as this transition will be used within a Raman setup to realize side-band cooling and improve the temperature and heating-rate measurements. We measure the isotope shifts of the transition as well as the branching fractions into the lower lying \(D\)-states. In addition, we measure the isotope shifts of the \(2F_{7/2} \rightarrow 1D[5/2]_{5/2}\) transition and the hyperfine structure constants \(A(2P_{3/2})\) and \(A(1D[5/2]_{5/2})\) for \(^{171}\)Yb\(^+\). We find that our results are in agreement with previous measurements (where available) but a factor of 5-9 more precise. The predictions for \(A(2P_{3/2})\) are in strong disagreement with our values and to our best knowledge, the value of \(A(1D[5/2]_{5/2})\) has not been measured nor calculated before. Thus, our results may serve as a benchmark for atomic structure calculations.

We conclude our results obtained in this study in chapter 8 and present possible improvements and future steps in the experiment.
Prospects of reaching the quantum regime in Li-Yb$^+$ mixtures

In this chapter we perform numerical simulations of trapped $^{171}\text{Yb}^+$ ions that are buffer gas cooled by a cold cloud of $^6\text{Li}$ atoms. This species combination has been suggested to be the most promising for reaching the quantum regime of interacting atoms and ions in a Paul trap. Treating the atoms and ions classically, we compute that the collision energy indeed reaches below the quantum limit for a perfect linear Paul trap. We analyze the effect of imperfections in the ion trap that cause excess micromotion. We find that the suppression of excess micromotion required to reach the quantum limit should be within experimental reach. Indeed, although the requirements are strong, they are not excessive and lie within reported values in the literature. We analyze the detection and suppression of excess micromotion in our experimental setup. Using the obtained experimental parameters in our simulation, we calculate collision energies that are a factor 2–11 larger than the quantum limit, indicating that improvements in micromotion detection and compensation are needed there. We also analyze the buffer-gas cooling of linear and two-dimensional ion crystals. We find that the energy stored in the eigenmodes of ion motion may reach 10–100 $\mu$K after buffer-gas cooling under realistic experimental circumstances. Interestingly, not

The content of this chapter and its appendices A.1–A.2 are based on *J. Phys. B*, 51:195001, September 2018 [62].
all eigenmodes are buffer-gas cooled to the same energy. Our results show that with modest improvements of our experiment, studying atom-ion mixtures in the quantum regime is in reach, allowing for buffer-gas cooling of the trapped ion quantum platform and to study the occurrence of atom-ion Feshbach resonances.

**2.1. Introduction**

A crucial step towards realizing quantum applications in atom-ion experiments is to reach the quantum (or s-wave) regime for atom-ion mixtures. While preparing atomic clouds at ultracold temperatures in the quantum degenerate regime is routinely performed in many groups, using for example Li atoms [63, 64, 65], it turned out that the Paul or radio-frequency (rf) trap, commonly employed for trapping the ions, limits the attainable temperatures in atom-ion mixtures, and the s-wave regime has so far not been reached in this system. This limitation stems from the oscillating electric fields employed in the rf trap, which causes the ion to perform a rapid micromotion. During an atom-ion collision energy may be transferred from the time-dependent trapping field into the atom-ion system [41, 42, 43, 50, 53, 54, 66, 67, 68, 69, 70]. Even in the limit of zero atomic temperature and an ion sitting at the rf node of the trapping field, the attractive atom-ion potential leads to a drag on the ion to a region of non-negligible rf amplitude during a collision. In fact, even runaway heating may occur when the atom is heavier than the ion. Cetina et al. [54] calculated that the lowest temperatures may be achieved for atom-ion combinations with large ion to atom mass ratios. They theorize that Yb+/Li, which has the largest mass ratio of any atom-ion combination allowing straightforward laser cooling, may enter the quantum regime after improving control over the trapping voltages to slightly beyond state-of-the-art to compensate excess micromotion.

In this chapter, we perform Monte-Carlo simulations of the classical scattering events between individual free $^6$Li atoms and $^{171}$Yb$^+$ ions trapped in a Paul trap. The simulation includes the attractive atom-ion potential as well as the full trapping potential of the ion and potential excess micromotion fields using realistic experimental parameters that we obtain from our experimental setup and from parameters reported in the literature. The atom’s initial velocity is drawn from a thermal distribution of given temperature, starting on a random position on a sphere around the ion. The sphere size is chosen carefully to take into account the potentially large ion orbits and accounts for realistic atomic densities. We track the ionic motion continuously while each atom is
2.2. Simulating buffer-gas cooled ions

introduced after the previous atom has escaped a second sphere around the ion again, defining the end of a collision. Thus, no back-action on the atomic cloud is assumed, justified by the large experimental atom numbers on the order of typically $10^5$ to $10^7$. Using this approach, we calculate that the $s$-wave regime of Yb$^+$/Li should be in reach with current technology and considering all known sources of excess micromotion in the ion. We further investigate the prospects of collisional cooling of single ions and crystals of ions into the motional ground state using a cloud of ultracold Li, taking into account experimental imperfections. We give a limit on the remaining number of motional quanta that can be expected and compute the cooling rate. Motivated by the prospects of an ultracold atom-ion system to form a solid-state emulator [30] we study the classical cooling dynamics for multiple trapped ions forming a Coulomb-crystal within the cloud of atoms and show that the cooling dynamics is very similar to that of a single trapped ion.

This chapter is organized as follows: First, we give the theoretical background of ion trapping and micromotion as well as the model for simulating buffer-gas cooling in Sect. 2.2. In Sect. 2.3 we describe the experimental parameters and limitations in our experimental setup. We use these parameters in the calculations of Sect. 2.4, where we study the thermalization of a single trapped ion experiencing each type of micromotion. In sections 2.5 and 2.6 we describe the buffer-gas cooling of linear ion crystals, while Sect. 2.7 describes the results for two-dimensional ion crystals. Finally, we draw conclusions in Sect. 2.8.

2.2. Simulating buffer-gas cooled ions

2.2.1. Ion trapping in a linear quadrupole trap

The potential of a Paul trap as a function of the ion position $\vec{r}$ can be written as:

$$\Phi(\vec{r}, t) = \frac{u_{dc}}{2} \sum_{i=1}^{3} \alpha_i r_i^2 + \frac{u_{rf}}{2} \cos(\Omega_{rf} t) \sum_{i=1}^{3} \alpha'_i r_i^2$$

(2.1)

with the positive, geometry and voltage-dependent prefactors $u_{dc}$ and $u_{rf}$ and trap drive frequency $\Omega_{rf}$. To describe a linear Paul trap as it is used in our experiment we have [71]

$$\alpha_1 = \alpha_2 = -\frac{1}{2} = -\frac{\alpha_3}{2} \quad \text{and} \quad \alpha'_1 = -\alpha'_2 = 1, \quad \alpha'_3 = 0.$$  

(2.2)
For this choice, the confinement along the 3-axis is supplied by a time-independent harmonic trapping potential \( \propto u_{dc} \), whereas the radial confinement is supplied by the oscillating field \( \propto u_{rf} \). Note that in reality the \( \alpha_{1,2} \) coefficients are chosen to slightly differ from each other to lift the degeneracy in the resulting radial trap frequencies.

The electric field is given by

\[
\vec{E}(\vec{r}, t) = -\nabla \Phi(\vec{r}, t) = -u_{dc} \left( r_3 \hat{e}_3 - \frac{1}{2} (r_1 \hat{e}_1 + r_2 \hat{e}_2) \right) - u_{rf} \cos(\Omega_{rf} t) (r_1 \hat{e}_1 - r_2 \hat{e}_2) ,
\]

with the unit vectors \( \hat{e}_i \) in the \( i \)-th direction. With that, the equation of motion for a single ion with mass \( m_{ion} \) and positive charge \(+e\) can be written as the Mathieu equation \[72\]

\[
\ddot{r}_i + \left( a_i + 2 q_i \cos(\Omega_{rf} t) \right) \frac{\Omega_{rf}^2}{4} r_i = 0 , \quad i \in \{1, 2, 3\} \equiv \{x, y, x\} ,
\]

with the parameters

\[
a_1 = a_2 = -\frac{1}{2} a_3 = -\frac{2e u_{dc}}{m_{ion} \Omega_{rf}^2} , \quad q_1 = -q_2 = \frac{2e u_{rf}}{m_{ion} \Omega_{rf}^2} , \quad q_3 = 0 ,
\]

which are the stability parameters of the Paul trap \[71\]. Usually, Paul traps are operated at a region where \( |a_i|, q_i^2 \ll 1 \), which can be achieved by properly choosing a suitable combination of \( \Omega_{rf} \) and the static and rf electrode voltages \( \propto u_{rf}, u_{dc} \). An approximate solution in first order in \( q_i \) can then be obtained by

\[
r_i(t) \approx r_i^{(1)}(\omega_i t + \phi_i) \left( 1 + \frac{q_i}{2} \cos(\Omega_{rf} t) \right) ,
\]

where the phase \( \phi_i \) and amplitude \( r_i^{(1)} \) are determined by the initial condition at \( t = 0 \).

The motion consists of a low frequency part, oscillating with the secular frequency \( \omega_i \approx \frac{1}{2} \Omega_{rf} \sqrt{a_i + \frac{1}{2} q_i^2} \), thus requiring \( a_i + \frac{1}{2} q_i^2 > 0 \) for a stable solution. In the two radial directions, the rf field drives the so-called micromotion that oscillates in phase with the rf drive and whose amplitude depends on the secular motion amplitude and \( q_i \)-parameters. Note that in a real ion trap, imperfections in the electrode alignment can lead to a small rf field component also in the axial direction, effectively setting \( q_z \neq 0 \). By averaging over the secular oscillation period \( T_i = \frac{2\pi}{\omega_i} \), one can obtain the
average kinetic energy in each coordinate,

\[
\tilde{E}_{\text{kin},i} = \frac{1}{2} m_{\text{ion}} \langle \dot{r}_i (t)^2 \rangle_{T_i} \approx \frac{1}{4} m_i r_i^{(1)} \left( \omega_i^2 + \frac{1}{8} q_i^2 \Omega_{\text{rf}}^2 \right), \quad (2.7)
\]

where the assumption \( \Omega_{\text{rf}} \gg \omega_i \) was used.

### 2.2.2. Excess micromotion

Besides the intrinsic micromotion of the ion caused by the radiofrequency drive, stray charges on the trap electrodes, imperfections of the trap assembly and electrical connection as well as finite-size effects can lead to various types of so-called excess micromotion [72] that affects the average kinetic energy of the ion and prevents reaching ultracold temperatures. Below, we will briefly describe the three different kinds of excess micromotion that occur in a linear Paul-trap, namely radial, axial and quadrature micromotion, and in Sect. 2.3 we will describe how these can be detected and compensated in our experiment.

#### In-phase micromotion

Stray electric fields \( E_{\text{rad}} \) in the radial direction may push the ions away from the rf node, where they experience the presence of the radiofrequency field even without any secular energy. This type of excess micromotion we will call radial micromotion. The modified Mathieu-equation of the system including \( \tilde{E}_{\text{rad}} \) reads [72]

\[
\ddot{r}_i + \left( a_i + 2 q_i \cos (\Omega_{\text{rf}}) \right) \frac{\Omega_{\text{rf}}}{4} r_i = \frac{eE_{\text{rad},i}}{m_{\text{ion}}}, \quad (2.8)
\]

with \( i \in \{x, y\} \equiv \{1, 2\} \). To lowest order in \( q_i \), the solution is given by

\[
r_i(t) \approx \left( r_i^{(0)} + r_i^{(1)} \cos (\omega_i t + \phi_i) \right) \left( 1 + \frac{q_i}{2} \cos (\Omega_{\text{rf}} t) \right), \quad (2.9)
\]

with the shifted equilibrium position \( r_i^{(0)} \approx eE_{\text{rad},i}/(m_{\text{ion}} \omega_i^2) \) of the secular motion. For both radial directions this additional shift leads to an energy

\[
E_{\text{emm},i} = \frac{1}{16} m_{\text{ion}} \left( q_i r_i^{(0)} \Omega_{\text{rf}} \right)^2 = \frac{4}{m_{\text{ion}}} \left( \frac{q_i eE_{\text{rad},i} \Omega_{\text{rf}}}{8 \omega_i^2} \right)^2, \quad (2.10)
\]
2. Prospects of reaching the quantum regime in Li-Yb\textsuperscript{+} mixtures

in lowest order. Typically, this micromotion can be compensated by applying an external static electric field to cancel the stray field at the position of the ion. Note that a stray field component in axial direction only changes the ion’s axial equilibrium position, not the kinetic energy of the system.

Axial micromotion

Axial excess micromotion is mainly caused by the finite size of the trap leading to a radiofrequency pickup on the dc end caps. This pickup leads to an additional, position-independent, oscillating field with amplitude \( E_{ax} \) in axial direction that modifies the axial Mathieu-equation to

\[
\ddot{r}_z + a_z r_z = \frac{eE_{ax} \cos (\Omega_{rf} t)}{m_{ion}},
\]

leading to the analytic solution of a driven harmonic oscillator,

\[
r_z(t) = \frac{eE_{ax} \cos (\Omega_{rf} t)}{m_{ion} (\omega_z^2 - \Omega_{rf}^2)} + r^{(1)}_z \cos (\omega_z t + \phi_z),
\]

thus increasing the average kinetic energy by the term

\[
E_{emm,z} = \frac{(eE_{ax} \Omega_{rf})^2}{4m_{ion} (\Omega_{rf}^2 - \omega_z^2)^2}.
\]

While it is hard to minimize this pickup by trap design, it can be reduced by appropriate low-pass filters connected to the end cap electrodes or injecting an rf field with opposite phase at one of the end cap electrodes [73].

Quadrature micromotion

Phase- or quadrature micromotion [72, 74] is caused by a phase difference \( \delta \phi_{rf} \) between the radiofrequency voltages on the opposing rf-electrodes. The phase micromotion can be approximately described by an additional homogeneous oscillating field in the direction of the electrodes [72]

\[
\vec{E}_{ph} \approx \frac{1}{4e} q_{ion} \delta \phi_{rf} \Omega_{rf}^2 R_{trap} \sin (\Omega_{rf} t) \hat{e}_x,
\]
2.2. Simulating buffer-gas cooled ions

where $R_{\text{trap}}$ is half the distance between the two rf-electrodes. The field leads to the modified Mathieu-equation

$$\ddot{r}_x + (a_x + 2q_x \cos (\Omega_{\text{rf}} t)) = \frac{1}{4} q_x R_{\text{trap}} \delta\phi_{\text{rf}} \Omega_{\text{rf}}^2 \sin (\Omega_{\text{rf}} t) .$$  \hspace{1cm} (2.15)$$

The solution in lowest order approximation then reads

$$r_x(t) = r_x^{(1)} \cos (\omega_x t + \phi_x) \left(1 + \frac{1}{2} q_x \cos (\Omega_{\text{rf}} t)\right) - \frac{1}{4} q_x R_{\text{trap}} \delta\phi_{\text{rf}} \sin (\Omega_{\text{rf}} t) ,$$  \hspace{1cm} (2.16)$$

leading to an additional term in the average kinetic energy in the x-direction of

$$E_{\text{phmm}} = \frac{1}{64} m_{\text{ion}} \left(q_x R_{\text{trap}} \delta\phi_{\text{rf}} \Omega_{\text{rf}}\right)^2 .$$  \hspace{1cm} (2.17)$$

Compensation of the quadrature micromotion is possible but technically challenging, for example by using two coherent rf drives with an adjustable phase difference between their respective outputs.

2.2.3. Modeling atom-ion collisions

We numerically simulate the classical atom-ion scattering process by launching individual atoms from a sphere of constant radius $r_0$ centered around the equilibrium position of the trapped ion, one at a time. The radius of the sphere is chosen to be large enough to allow for potentially large orbits of the ionic motion and to resemble realistic atomic densities (since we will only consider a single atom at a time inside the sphere). During the whole propagation, we simulate the full radiofrequency potential of the Paul trap, including potentially present excess micromotion. A collision event is finished after the atom has left a second sphere with a slightly bigger radius $r_1$, also centered around the ion’s equilibrium position. The use of spheres ensures a simple way to simulate isotropic interaction with a homogeneous atomic cloud. While the ionic motion is continuously propagated, the scattered atom is removed and a new atom is introduced, thus no back-action on the atomic cloud is assumed. In the following we will explain in detail the atom-ion scattering potential, the sampling of the atoms, the propagation method and the energy determination of the ion after each scattering event.
The atom-ion scattering is caused by the long range attractive \( r^{-4} \) atom-ion potential that originates from the induced dipole moment of the atom [75]. At short ranges, we add a repulsive \( r^{-6} \) term to simulate a hard core potential,

\[
V_{a-i}(r) = C_4 \left( -\frac{1}{2r_{a-i}^4} + \frac{C_6}{r_{a-i}^6} \right), \quad r_{a-i} = ||\vec{r}_a - \vec{r}_i||,
\]

where \( C_6 \) is given as a fraction of \( C_4 \), leading to a zero crossing of the potential at a distance of \( r_{hc} = \sqrt{2C_6} \). The attractive \( r^{-4} \) potential leads either to glancing collisions, where mainly the momentum directions of the partners slightly change, or to Langevin collisions where atom and ion are spiraling into each other, enabling for a large energy and momentum transfer. Langevin collisions occur when the impact parameter \( b \) is less than the Langevin range \( b_c = (2C_4/E_{col})^{1/4} \) [75]. Notably, the Langevin collision rate \( \Gamma_L = \frac{2\pi\rho_a}{\sqrt{C_4/\mu}} \) is only dependent on the atomic density \( \rho_a \) and the \( C_4 \) potential as well as the reduced mass \( \mu \) of the two body system but not on the collision energy \( E_{col} \).

To fairly sample the flow of atoms, the atom launching coordinates are obtained from a uniform distribution on the sphere surface at the beginning of each collision event. To get a starting position, two points \( p \) and \( q \) are randomly picked from the interval \([0, 1]\). The azimuthal angle \( \phi \) is then given by \( \phi = 2\pi \cdot p \) and the polar angle \( \theta = \arccos (2q - 1) \) [76], from which the Cartesian coordinates are derived,

\[
r_{a,1} = r_0 \cos (\phi) \sin (\theta), \quad r_{a,2} = r_0 \sin (\phi) \sin (\theta), \quad r_{a,3} = r_0 \cos (\theta).
\]

The initial velocity \( \vec{v}_a \) of the atoms is then sampled from the probability distribution \( P_\Phi(\vec{v}_a, T_a) \) of the flux of thermal atoms

\[
\Phi(\vec{v}_a) = \rho_a 4\pi r_0^2 \hat{e}_r \cdot \vec{v}_a,
\]

at a given temperature \( T_a \) and density \( \rho_a \) through the sphere,

\[
P_\Phi(\vec{v}_a, T_a) d^3 v_a = \frac{\Phi(\vec{v}_a)}{\rho_a 4\pi r_0^2} \frac{m_a^2}{2\pi (k_BT_a)^2} e^{-\frac{m_a v_a^2}{2k_BT_a}} d^3 v_a
\]

\[
= \frac{m_a^2}{2\pi (k_BT_a)^2} v_{a,r} e^{-\frac{m_a v_{a,r}^2}{2k_BT_a}} dv_{a,r} e^{-\frac{m_a v_{a,\phi}^2}{2k_BT_a}} dv_{a,\phi} e^{-\frac{m_a v_{a,\theta}^2}{2k_BT_a}} dv_{a,\theta},
\]

meaning that the velocity components \( v_{a,\phi} \) and \( v_{a,\theta} \) tangential to the sphere surface are picked from one-dimensional Gaussian distributions with a standard deviation of
\[
\sigma = \sqrt{k_B T_a/m_a} \text{ each, whereas the perpendicular velocity } v_{a,r} \text{ is picked from a Weibull-distribution with shape parameter } k = 2 \text{ and scale parameter } \lambda = \sqrt{2k_B T_a/m_a}. \text{ Only atoms flying towards the center of the sphere will have a chance to collide with the ions, therefore it is enforced that } v_{a,r} < 0. \text{ The Cartesian components of the velocity are then obtained by a coordinate transformation of the spherical components. We check the functionality of the random number generator in appendix A.1.}
\]

After the atom is introduced, the full trapped-ion-atom system is propagated forward in time by an adaptive step-size Runge-Kutta algorithm of fourth order [77], including the full radiofrequency ion trap potential and, if desired, additional excess micromotion. The algorithm maintains a desired relative accuracy in each coordinate \( p_{\text{tol}} \) in each coordinate as explained in appendix A.1. This allows for a fast propagation when atom and ion are far away from each other and an accurate propagation when the interaction is strong. At the end of a collision event, when the atom passes the second sphere of radius \( r_1 \), all ion’s coordinates at this time are intermediately stored as initial coordinates for the next collision event and the energy of the ion is determined. For this, the atom is removed from the simulation and the ion motion is propagated further for a fixed amount of time \( t_{\text{kin}} \gg 2\pi/\omega_i \) using \( N_{\text{kin}} \) fixed time steps of duration \( \Delta t_{\text{kin}} \), sufficiently small to resolve micromotion. During this additional propagation all ion trajectories are stored. From the velocities \( \vec{v}_{i,n} \) at each point in time the average kinetic energy

\[
\bar{E}_{\text{kin}} = \frac{1}{N_{\text{kin}}} \frac{1}{2} m_{\text{ion}} \sum_{k=1}^{N_{\text{kin}}} \sum_{n=1}^{N_{\text{ions}}} \vec{v}_{i,n}(t_k)^2 = \frac{3N_{\text{ions}}}{2} k_B T_{\text{kin}},
\]

is computed, which can be used to determine the collision energy in the relative coordinate frame of the two body atom-ion system. The expression contains both the energy of the secular harmonic oscillator motion of the ion as well as the micromotion energy, caused by intrinsic and potentially present excess micromotion. Here, we defined the quantity kinetic temperature \( T_{\text{kin}} \) that includes both micromotion and secular motion energy, thus it is technically not a temperature but just the average kinetic energy scaled with \( 3N_{\text{ions}}/2k_B \), whereas in literature the ion temperature often refers only to the secular motion. The decomposition into micromotion and vibrational energy will be discussed in section 2.5. After the energy of the ion has been determined in the simulation, the time and ion coordinates are reset to the stored values from the end of the collision event and a new atom is introduced.
2. Prospects of reaching the quantum regime in Li-Yb\(^+\) mixtures

<table>
<thead>
<tr>
<th>Parameter</th>
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<th>Section</th>
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<tr>
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<td>rf-drive frequency</td>
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<tr>
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<td>rad. (q)-parameter</td>
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<tr>
<td>(q_z)</td>
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<td>atom escape sphere rad.</td>
<td>A.1</td>
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<td>(2^{14})</td>
<td>Fourier grid size</td>
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<td>(\Delta t_{kin})</td>
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<td>dc offset field</td>
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<td>rf phase mismatch</td>
<td>2.4.4 &amp; 2.6.2</td>
</tr>
</tbody>
</table>

Table 2.1.: Parameters used for the numerical simulation of the atom-ion collisions, unless given otherwise in the text. If varied, the last column refers to the respective section where it is investigated.

2.2.4. Collision energy and \(s\)-wave limit

The atom-ion scattering enters the \(s\)-wave regime, when the collision energy is lower than the first centrifugal barrier, such that only the partial wave with angular momentum quantum number \(l = 0\) (the \(s\)-wave) contributes significantly to the scattering problem \([49]\). For the long range atom-ion potential of \(^{171}\)Yb\(^+\)/\(^6\)Li the \(s\)-wave limit is reached at a collision energy of

\[
k_B \cdot T_s = \frac{\hbar^4}{2 \mu^2 C_4} = 8.6 \mu K.
\]  

(2.23)

The collision energy is given by the energy in the relative atom-ion coordinate. In the experimentally relevant situation in which the ion has a much larger kinetic energy than the atoms \(T_{kin} \gg T_a\), the collision energy is given by:

\[
E_{col}/k_B = T_{col} \approx \frac{3}{2} \frac{\mu}{m_{ion}} T_{kin}.
\]  

(2.24)
Therefore, to reach the quantum regime in the limit where $T_a \to 0$, the requirement for the ion is $T_{\text{kin}} < 168 \mu K$ [40]. In this work, we use $T_a = 2 \mu K \ll T_s$ such that $T_{\text{kin}} \gg T_a$ is fulfilled in most circumstances. At the same time, this choice still allows for a classical treatment of the atomic bath [52].

### 2.3. Micromotion detection and compensation

The experimental setup is described in detail in chapter 3 and Ref. [78]. The linear Paul trap is made out of four blade electrodes with a distance of $R_{\text{trap}} = 1.5 \text{ mm}$ to the trap center. End caps with a spacing of 10 mm are used to confine the ion along the axial ($z$) direction. Two sets of additional electrodes can be used for compensation of stray electric fields. Oscillating voltages at a frequency of $\Omega_{rf} = 2\pi \times 2 \text{ MHz}$ and an amplitude of $V_0 = 75 \text{ V}$ are applied to the blades and dc voltages of $V_{dc} \approx 15 \text{ V}$ to the end caps. This results in radial and axial trap frequencies of $\omega_{\text{rad}} \approx 2\pi \times 150 \text{ kHz}$ and $\omega_{\text{ax}} \approx 2\pi \times 42 \text{ kHz}$. Below, we describe how we detect and compensate micromotion in our setup and give limits on the attainable experimental parameters. More details on the micromotion detection and compensation can be found in chapter 4.

A radial stray field component $E_{\text{rad},i}$ leads not only to excess micromotion but also to a shift in equilibrium position as shown in Fig. 2.1. Within the horizontal direction (1), this can be detected by tracking the ions position for different radial trap frequencies, shifting the ions position by $r_h \approx eE_{\text{rad},h} \omega_{\text{rad}}^2 / m_{\text{ion}} \omega_h^2$, for $\omega_x \approx \omega_y = \omega_h$. We measure the shift of the ion by imaging from the top. We extract the ion’s horizontal position from averaging over five camera images at each radial trap frequency setting and fitting a Gaussian function. From these measurements we conclude that $E_{\text{emh},h} < 0.5 \text{ V/m}$ under optimal circumstances.

The ion’s vertical position cannot be obtained with the camera as the imaging system and vacuum system was designed to only image the ions from the top. Instead, we use the magnetic field dependence of the $(^2S_{1/2}, F = 0, m_F = 0) \leftrightarrow (^2S_{1/2}, F = 1, m_F = 1)$ hyperfine splitting in $^{171}\text{Yb}^+$ [79] for a determination of position shifts as a function of trap frequency. To do so, we apply a vertical magnetic field gradient of $g_v = 0.15 \text{ T/m}$ as shown in Fig. 2.1, which leads to a frequency shift of $2.1 \text{ kHz/µm}$. By comparing the frequency shift at radial confinements of $\omega_{\text{rad}} = 2\pi \times 80 \text{ kHz}$ and $\omega_{\text{rad}} = 2\pi \times 230 \text{ kHz}$ using microwave Ramsey spectroscopy, we measure a dc electric field of $E_{dc} = 0.29(2) \text{ V.m}^{-1}$ for 1 V applied to the compensation electrodes. As the
2. Prospects of reaching the quantum regime in Li-Yb⁺ mixtures

Figure 2.1.: Sketch of the ion trap seen from the axial (z) direction. We refer to the other horizontal direction with h and to the vertical (imaging) direction with v. Stray electric fields lead to position shifts in the horizontal (1), vertical (2) or both (3) directions and cause micromotion due to the non-vanishing rf field amplitude. A vertical magnetic field gradient \( g_v \) is used to detect the vertical position of the ion as mentioned in the text. Also shown is the radial basis (x and y) of the secular ion motion. The picture was adapted from Ref. [78] and updated.

set compensation voltages typically need to be adjusted by less than 1 V from day to day, we estimate that \( E_{\text{emm,v}} < 0.3 \text{ V/m} \) starting at optimal compensation during an experimental run.

The axial micromotion is obtained by measuring the line broadening of the 4.2 MHz wide \( ^2D_{3/2} \rightarrow ^3D[3/2]_{1/2} \) transition at 935 nm wavelength in Yb⁺ [79]. For this, we use a laser beam aligned along the trap axis [72, 80]. We obtain an upper bound to the amplitude of the oscillating electric field in the trap center of \( E_{\text{ax}} \leq 15 \text{ V}\cdot\text{m}^{-1} \), limited by the observed linewidth of the \( ^2D_{3/2} \rightarrow ^3D[3/2]_{1/2} \) transition at optimal compensation. By measuring the axial micromotion at various ion positions along the trap axis, we obtain \( q_z \leq 0.0023 \) at the settings used.

Aligning the beam under 45° with respect to the trap axis allows us to also check for quadrature micromotion, but none was detected. The observed transition linewidth results in the limit \( \delta \phi_{\text{rf}} < 0.65 \text{ mrad} \). Using a transition with a narrower linewidth, for example the 22 Hz wide \( ^2S_{1/2} \rightarrow ^2D_{5/2} \) clock transition at 411 nm in Yb⁺ [81], could improve these limits significantly.
2.4. A single ion in the cold buffer gas

In this section, we present the simulation results for collisions between a single trapped ion in a Paul trap with $^6$Li atoms using parameters that can be achieved with the ion trap used in our experiment. We investigate the influence of atomic bath temperature as well as the different kinds of micromotion on the ion’s average kinetic energy for realistic parameters. For simplicity, we start our calculations with an ion that has no energy and observe how this ion thermalizes with the atomic bath in a similar way as described in Refs. [43, 54]. Although chosen for convenience, this situation is also of experimental relevance, as the ion may be laser-cooled close to its ground state of motion before the atoms are introduced [43].

2.4.1. Influence of the atomic bath temperature

We simulated collisions for an atomic bath temperature $T_a$ between 0 – 50 µK. The ion’s averaged kinetic energy after equilibration in units of $T_{\text{kin}}$ and typical 1/e number of collisions to equilibrate $N_{\text{col}}$ were determined by fitting an exponential function of the form

$$T(n_{\text{col}}) = (T_{\text{kin}} - T_0) \left(1 - e^{-n_{\text{col}}/N_{\text{col}}} \right) + T_0,$$

(2.25)

to the results obtained by averaging at least 300 individual runs. The results are shown in Fig. 2.2. The errors given in the plot correspond to the standard errors of the fit parameters. The average kinetic energy of the ion (left) in units of $T_{\text{kin}}$ shows a strictly linear dependence with a slope of 1.79(2) and offset of 7.60(14) µK. The dashed line shows the hypothetical case in which each secular mode of the ion equilibrates with the temperature of the atoms, according to the approximate prediction of Eq. 2.7. Its slope reads 1.68 using the trap parameters of the simulation. In particular, the deviation from unity slope is given by the extra energy stored in the micromotion amplitude, which is approximately $\frac{1}{2} k_B T_a$ extra per radial direction [72], such that the energy of the atomic bath excites five kinetic degrees of freedom instead of three, explaining the slope of approximately 5/3. The deviation in slope of the simulated points with respect to the prediction is expected to be caused by the approximations made to obtain the prediction (i.e., $|a_i|$ and $q_i^2 \ll 1$, see Sect. 2.2.1). The offset can be seen as the direct influence of micromotion-induced heating, transferring energy from the trap drive rf field into the secular motion of the ions, mediated by the atoms. The number of collisions required to equilibrate (right) follows a square root
2. Prospects of reaching the quantum regime in Li-Yb⁺ mixtures

![Graphs showing equilibrium average kinetic energy and number of collisions required to equilibrate versus temperature.]

**Figure 2.2.** Equilibrium average kinetic energy in units of $T_{\text{kin}}$ of a single ion colliding with atoms (left) and number of collisions required to equilibrate (right) versus temperature of the atoms. The results were fit with a linear function (solid line, left) or a square root function (solid line, right) respectively. The dashed line corresponds to a hypothetical case without micromotion-induced heating as explained in the text.

function, which is to be expected, since the thermalization rate $\Gamma_{\text{eq}} = 1/N_{\text{col}}$ should be directly proportional to the fraction of events that lead to thermalization, namely Langevin collisions, divided by the number of total events, $\Gamma_{\text{eq}} \propto \frac{\Gamma_L}{\Phi(\vec{v}_a)}$, with $\Gamma_L$ the Langevin rate and $\Phi(\vec{v}_a)$ the flux into the sphere on which the atoms start as defined in Eq. 2.20. Thus, $N_{\text{col}} \propto \Phi(\vec{v}_a) \propto \sqrt{T_a}$. From the fit, we obtain a proportionality factor of $412(8)/\sqrt{\mu K}$.

### 2.4.2. Influence of radial excess micromotion

In this paragraph, we investigate the influence of radial excess micromotion caused by a stray electric field $E_{\text{rad}}$ on the average kinetic energy of a single ion when immersed in a cold atomic bath of $T_a = 2 \mu K$. We scanned $E_{\text{rad}}$ over a range of $0.0 - 0.6 \text{ V/m}$ and determined the ion’s average kinetic equilibrium energy in units of $T_{\text{kin}}$ and the typical number of collisions required to equilibrate $N_{\text{col}}$ according to Eq. 2.25 by averaging over at least 300 individual runs for each point. We additionally checked the influence of the radial direction of $E_{\text{rad}}$. The results are shown in Fig. 2.3. The temperatures (blue) were calculated using a radial electric field in $x$-direction only. The results were fit with a quadratic function (solid blue line),

$$T_{\text{kin}} = T_1 + \theta_{E_{\text{rad}}} E_{\text{rad}}^2,$$

leading to a quadratic rise factor of $\theta_{E_{\text{rad}}} = 2680(15) \mu K \cdot (\text{V/m})^{-2}$. The dashed blue curve represents the approximate theoretical amount of kinetic energy due to the
2.4. A single ion in the cold buffer gas

Figure 2.3.: Equilibrium temperature of a single ion colliding with atoms at 2 µK (left) and number of collisions required to equilibrate (right) versus radial electric offset field. The results (blue points) were fit with a quadratic function (solid blue curve). The red points correspond to the average kinetic energy of an ion initialized at zero secular temperature without an atomic bath, along with a quadratic fit (red dashed curve) and the approximate theoretical amount of micromotion energy (blue dashed curve). The dashed gray lines indicate the s-wave temperature limit for $T_a \to 0$. The inset shows the difference between the solid and dashed blue curve, resembling the micromotion-induced heating. Other colors are explained in the text.

presence of excess micromotion, according to Eq. 2.10, with a quadratic rise factor of $2360 \mu K \cdot (V/m)^{-2}$. Also shown is the average kinetic energy for an ion without an atomic bath present, initialized at zero temperature (red points) along with a quadratic fit (red dashed line). The difference between the solid blue curve and the dashed red curve corresponds approximately to the amount of energy stored in the intrinsic micromotion and the secular motion. The point at $E_{rad} = 0.3 V/m$ was simulated once with a factor 10 smaller tolerance parameter $p_{tol}$ in the propagator to check for numerical errors. The values in orange were taken using a dc field with equal components $E_{rad,x} = E_{rad,y}$ in both radial directions, the values in green (behind the orange points) with a dc field with opposite components, $E_{rad,x} = -E_{rad,y}$, to check the influence of the direction of $E_{rad}$, showing no deviation from the fitted curve. The number of collisions required to equilibrate (right) seems to slightly decrease with increasing field amplitude.

2.4.3. Influence of axial micromotion

In this paragraph, we investigate the influence of a homogeneous oscillating electric field along the axial direction of the trap on the average kinetic energy of a single ion when immersed in a cold atomic cloud at 2 µK. We scanned the field amplitude $E_{ax}$
2. Prospects of reaching the quantum regime in Li-Yb$^+$ mixtures

Figure 2.4.: Equilibrium temperature of a single ion colliding with atoms at 2 µK (left) and number of collisions required to equilibrate (right) versus axial rf-field amplitude. The temperatures (blue) were fit with a quadratic function (solid blue curve). The red points correspond to an ion initialized at zero secular temperature without the presence of an atomic bath, in agreement with the approximate theoretical amount of micromotion energy (dashed blue curve). The dashed gray lines indicate the s-wave temperature limit. The inset shows the difference between the solid and dashed blue curve, resembling the micromotion-induced heating. Colors are explained in the text.

from 0 – 15 V/m and determined the ion’s average kinetic equilibrium energy in units of $T_{\text{kin}}$ and the typical number of collisions required to equilibrate $N_{\text{col}}$ according to Eq. 2.25 by taking the average over at least 300 individual runs for each point. The results are shown in Fig. 2.4. The temperatures (blue) were fit with a quadratic function (solid blue curve),

$$T_{\text{kin}} = T_1 + \theta_{E_{\text{ax}}} E_{\text{ax}}^2,$$

leading to a quadratic rise factor of $\theta_{E_{\text{ax}}} = 7.44(3) \mu \text{K} \cdot (\text{V/m})^{-2}$. The dashed blue curve represents the approximate theoretical amount of kinetic energy due to the axial oscillating electric field, according to Eq. 2.13, with a quadratic dependence of $6.92 \mu \text{K} \cdot (\text{V/m})^{-2}$, in agreement with the points in red, showing the average kinetic energy of a crystal at zero secular energy without atoms present.

Due to the large axial oscillation amplitudes at high values of $E_{\text{ax}}$, a fixed starting sphere causes the atoms to occasionally launch very close to the ion, thus introducing unrealistic jumps in the potential energy that can lead to unstable behavior. Therefore, the blue points were not obtained using a starting sphere with fixed origin at the ion’s equilibrium position, but a comoving sphere around the ion’s immediate position. As a consequence, there are events where the ion is moving away from the introduced atom such that the atom is immediately registered as having escaped, leading to an increased number of required collisions, (Fig. 2.4 right, blue points) as compared to the non-comoving case (green points). This effect seems to increase with field amplitude.
2.4. A single ion in the cold buffer gas

Figure 2.5.: Equilibrium temperature of a single ion colliding with atoms at 2 µK (left) and number of collisions required to equilibrate (right) versus phase mismatch of the two radial rf-components of the potential. The temperatures (blue) were fit with a quadratic function (solid blue curve). The red points correspond to an ion initialized at zero secular temperature without the presence of an atomic bath, in agreement with the approximate theoretical amount of micromotion energy (dashed blue curve). The dashed gray lines indicate the s-wave temperature limit. The inset shows the difference between the solid and dashed blue curve, resembling the micromotion-induced heating.

A comoving starting sphere means that especially very slow atoms that would usually cause a Langevin collision are overseen. Therefore, the average contribution of the atom to the collision energy increases. Since the ion temperature in this regime is dominated by the micromotion energy anyways, this effect can be ignored.

2.4.4. Influence of quadrature micromotion

The effect of phase micromotion on the equilibrium average kinetic energy of a single ion in an atomic gas of 2 µK is investigated. We scanned the phase difference δφrf from 0–0.65 mrad, corresponding to the expected experimental upper limit from the linewidth broadening measurement as discussed in Sect. 2.3. We determined the resulting equilibrium average kinetic energy in units of $T_{\text{kin}}$ as well as $N_{\text{col}}$ according to Eq. 2.25 by averaging over at least 300 individual runs per point. The results are shown in Fig. 2.5. The temperatures (blue) were fit with a quadratic function (solid blue line),

$$T_{\text{kin}} = T_1 + \theta_{\delta \phi_{\text{rf}}} \delta \phi_{\text{rf}}^2,$$

leading to a quadratic rise factor of $\theta_{\delta \phi_{\text{rf}}} = 3980(15) \mu K \cdot \text{mrad}^{-2}$. Also shown is the approximate theoretical amount of kinetic energy stored in the phase micromotion (dashed blue), according to Eq. 2.17, with a quadratic increase of $3651.2 \mu K \cdot \text{mrad}^{-2}$ for the parameters used in the simulation. As in the case for axial micromotion, the
red points show the average kinetic energy of an ion without an atomic bath present, in agreement with the dashed blue line. All points of the plot were simulated using a comoving start and escape sphere for the atoms to prevent numerical instabilities, thus leading to an increasing number of collisions required to equilibrate (right).

2.4.5. Summary

We have seen that the intrinsic micromotion-induced heating of the ion in the simulated system leads to an ion temperature of \( T_{\text{kin}} = 7.60(14) \, \mu\text{K} \) for the limit of \( T = 0 \, \mu\text{K} \) and rises linearly with the atomic bath temperature as expected, redistributing the atomic bath temperature on the motional degrees of freedom of the ion. From this, a collision energy of \( E_{\text{col}}/k_B = 0.38(1) \, \mu\text{K} \) can be deduced, much lower than the \( s \)-wave limit of \( T_s = 8.6 \, \mu\text{K} \) for the system. From the excess micromotion scans, we obtain the same result when the excess micromotion is is set to 0 and otherwise a quadratic dependence of the scanned parameter, as expected. The quadratic rise is about 7.5–13.6% larger than the excess micromotion energy of an isolated ion, indicating additional heating due to the collisions with the much colder atoms. This effect is found to be strongest in the radial case and weakest in the axial case. We will discuss the accessibility of the desired values for each excess micromotion parameter in section 2.8.

2.5. Ion crystals

In this section, we briefly introduce the theoretical and numerical framework to describe the normal modes of oscillations in an ion crystal. We present and test a numerical method to extract the energy stored in the secular motion of each individual mode. The section is structured as follows. First, we present the underlying physics and a method to numerically find the ion equilibrium positions. Starting from these positions, we expand the potential energy in second order and express the motion in a normal mode basis, diagonalizing the approximate potential energy. Last, we present a numerical method to extract the secular energy stored in each mode from the stored trajectories of each ion by Fourier transformation of the normal mode coordinates.

By treating the mutual Coulomb interaction of the ions as well as the trapping itself in harmonic approximation, the ion crystal can be described as a system of coupled harmonic oscillators. This system can be decomposed into normal mode coordinates.
2.5. Ion crystals

and frequencies. This procedure is described in detail in Ref. [82] for a linear ion crystal. For a given set of secular trap frequencies and number of ions, the equation of motion reads

\[ m_{\text{ion}} \ddot{\vec{r}}_n = \vec{F}_n = -m_{\text{ion}} \hat{\omega}^2 \vec{r}_n + \frac{e^2}{4\pi \varepsilon_0} \sum_{m \neq n} \frac{\vec{r}_n - \vec{r}_m}{||\vec{r}_n - \vec{r}_m||^3} , \tag{2.29} \]

where the first term describes the three-dimensional trapping of each ion with the trap frequency matrix \( \hat{\omega} = \text{diag} (\omega_x, \omega_y, \omega_z) \) and the second term is the mutual Coulomb interaction of the \( N \)-ion system. To obtain the transformation matrix to transform the system into normal mode coordinates, one first has to find the equilibrium positions \( \vec{r}_n^{(0)} \) of the ions within the trap, defined as \( \vec{F}_n(\vec{r}_n^{(0)}) = 0 \). We do this in a two-step process: First, we numerically simulate the cooling of an \( N \)-ion system in our trap until it crystallizes by introducing an additional velocity-dependent force in the equation of motion,

\[ m_{\text{ion}} \ddot{\vec{r}}_n = \vec{F}_n - \kappa \dot{\vec{r}}_n, \quad \kappa > 0 . \tag{2.30} \]

As a second step, we use the numerically obtained equilibrium positions as a guess for numerically finding the positions where the force on the ions disappears. This procedure was found to be more stable than immediate minimization of force on the ions, especially for higher dimensional crystals.

Treating the coordinates of the ions as small deviations from their equilibrium positions, \( \vec{r}_n(t) \approx \vec{r}_n^{(0)} + \vec{\rho}_n(t) \), the potential energy of the system can be expanded to second order in \( \vec{\rho}_n \) to

\[ U = \sum_{n=0}^{N_{\text{ions}}} \left( m_{\text{ion}} \frac{3}{2} \omega_x^2 \vec{r}_n^2 + \frac{1}{2} \frac{e^2}{4\pi \varepsilon_0} \sum_{n \neq m} \frac{1}{||\vec{r}_n - \vec{r}_m||} \right) \approx \frac{1}{2} m_{\text{ion}} \omega_x^2 \sum_{i,j=1}^{3} \sum_{m,n=1}^{N_{\text{ions}}} A_{3(m-1)+i,3(n-1)+j} \rho_m,i \rho_n,j , \tag{2.31} \]

with the \( 3N_{\text{ions}} \times 3N_{\text{ions}} \) Hessian matrix \( A_{3(m-1)+i,3(n-1)+j} = \frac{\partial^2 U}{\partial r_m,i \partial r_{n,j}} \bigg|_0 \), where \( r_m,i \) is the coordinate of ion \( m \) in the \( i \)-th direction and the 0 denotes its evaluation at equilibrium positions. For clarity we rename the indices of \( A \) to \( u = 3(m-1) + i, v = 3(n-1) + j, u, v \in \{1, \ldots, 3N_{\text{ions}}\} \). Diagonalization of the symmetric Hessian matrix leads to the diagonal form \( D_{u,v} \) that can be obtained from the transformation \( D = S^T A S \), where \( S \) is the matrix of eigenvectors of \( A \). The \( 3N_{\text{ions}} \) eigenmode frequencies \( f_{qu} \) are then given by \( 2\pi f_{qu} = \omega_{qu} = \omega_z \sqrt{D_{u,u}} \) and the potential energy
2. Prospects of reaching the quantum regime in Li-Yb\(^{+}\) mixtures

in secular approximation reads

\[ U_{\text{sec}} = \frac{1}{2} m_{\text{ion}} \sum_{u=1}^{3N_{\text{ions}}} \omega_{q_u}^2 q_u^2, \tag{2.32} \]

with \( q_u = \sum_{n=1}^{N_{\text{ions}}} \sum_{j=1}^{3} S_{u,3(n-1)+j} \rho_{n,j} \) the normal mode coordinates.

Once transformed to these coordinates, the trajectories stored in each kinetic energy determination are Fourier transformed numerically using a standard Cooley-Tukey fast Fourier transform (FFT) algorithm \[83\]. The Fourier spectra of the normal coordinates then contain only a peak at the respective mode frequency along with peaks at the micromotion sidebands. To obtain the energy stored in each mode, we compute the average kinetic energy of each normal coordinate \( q_m \),

\[ \bar{E}_{m,\text{tot}} = \frac{1}{2} m_{\text{ion}} \frac{1}{N_{\text{fft}}} \sum_{k=1}^{N_{\text{fft}}} \bar{q}_m(t_k)^2, \tag{2.33} \]

where \( m \) is the mode index and \( k \) the time index of the Fourier time grid of spacing \( \Delta t_{\text{fft}} \). Since this energy still contains micromotion, we make use of the Fourier relation for time derivatives,

\[ (\mathcal{F} \ddot{q}_m)(f) = -i2\pi f \tilde{q}_m(f), \tag{2.34} \]

where \( \tilde{q}_m(f) = (\mathcal{F}q_m)(f) \) is the Fourier transform of the normal coordinate \( q_m(t) \), and Parseval’s theorem for the discrete Fourier transformation,

\[ \sum_{k=1}^{N_{\text{fft}}} ||\dot{q}_m(t_k)||^2 \Delta t_{\text{fft}} = \sum_{k=1}^{N_{\text{fft}}} || -i2\pi f_k \tilde{q}_m(f_k)||^2 \Delta f_{\text{fft}} \]

\[ = (2\pi)^2 \Delta f_{\text{fft}} \sum_{k=1}^{N_{\text{fft}}} f_k^2 \tilde{q}_m(f_k)\tilde{q}_m^*(f_k), \tag{2.35} \]

with which we can replace the expectation value of the squared normal mode velocity \( \dot{q}_m(t) \) and obtain

\[ \bar{E}_{m,\text{tot}} = \frac{1}{2} m_{\text{ion}} (2\pi)^2 \Delta f_{\text{fft}} \sum_{k=1}^{N_{\text{fft}}} f_k^2 \tilde{q}_m(f_k)\tilde{q}_m^*(f_k) = \frac{1}{2} k_B T_m, \tag{2.36} \]

using the identity for the Fourier frequency grid spacing \( \Delta f_{\text{fft}} = (N_{\text{fft}}\Delta t_{\text{fft}})^{-1} \). To test
the validity of this method, the total kinetic energy of all modes

$$E_{\text{tot}, \text{fft}} = \sum_{m=1}^{3N_{\text{ions}}} \bar{E}_{m, \text{tot}} = \frac{3N_{\text{ions}}}{2} k_B T_{\text{fft}}, \quad (2.37)$$

can be compared with the average kinetic energy defined in Eq. 2.22, which is presented in Sect. A.2. Since typically all secular frequencies are separated far from the micromotion frequency, the high frequency parts of the spectrum can be cut off easily by reducing the limit of the sum in Eq. 2.36 to a value $N_c = f_c/\Delta f_{\text{fft}}$, where $f_c$ is the desired cut-off frequency. To obtain only the secular energy part for each of the modes $\bar{E}_{m, \text{sec}}$, the cut-off frequency should be chosen centered between the highest normal mode frequency and the lowest micromotion sideband. We define the temperature of each mode by $T_{m, \text{sec}}$ and the total secular temperature as $T_{\text{sec}}$ as

$$\bar{E}_{\text{sec}} = \sum_{m=1}^{3N_{\text{ions}}} \bar{E}_{m, \text{sec}} = \sum_{m=1}^{3N_{\text{ions}}} \frac{1}{2} k_B T_{m, \text{sec}} = \frac{3N_{\text{ions}}}{2} k_B T_{\text{sec}}. \quad (2.38)$$

The approximate eigenmode frequencies $f_{q_m}$ can be found by searching the peak position of the Fourier spectrum for the respective mode within an accuracy of the Fourier frequency grid size $\Delta f_{\text{fft}} = 1/(N_{\text{fft}} \Delta t_{\text{fft}})$ leading to a relative error typically on the order of $\frac{1}{2} \Delta f_{\text{fft}}/f_{q_m}$.

A typical spectrum of the Fourier amplitudes for a linear four-ion crystal is shown in Fig. 2.6. The Fourier spectra of all spatial coordinates (left) show each multiple peaks at the twelve different mode frequencies. The spectrum also contains the micromotion sidebands around the trap drive frequency of $f_{\text{rf}} = 2$ MHz and a possible cutoff value (gray bar) for the secular energy determination. While some of the peaks at around 130 kHz are too close to be distinguished, the Fourier spectra of the normal mode coordinates (right) show only one peak each, allowing for the numerical frequency and energy determination within each mode. Note that the plots are cut off at the relevant eigenmode frequency scale, not showing the micromotion sidebands around the trap drive frequency $f_{\text{rf}} = 2$ MHz. The twelve normal modes of the four-ion crystal are visualized in Fig. A.11 in appendix A.2, along with their respective frequencies obtained from the diagonalization of the secular case as presented in this section and the frequency peak positions of the Fourier spectra. Typically, these modes are assigned with the names given in the right column [84].
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Figure 2.6.: Fourier amplitudes for the twelve spatial coordinates (left) and for the twelve normal coordinates (right) for a simulated linear four-ion crystal at an average kinetic energy of around 5 $\mu$K. Each spatial coordinate shows contributions of multiple frequencies, whereas the normal modes are clearly decoupled and show only a single peak at the respective mode frequency. For the spatial coordinates, the micromotion sidebands around $f_{rf} = 2$ MHz and the cutoff frequency (gray bar) for the secular energy determination are shown as well. The Fourier spectra were obtained using $N_{\text{fft}} = 16384$ steps of $\Delta t_{\text{fft}} = 50$ ns.

2.6. Ion crystals in the cold buffer gas

In this section, we investigate the influence of the number of ions as well as that of all types of micromotion in an ion crystal. We further analyze the case where an additional oscillating electric quadrupole field in axial direction is present, leading to a non-vanishing $q_z$-parameter, which is typically the case under realistic experimental conditions. In this section, we assume that the entire crystal is immersed in the atomic cloud, and each ion is equally likely to collide with an atom. In particular, we dice the ion at which the atom is introduced before calculating each collision event.

2.6.1. Influence of the number of ions

First, the influence on the achievable temperature of the crystal $T_{\text{kin}}$ (see Eq. 2.22) and typical number of collisions required to equilibrate $N_{\text{col}}$ as defined in Eq. 2.25 was investigated. The results for one to six ions trapped using no axial or excess radial micromotion is shown in Fig. 2.7. For one and two ions at least 300 runs were averaged, whereas due to the computational effort for three to six ions, only 40 runs each were simulated, thus leading to worse statistics and thus larger errors. For the final temperature of the crystal (left) a weak dependence on the number of ions can
2.6. Ion crystals in the cold buffer gas

Figure 2.7.: Final temperature $T_{\text{kin}}$ (left) and the number of collisions required to equilibrate (right) versus number of ions in a linear crystal colliding with atoms at $2\,\mu\text{K}$. The kinetic energy shows a weak dependence on the number of ions, whereas $N_{\text{col}}$ is strictly linear.

be observed. The results were fit with a heuristic fit function (blue line),

$$T_{\text{kin}} = T_1 + \theta_i (N_{\text{ions}} - 1)^2,$$

leading to $T_1 = 11.4(2)\,\mu\text{K}$ and a quadratic rise factor of $\theta_i = 0.17(2)\,\mu\text{K}$. The number of collisions required for thermalization (right) is strictly linear in number of ions. The linear fit (solid line) leads to an increase of $626(20)$ collisions per additional ion. The behavior is to be expected since the number of modes of the crystal that need to be cooled increases linearly as well. While in the simulation only one atom is introduced at a time, in the experiment the density of atoms ideally is the same all along the ion crystal, thus increasing the actual collision rate by the factor $N_{\text{ions}}$. Consequently, the thermalization time for an $N_{\text{ions}}$-crystal is expected to be the same as for one ion.

2.6.2. Influence of excess micromotion

Similar to the single ion case, the effect of radial excess micromotion as well as axial micromotion and quadrature micromotion was investigated. Additionally, the dependence of the secular energy was studied. The obtained results can be found in appendix A.3. The behavior of the final average kinetic energy versus the scanned micromotion parameter is in perfect agreement with the single ion case.
Figure 2.8.: Equilibrium temperature of a linear four-ion crystal colliding with atoms at 2 \( \mu \)K (left) and secular temperature (right) versus \( q_z \) parameter. The left points (blue) were fit with a quadratic function and an offset (solid curve). The dashed curve shows the approximate theoretical behavior as explained in the text. The dashed gray lines indicate the s-wave temperature limit for \( T_a \to 0 \) \( \mu \)K. The red dots were obtained from a simulation with zero secular energy and no atoms present.

2.6.3. Influence of a non-vanishing axial rf-gradient

To study the effect of a non-vanishing axial rf-gradient \( q_z \), the parameter was scanned from 0 to 0.005. The value in our ion trap is around \( q_z^{\exp} = 0.0023 \) for similar trapping parameters as used in the simulation. The resulting equilibrium Temperatures \( T_{\text{kin}} \) and \( T_{\text{sec}} \) are shown in Fig. 2.8 (blue). The points were obtained by averaging over at least 30 individual runs for each value of \( q_z \) and fitting the averages according to Eq. 2.25. The results for the average kinetic energy (left) were fit using a quadratic function with offset (solid line), \( T_{\text{kin}}(q_z) = T_1 + \theta_{q_z} q_z^2 \), leading to a quadratic rise factor of \( \theta_{q_z} = 8.29(6) \cdot 10^7 \mu \)K with offset \( T_1 = 13.0(6) \mu \)K. The approximate theoretical dependence of the average kinetic energy according to Eqs. 2.9–2.10 is shown as a dashed line. The quadratic rise of the theoretical curve is given by \( \theta_{q_z}^{\text{theo}} = 7.80 \cdot 10^7 \mu \)K. The points in red show the average kinetic energies due to the influence of \( q_z \) in the non-interacting case where the ions were initialized without secular energy. A quadratic fit of the red points leads to a rise factor of \( \theta_{q_z}^{(0)} = 7.81(1) \cdot 10^7 \mu \)K, in good agreement with the prediction from the approximate solution, which is to be expected as the approximation holds for \( q_z^2 \ll 1 \). The secular temperature (right) shows an almost linear dependence on \( q_z \) and resembles the actual influence of the additional micromotion-induced heating due to a non-vanishing \( q_z \).
2.6. Micromotion-induced heating on the individual modes

In this section, we analyze the effect of each type of micromotion on the individual modes of a four-ion crystal. The secular temperature of each mode was obtained as described in Sect. 2.5 from the simulations of the linear four-ion crystal in Sect. 2.6.2 and 2.6.3. The resulting temperatures for the twelve individual modes as presented in Fig. A.11 are shown in Fig. 2.9 for radial excess micromotion (left top) axial micromotion (right top) and quadrature micromotion (left bottom). In each of the three cases the radial modes equilibrate to a slightly higher temperature than the axial modes, when the scanned excess micromotion parameter is low. For high values the temper-
2. Prospects of reaching the quantum regime in Li-Yb⁺ mixtures

ature of the modes with excess micromotion dominate, which is the x-direction (red) for both radial and quadrature micromotion and the z-direction (black) in the case of axial micromotion. A further sub-separation of the radial and axial modes is not resolved.

Interestingly, for a non-vanishing axial gradient, expressed by $q_z$, the situation is quite different, as it is shown in Fig. 2.9. In this case, the modes separate for high $q_z$ into different groups, starting with the x and y zigzag modes (red and blue crossed circles) at the lowest temperature for $q_z = 0.005$. The next group is formed by the x and y center-of-mass modes (red and blue squares) along with the drum modes (red and blue triangles) and the z anti-stretch mode (black triangles). Approximately located at average mode temperature the two tilt modes (red and blue circles) are found. At higher temperature, the three remaining axial modes, i.e. Egyptian (black crossed circles), center-of-mass (black squares) and stretch (black circles) are located. This behavior is mainly caused by the participation of the outer ions to these modes, since these can exchange the largest amount of energy during a collision due to their large micromotion amplitudes. While the contribution of the outer ion’s motion to the zigzag modes is lowest and the mode is moving perpendicular to the micromotion direction, the radial center-of-mass and drum modes show larger and equal coupling as indicated by the arrow length in the mode visualization insets and in table A.11. The anti-stretch mode shows less coupling strength for the outer ions but moves in the direction of micromotion, thus enhancing the probability for a high energy exchange within a collision. The strongest radial contribution of the outer ion’s motion is to the two tilt modes, leading to the highest radial mode temperatures. As in the case of an homogeneous oscillating axial field, the highest temperatures are found within axial modes, dominated by the one with the largest contribution of the outer ion’s motion, the stretch mode.

2.7. Two-dimensional ion crystals

By adjusting the axial and radial trapping fields, it is possible to change the shape and dimensionality to form two dimensional ion crystals [85, 86, 87, 88]. Even with perfect micromotion compensation, there are always ions within any nonlinear crystal that have their quasi-equilibrium position outside the radiofrequency node axis, thus experiencing a non-vanishing oscillating electric field, leading to additional, unavoidable micromotion. Therefore, immersing the complete ion crystal in a cloud of
ultracold atoms will always lead to micromotion-induced heating of the normal modes. To avoid this effect, one can utilize the large spacing between the ions, enabling the experimental possibility to overlap a dense and small atomic cloud only with a single ion sitting at the axial radiofrequency node within a larger ion crystal.

To simulate a stable 7-ion hexagonal ion crystal, we change the trap parameters to $f_z = 95.459\text{ kHz}$, $q_x = q_y = 0.261$, and $\alpha_x = 1.0, \alpha_y = -2.0$ to achieve $f_x = 211.002\text{ kHz}$ and $f_y = 127.229\text{ kHz}$ as radial secular trap frequencies, all within experimental reach with the ion trap used in our experiment. Due to the stronger confinement in the $x$-direction, the crystal forms in the $y - z$ plane. Its geometry along with its approximate (secular) mode structure is depicted in Fig. 2.10. Notably, in contrast to a linear crystal, the mode with the highest frequencies are not center-of-mass modes, but the two planar blink modes, where the ion density oscillates in $y$- and $z$-direction respectively. Also the mode with the lowest frequency is not a center-of-mass mode but the $x$ rotate mode, where all six ions defining the hexagon oscillate in phase clockwise/counterclockwise around the central ion within the crystal plane.

To simulate the thermalization of the secular modes, we initialize the ion crystal with negligible secular energy by first switching on a strong velocity-dependent damping force as defined in Eq. 2.30 that is adiabatically turned to zero. To give the ion crystal an initial secular energy, we add to each ion’s velocity components a velocity sampled from a Maxwell-Boltzmann distribution at a given temperature before the first collision occurs. We only let the central ion collide with atoms at $T_a = 2\text{ µK}$. We obtain the secular temperatures for each mode as in the case for the linear ion crystal by integrating over the Fourier spectra of the normal mode coordinates. Due to the orders of magnitude larger micromotion sidebands around the trap frequency of 2 MHz, it is necessary to increase the frequency resolution by a factor of four and only take a narrow range around the respective peaks for the integrals into account. Otherwise, the integrals suffer from a non-negligible micromotion floor of the Fourier spectra even around the secular frequencies that can only be suppressed by further increasing the Fourier resolution towards unfeasible computational effort. To compensate for the already large increase in computation time due to the large micromotion amplitudes and increased number of particles compared to the four-ion linear crystal, the atom start sphere size was chosen to be fixed and only $r_0 = 0.3\text{ µm}$ around the central ion, thus increasing the likelihood of Langevin collisions but also cutting down the propagation times during a collision. The results for all 21 modes of a planar seven-ion crystal initialized at $25\text{ µK}$ are shown in Fig. 2.11. The values were averaged over 120 individual runs. The thermalization of the modes can be classified into three
2. Prospects of reaching the quantum regime in Li-Yb\(^+\) mixtures

<table>
<thead>
<tr>
<th>motion</th>
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<tr>
<td>x y z</td>
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<td>z blink</td>
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<td></td>
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<td></td>
<td>y tilt</td>
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<td></td>
<td>z tilt</td>
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<tr>
<td></td>
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<td></td>
<td>x rotate</td>
<td>35.6</td>
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**Figure 2.10.** Visualization of the normal mode movement for a trapped planar seven-ion crystal. The arrows indicate the direction and amplitude of the respective mode within the plane (black) and perpendicular to the plane (red). For each mode the respective eigenfrequency \(f_{q,u}^{th}\) obtained from diagonalization of the secular approximation is shown.

- The modes where the central ion’s motion is not participating at all do not show significant cooling dynamics (left), besides the \(y\) drum (orange dashed) and \(y\) wave (dark red dashed) mode, showing a relatively slow cooling and heating, possibly due to enhanced nonlinear Coulomb interactions between the ions in these two modes.

- The modes where the central ion participates rather weakly (right, black dashed), as indicated by the length of the vectors in Fig. 2.11, show a slow cooling dynamic over the observed number of collisions.
2.8. Conclusions

Figure 2.11.: Thermalization of the secular modes of a hexagonal planar seven-ion crystal initialized at a secular temperature of 25 µK when only the central ion is colliding with atoms at 2 µK. The modes without motional components of the central ion (left) show almost no dynamic, whereas all other modes (right) thermalize to temperatures below 20 µK.

- The modes where the central ion participates most (right, solid red), \(x/z\) blink, \(x\) drop, \(z\) pendulum and \(x\) double rotation, thermalize the fastest.

The different initial temperatures of each mode are caused by the different coupling strength and number of modes each ion is involved in and could in principle be corrected for, but this is not necessary for the qualitative analysis of the behavior. Remarkably, the achieved minimum temperatures of the modes that thermalize are all found to be between 5 µK and 15 µK, comparable to the secular temperatures achieved using the linear four-ion crystal at perfect micromotion compensation, although the average kinetic energy of the planar crystal \(T_{\text{kin}} = 700\) mK is five orders of magnitude larger due to the large micromotion amplitudes of the outer ions.

2.8. Conclusions

In this chapter we have presented numerical simulations of classical Yb\(^+\)/Li collisions for ions trapped in a Paul trap. We presented and tested a numerical framework to simulate and analyze the collisions using parameters that can be achieved in our experiment, including all types of micromotion that are observable in real ion traps. We analyzed the effect of the micromotion on the achievable average kinetic energy of a single ion. For an ion in an ideal Paul trap and in the limit where \(T_a \to 0\), this energy is found to be at \(T_{\text{kin}} = 7.60(14)\) µK. Owing to the large mass ratio, this leads to a collision energy of \(T_{\text{col}} = 0.4\) µK which lies well below the s-wave temperature limit.
In this situation, the ion is cooled close to its ground state of motion with $\bar{n} = 1.2$ motional quanta remaining in the secular motion on average.

For the limits of all types of excess micromotion found in our experiment, the determined collision energies are a factor of 2–11 higher than the s-wave temperature limit, as it is shown in table 2.2. This indicates that better micromotion detection and compensation is required. In particular, using a narrow linewidth laser would allow to put better limits on the axial and quadrature micromotion amplitudes. Another option may be to use the atoms themselves for accurate micromotion detection as described in Ref. [29].

<table>
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<th>Value</th>
<th>$T_{\text{kin}}$ [$\mu$K]</th>
<th>$T_{\text{col}}$ [$\mu$K]</th>
<th>$T_{\text{sec}}$ [$\mu$K]</th>
<th>$\bar{n}_{\text{min}}$</th>
<th>$\bar{n}_{\text{max}}$</th>
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<td>single ion</td>
<td>$E_{\text{rad}}$</td>
<td>0.3 V/m</td>
<td>257(2)</td>
<td>16(3)</td>
<td>20.9(2)</td>
<td>2.6(1)</td>
</tr>
<tr>
<td></td>
<td>$E_{\text{ax}}$</td>
<td>15 V/m</td>
<td>1686(8)</td>
<td>89(4)</td>
<td>86.5(5)</td>
<td>7.0(1)</td>
</tr>
<tr>
<td></td>
<td>$\delta \phi_{\text{rf}}$</td>
<td>0.65 mrad</td>
<td>1694(7)</td>
<td>89(4)</td>
<td>75.7(7)</td>
<td>6.4(1)</td>
</tr>
<tr>
<td>four ions</td>
<td>$E_{\text{rad}}$</td>
<td>0.3 V/m</td>
<td>247(2)</td>
<td>16(3)</td>
<td>20.9(2)</td>
<td>2.5(1)</td>
</tr>
<tr>
<td></td>
<td>$E_{\text{ax}}$</td>
<td>15 V/m</td>
<td>1685(7)</td>
<td>89(4)</td>
<td>86.5(5)</td>
<td>7.3(1)</td>
</tr>
<tr>
<td></td>
<td>$\delta \phi_{\text{rf}}$</td>
<td>0.65 mrad</td>
<td>1706(6)</td>
<td>90(4)</td>
<td>75.7(7)</td>
<td>6.3(1)</td>
</tr>
<tr>
<td></td>
<td>$q_z$</td>
<td>0.0023</td>
<td>452(4)</td>
<td>26(4)</td>
<td>26.9(1)</td>
<td>2.5(1)</td>
</tr>
<tr>
<td>desired</td>
<td>$E_{\text{rad}}$</td>
<td>$&lt; 0.24$ V/m</td>
<td>168.4</td>
<td>8.6</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>$E_{\text{ax}}$</td>
<td>$&lt; 4.58$ V/m</td>
<td>168.4</td>
<td>8.6</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>$\delta \phi_{\text{rf}}$</td>
<td>$&lt; 0.20$ mrad</td>
<td>168.4</td>
<td>8.6</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>$q_z$</td>
<td>$&lt; 0.0014$</td>
<td>168.4</td>
<td>8.6</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 2.2: Simulation results for the different types of micromotion for the single and four-ion case. The collision energies $k_B T_{\text{col}}$ are all well above the s-wave energy of $E_s = k_B 8.6 \mu$K for the given experimental limits. Also shown are the corresponding minimum and maximum normal mode occupation numbers $\bar{n}_{\text{min/max}}$ and the desired values to reach collision energies below $E_s$ for each micromotion case.

The limits for each experimental parameter that lead to s-wave collisions energies are presented in table 2.2. Although all lie beyond the limits of our current setup, they are not excessive. For example, Härter et al. [89] report a field of $E_{\text{rad}} \leq 0.02$ V/m and $E_{\text{ax}} \leq 2.1$ V/m in a similar system. For the quadrature micromotion, we expect the given experimental limit of $\delta \phi_{\text{rf}} = 0.65$ mrad to be overestimated by at least an order of magnitude due to the limitations of our detection techniques, as we show in Sect. 2.3. The rf phase shift mainly results from unequal length of the connectors, which is approximately less than $\Delta x_{\text{rf}} \approx 0.5$ mm. Thus, we expect a phase mismatch on the order of $\delta \phi_{\text{rf}} \leq \frac{\Delta x_{\text{rf}}}{v_{\text{rf}}} \Omega_{\text{rf}} \approx 0.04$ mrad for an assumed signal propagation velocity of $v_{\text{rf}} \approx c_{\text{light}}/2$ half the speed of light. Similarly, we expect that the true axial
micromotion amplitude lies significantly below the experimental limit stated. We conclude that Yb\(^+\)/Li may reach the quantum regime with state-of-the-art micromotion compensation. We do note however that our present analysis is based on classical theory. For excellent micromotion compensation, a quantum description such as the one developed in Ref. [52] should be generalized to include excess micromotion and used to predict thermalization in the ultracold regime.

We found that a buffer-gas cooled linear ion crystal behaves similar as a single ion and the presence of more than three modes of ion motion does not significantly influence the achievable collision energies and thermalization rates. A non-vanishing axial gradient expressed as a \( q_z \)-parameter leads to a collision energy of \( T_{\text{col}} = 26.3 \, \mu \text{K} \) for a four-ion crystal and the experimental value of \( q_{\text{exp}}^z = 0.0023 \). Also shown in table 2.2 are the mean secular energies of the single ion and four ion case along with the mean thermal occupation numbers for the mode with the lowest frequency (center-of-mass).

Within all simulations, we do not observe runaway heating of the ion, as expected, since the mass of the ion is much larger than the mass of the atom [50]. In the simulations it takes around \( N_{\text{col}} \approx 550 - 600 \) collisions for a single ion to equilibrate within an atomic cloud with a density of \( \rho_a = \frac{1}{4/3 \pi r_0^3} \approx 1.1 \cdot 10^{18} \, \text{m}^{-3} \) (i.e. one atom within the interaction sphere at a time). Within a simulation run using a non-comoving sphere we observe an average flux \( \Phi_a \) of 10000 collisions within 120 ms propagation time, which translates into

\[
\Gamma_L t_{\text{col}} = \frac{2 \pi \rho_a}{\mu} \sqrt{\frac{C_4}{\mu N_{\text{col}}} \Phi_a} \approx 35 - 38
\] (2.40)

Langevin collisions that are required for reaching the equilibrium temperature. As only Langevin collisions lead to a significant change in momentum and energy of the colliding pairs [75], the back-action on the atomic cloud temperature in a real experiment with atom numbers typically on the order of \( 10^5 \) to \( 10^7 \) can be safely neglected. Luckily, the chance for an inelastic collision happening during the interaction time, leading to charge transfer or molecule formation is less than 0.76% as we recently measured [80]. The cooling rate for a linear ion crystal is comparable to the single ion case, under the assumption of a homogeneous atomic density all along the ion crystal. Interestingly, the secular modes of a linear ion crystal equilibrate to slightly higher temperatures than average when moving in a micromotion direction.

We have shown that collisional cooling of a planar seven-ion crystal by a localized atomic cloud interacting with only the central ion should be possible. The technique
2. Prospects of reaching the quantum regime in Li-Yb$^+$ mixtures

enables cooling of all the ten modes where the colliding ion participates in. The achieved temperatures of these modes are all below 12 $\mu$K, corresponding to mode occupation numbers of $\bar{n}_m = \frac{k_B T_m}{\hbar \omega_m} = 2 - 11$ phonons. Shuttling the ion crystal to overlap one of the outer ions with a small atomic cloud at the position of optimal micromotion compensation should in principle increase the number of cooled modes up to 18 out of the 21 total modes. Such localized micro-clouds could be implemented by using a dimple trap as it is described in Ref. [90]. There, the atomic cloud is trapped by a strongly focused laser beam with a waist of $\leq 1.8 \mu$m, much smaller than the interionic distance, e.g., 14.6 $\mu$m for the ion crystal investigated in this chapter.

Our results show that with modest improvements in micromotion compensation and detection, reaching the quantum regime of atom-ion collisions can be achieved in our experiment, enabling buffer-gas cooling of the trapped ion quantum platform close to the motional ground state and the observation of atom-ion Feshbach resonances.
This chapter describes the core components of the experimental setup that were used for the measurements in the following chapters, including the vacuum chamber, the optical setup, the magnetic field coils, the microwave setup, the computer control and home-built electronics for switching high currents. The presented system is an updated version of the setup described in [78].

3.1. Vacuum system

The vacuum chamber consists of a main part, where atoms and ions are trapped, and the lithium oven part. Both are interconnected by a differential pumping stage that also acts as a Zeeman slower (see Sect. 3.1.2 and 3.3.5 for details). All parts were custom designed or selected to fulfill the core requirement of our experiment, namely the combination of a cold atom and trapped ion experiment in the same vacuum system, involving

- the creation of a high flux of cold atoms to be trapped while not distorting the ion trapping conditions,
3. Experimental Setup

- flexible optical access for all light fields required to cool and trap both atoms and ions,
- the possibility to create large magnetic fields (up to $\sim 1000 \text{ G}$) for trapping and evaporative cooling of the atoms,
- a low magnetic permeability to prevent magnetization of the components due to the required large magnetic fields.

3.1.1. Main vacuum chamber

A CAD drawing of the main vacuum chamber is shown in Fig. 3.1 and described in detail in the PhD thesis of Jannis Joger [78]. The drawing shows a cut through the main vacuum chamber, revealing the trapping and interaction zone (1), formed by the ion trap (see Sect. 3.2). The trap is mounted to a flange (2), equipped with electrical feedthroughs for driving the trap electrodes, the Yb oven and an rf coil. The Zeeman slower (3) is connected under an angle of $48^\circ$ with respect to the ion trap axis and...
3.1. Vacuum system

slows an atomic beam coming from the oven chamber (4) (described in Sect. 3.1.2) pointing slightly below the ion trap to not disturb the trapped ions or coat the trap electrodes with $^6$Li atoms.

The coils shown are all used to create the MOT and described in detail in Sect. 3.3. The largest set (5) we name the MOT coils. To allow for high current operation, they are clamped to large water cooled copper blocks and create the required magnetic quadrupole field. The field minimum can be shuttled horizontally with the help of two small coils that are mounted around the flange holding the ion trap (2) and on the opposite side. Here, a large cross (6) connects the main chamber to an ion pump (7) and a titanium sublimation pump (8) that are required for maintaining ultra high vacuum (UHV) conditions. An ion gauge (9) is mounted at the top side of the cross and can be used to monitor the pressure. Just above and below the ion trap, another set of small coils (10), fitted into the re-entrant viewports, is used to shuttle the field minimum vertically. When switched to Helmholtz configuration, these coils can be used to generate large magnetic fields required for evaporative cooling of $^6$Li by making use of a broad Feshbach resonance near 832 G [91]. We name these coils upper/lower Feshbach coils (ufc, lfc) in the further text. Details on the design and manufacturing process of the Feshbach coils and their cooling bodies are documented in Ref. [78].

The main chamber provides optical access from the top and bottom for high NA fluorescence imaging of the ions, absorption imaging of the atoms and the creation of a magneto-optical trap (MOT) of the atoms from the atomic beam via the two aforementioned re-entrant viewports. Further optical access for ion trapping and cooling is provided via four anti-reflective (AR) coated CF16 viewports that are distributed under $45^\circ$ with respect to the ion trap axis (not visible in the drawing). On the opposite side of the Zeeman slower, another AR coated CF16 viewport (11) is used to send in the light required for slowing the atomic beam. This window is equipped with heat tape (not shown) and continuously heated to around 90°C to prevent coating with the $^6$Li-vapor, as it is directly exposed to the atomic beam. In addition, three AR coated CF63 viewports on both axial sides (12) of the ion trap and on the opposite side (13) of the ion trap mount flange provide optical access for further laser beams as it is described in Sect. 3.8.
3. Experimental Setup

3.1.2. Atomic oven chamber

To maintain ultra high vacuum (UHV) conditions in the main vacuum chamber during operation, the Zeeman slower acts as a differential pumping tube. The atomic oven part can be separated from the main chamber with a gate valve\(^1\) to exchange the lithium reservoir without breaking the vacuum in the main part. A cut through the atomic oven part including the Zeeman slower is depicted in Fig. 3.2, showing all relevant parts and the flux of the atomic beam (light red). The oven chamber and Zeeman slower follow a design developed in the group of Prof. Selim Jochim [92, 93]. The lithium reservoir (1) consists of a simple cylindrical box with 25 mm outer diameter and 26 mm outer length and a collimator tube attached to a CF16 flange, as shown in Fig. 3.2 (1), holding 1 g of \(^6\)Li (depicted in dark gray). The employed \(^6\)Li stems from an enriched sample of 95% purity\(^2\). Before filling the oven, the rough chunks were cut into blank pieces under a protective layer of mineral oil to remove oxide layers. Immediately before filling, we washed the blank pieces with cyclohexane to minimize the amount of undesired materials in the vacuum system. To avoid liquid lithium from exiting the oven during operation and reacting with the CF16 gasket, we weighted the filling to be less than a gram. As an additional safety measure, a nickel gasket\(^3\) is used at the connection to the vacuum cross, being much more resistant against corrosion [94, 95]. The oven is heated by a commercially available 200 W barrel heating element\(^4\) (not shown), which is sufficient to keep the oven at 400 – 420\(^\circ\)C during the experiment, even without thermal insulation. The heating element is controlled via solid state relay\(^5\) connected to a PID regulator\(^6\), set to heat the oven in around 5 min after switching it on, using a ramp rate of 5000 K/h. To keep the thermal load on the optical table low, we insulated the heating element with several layers of rock-wool coated aluminum foil (not shown), minimizing the power to 45(4) W. The insulation allows for a cool down of the oven with a time constant of 12(1) min.

The beam exiting the oven has a divergence angle of approximately 12.4\(^\circ\) but gets collimated by an aperture with a diameter of 5 mm, as depicted in Fig. 3.2 (2). The reduced angle allows the beam to pass the gate valve (5) without contamination of its

\(^1\) Vacom 5GVM-16CF-MV-S
\(^2\) Sigma Aldrich 340421-10G
\(^3\) Vacs SEV ICN-034G
\(^4\) Watlow MB1A1AN4-X16
\(^5\) Watlow DIN-a-mite A DA10-24C0-0100
\(^6\) Watlow EX-ZONE PM Express PM6C1CA-AAAABAA
3.1. Vacuum system

Figure 3.2.: CAD drawing of the atomic oven part of the vacuum chamber including the Zeeman slower. Lithium vapor is depicted in light red. Numbers explained in the text.

mechanics. The beam can be mechanically shut using a rotary feedthrough\textsuperscript{7} (3) with an attached, polished stainless steel plate. The rotation can be controlled with a servo\textsuperscript{8} (not shown) for shutting the beam after the loading of atoms within an experimental sequence. When the stainless steel plate is put under 45° angle to the atomic beam, it can be used to couple out a laser beam through the (uncoated) viewport\textsuperscript{9} on top (4), which is helpful for alignment of the Zeeman slower beam (see also Sect. 3.8). The atomic beam exits the Zeeman slower (6) with a divergence angle of approximately 0.54° and a diameter of 13 mm, small enough to prevent a coating of the lower inverted viewport of the main vacuum chamber. In case the atomic oven needs to be replaced, the gate valve (5) can be closed and the oven chamber can be filled with, e.g., argon via a separate all-metal valve\textsuperscript{10} (8) before a new oven is attached.

The Zeeman slower (6) is connected to the water cooling system (7). The water is guided successively through four channels between the vacuum tube and the outer coil-carrying tube, as described in Ref. [93]. The outer tube is equipped with eight coils of the same width but decreasing number of turns (from right to left) to tailor an axial magnetic field that provides optimal loading conditions. The working principle

\textsuperscript{7} Hositrad Rotary Feedthrough Economy, magnetically coupled
\textsuperscript{8} Radiant Dyes Low Cost Mini Shutter driven with a TTL controlled Arduino Mega 2560.
\textsuperscript{9} Hositrad HOVPZ64Q
\textsuperscript{10} Vacom 4AVM-63CF-MM-S
of the Zeeman slower and details about the coils and magnetic fields are described in Sect. 3.3.5. The inner tube does not have an optimal (conical) shape for differential pumping (see also [93]) as it was not possible to create such a shape in our mechanical workshop. Instead, the inner part has three different diameters to approximate a conical shape. To bridge the magnetic field of the Zeeman slower to the one created by the MOT coils, the flange connecting the slower tube to the main vacuum chamber needed to be hidden under the smallest coil.

3.2. Ion trap

The central part of our experiment is formed by the ion trap shown in the CAD drawings in Fig. 3.3. Part (a) shows a view from the vacuum-pumping side of the main chamber, (b) shows a cut through the radial plane viewed from the axial direction of the ion trap. The ion trap (2) is held by a single piece of stainless steel of low magnetizability (1) that is mounted on a CF63 flange. Ceramic tubes are used as insulation for the electrodes\textsuperscript{11}. The radial cut reveals the pair of rf and dc blade electrodes used to create the dynamical trapping field for radial confinement. The inter-blade distance is 3 mm each. Above and below the trap center, two sets of compensation electrodes can be used to apply DC voltages to compensate for potential unwanted electric fields, originating from, e.g., charges sticking to nearby surfaces. Cutouts in the trap holder (1) guarantee for horizontal optical access under 45° and for imaging from above. The end cap electrodes used for axial confinement of the ion provide further optical access via a hole of 2 mm diameter. The minimum distance between the two end cap electrodes is 10 mm. A stainless steel tube (4) filled with a few small blank-cut chunks of 99.9\% Yb\textsuperscript{12} serves as a source of neutral Yb atoms. The oven is heated by sending a current through a welded-on tantalum wire to generate a small flux of Yb atoms towards the ion trap, where they are ionized, trapped and cooled as described in Sect. 4.1. The mirror (3) is used for initial trapping of the atoms in a MOT below the ion trap to prevent direct exposure of the trap electrodes with the beam of $^{6}$Li atoms coming from the Zeeman slower. Note that the use of a mirror MOT also compactifies the system, as a conventional MOT would require optical access from the top and the ion trap mount side as well. Loading of the MOT and transport of the atomic cloud into the ion trap is described in chapter 5.

\textsuperscript{11} The full trap assembly manual and a list of parts and materials can be found in Ref. [78]
\textsuperscript{12} Sigma Aldrich 548804-5G
3.3. Magnetic field coils

We use four pairs of coils to produce magnetic fields for trapping, shuttling, optical pumping and evaporative cooling of the $^6\text{Li}$ atoms. Additionally, eight coils form a Zeeman slower (ZSL) used for slowing the atomic beam before initial trapping in the MOT. All of these coils have been designed and built within our group. They were modeled carefully using the theoretical framework provided in appendix A.5.

3.3.1. MOT coils

Together with the ZSL, the MOT coils produce the fields for the first stage of the atom trapping scheme, a magneto-optical trap (MOT). Each MOT coil consists of 98 turns of flat wire$^{13}$, divided into two layers of 49 radially stacked turns. Each layer was wound separately before being glued on top of the other layer using epoxy glue$^{14}$. The current runs from the outside to the inside of the first layer and then back to the outside in the second layer. The inside ends of both layers are connected to each other using brass screws. The MOT coils were designed to fulfill two major requirements. Due to the enhanced size of the vacuum chamber when compared to other cold lithium experiments, the MOT coils need a larger diameter to assure a smooth transition of the radial (horizontal) magnetic field to the axial field of the Zeeman slower. The second requirement is to produce a stable magnetic field gradient of around $g_z = 44\text{ G/cm}$ in the axial (vertical) direction for forming a $^6\text{Li}$ MOT. The coils are powered by a power supply$^{15}$ running at 54 A to produce the desired gradient. In this setting the pair of

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$^{13}$ Multogan/Damid 200 Grad 2 5.00 × 1.40 mm$^2$
$^{14}$ EPO-TEK T905BN-3
$^{15}$ Delta SM 45-70 D
3. Experimental Setup

coils consume around 1.2 kW. To prevent overheating, each MOT coil is clamped to a massive water cooled copper cooling body with regular heat sink grease in between.

3.3.2. Radial compensation coils

Since the MOT is not created in the exact center of the vacuum chamber but below a mirror, the magnetic field minimum produced by the MOT coils needs to be slightly shifted. For the horizontal shift, we use a pair of compensation coils, one wound around the ion trap holding flange and one on the opposite side. The compensation coils are wound axially around an aluminum ring that also serves as a sleeve to fit onto the flange. Each coil consists of two layers of 15 inner turns and 14 outer turns of copper wire with a conductor diameter of 2.0 mm. The coils are designed to produce a homogeneous field of around 13.3 G at 20 A at the position of the MOT to shift the quadrupole field minimum by around 6 mm below the mirror. Temperature sensors are connected to the remote shutdown of the power supply\textsuperscript{16} to avoid overheating in case of wrong current settings.

3.3.3. Axial compensation coils

The axial compensation coils are designed to fit exactly around the two large axial viewports and consist of 62 turns each, wound as four layers of copper wire with a conductor diameter of 1.0 mm. They are typically switched off and only used for defining an axial field for optical pumping of atoms and ions within the sequences and thus require no additional cooling. To ensure fast switching, these coils are connected to a four quadrant power supply\textsuperscript{17}. For the maximum current of 10 A, the coils produce an axial field of 20 G at the position of the MOT.

3.3.4. Feshbach coils

The smallest coil pair in the experimental setup are the Feshbach coils, whose main purpose is to produce large homogeneous magnetic fields during the evaporative cooling of the atoms, as described in Sect. 5.2.2. They consist of 16 radially stacked turns of flat wire\textsuperscript{18} each and are placed as close as possible to the experiment within the

\textsuperscript{16} Delta SM 18-50
\textsuperscript{17} Kepco BOP 20-10
\textsuperscript{18} Meffert 50063010070 6.30 × 1.00 mm\textsuperscript{2}
inverted viewports. The coils were designed to produce a homogeneous field of 900 G at a current of 320 A in Helmholtz configuration at the center of the vacuum chamber. As a second purpose, they are used to capture the magneto-optical trap from the slow MOT coils in anti-Helmholtz configuration and to transport the magnetically trapped atoms into the ion trap. This is done by controlling each coil current via the analog inputs of two individual power supplies as described in Sect. 5.1.4. To prevent overheating of the coils, they are each glued on top of two water cooling bodies. A detailed description of the design can be found in the PhD thesis of Jannis Joger [78].

### 3.3.5. Zeeman slower

To efficiently load the MOT, we employ a Zeeman slower [96] to enhance the flux of atoms that are slow enough to be captured by the MOT. The Zeeman slower is shown in Fig. 3.2 (6). The working principle is as follows: Atoms flying through the Zeeman slower experience a position-dependent magnetic field and thus a position-dependent Zeeman splitting. A counter-propagating laser beam, detuned by $\delta_L = -104$ MHz from the Doppler cooling transition used for the MOT, resonantly scatters photons on atoms that have the right position and velocity to compensate for $\delta_L$ via the Zeeman shift $\delta_Z$ and Doppler shift $\delta_D$ of the transition. To address as many atoms as possible, the slowing laser beam is focused onto the atomic oven, overlapped with the conical shape of the atomic beam. The laser creates a velocity and position-dependent slowing force [93] of the form

$$ \vec{F}_{sp}(\vec{x}, \vec{v}) = \hbar \vec{k} \cdot \frac{\Gamma}{2} \frac{s}{1 + s} + \frac{s}{(2\delta(\vec{x}, \vec{v})/\Gamma)^2} , $$

(3.1)

given by the momentum of the cooling photons $\vec{p} = \hbar \vec{k}$ times the scattering rate, where $\Gamma$ is the natural linewidth of the transition and $s$ is the saturation parameter. The detuning $\delta(\vec{x}, \vec{v})$ is given by the sum [93]

$$ \delta(\vec{x}, \vec{v}) = \delta_L + \delta_D(\vec{v}) + \delta_Z(\vec{r}) , $$

(3.2)

with the Doppler shift $\delta_D(\vec{v}) = \vec{v} \vec{k}$ and the Zeeman shift $\delta_Z(\vec{x}) \approx -\mu_B B(\vec{x})/\hbar$, where $\mu_B$ is the Bohr magneton and $B(\vec{x})$ the absolute value of the magnetic field. When designed properly, the magnetic field ensures that once resonant, a photon-scattering atom remains resonant and thus keeps being slowed down until it reaches the MOT.

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19 Delta SM 15-400
where it is trapped. This can be achieved by designing the magnetic field as close as possible to a square root shape along the Zeeman slower axis to ensure a constant slowing force for a resonant atom.

<table>
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<td>264</td>
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<td>198</td>
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<td>64</td>
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<td>0.19</td>
</tr>
<tr>
<td>$I$ [A]</td>
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<td>6.4</td>
<td>6.4</td>
<td>6.4</td>
<td>6.4</td>
<td>6.4</td>
<td>6.4</td>
<td>5.4</td>
</tr>
</tbody>
</table>

**Table 3.1.**: Coil configuration of the Zeeman slower including the counted number of turns $N$, measured Resistances $R$ at room temperature and operating currents $I$.

The field is created by a set of eight coils wound using insulated copper wire of 1 mm conductor diameter, certified to withstand temperatures of up to 180°C. To estimate the required currents and number of turns, we performed trajectory simulations solving Newton’s equations to account for a successful and smooth slowing of atoms for different numbers of turns, currents and saturation parameters. From the results of the simulations we decided for a coil configuration that is given in Tab. 3.1. Due to spatial restrictions, the magnetic field produced by the eight coils of the Zeeman slower and the MOT coils deviates significantly from the desired square root shape, as it is shown in Fig. 3.4 (left). An example of a phase portrait for this configuration is shown in Fig. 3.4 (right), where a saturation parameter of $s = 5$ was used. Although the magnetic field profile is not perfectly square-root-shaped, all trajectories with starting velocities from 150-750 m/s end in the capture volume of the MOT.

In operation, the water cooled Zeeman slower dissipates 330 W and heats up to around 110°C at the surface of the biggest coil due to the poor heat transport between the insulated, air-surrounded wires and the stainless steel body of the slower. In a future setup, this could be improved by the use of flat wire and thermal grease or at least glue between the turns to avoid air pockets.

### 3.4. Ion laser setups

In this section we briefly present the laser setups used to ionize and cool Yb$^+$ ions in our experiment. Unless otherwise noted, all optical fibers used (depicted as loops) are single mode fibers and for simplicity their couplers are not shown in the sketches. Focal lengths are given in mm and the distances between lenses are not drawn to scale.
3.4. Ion laser setups

Figure 3.4.: Calculated axial magnetic fields (left) of the Zeeman slower coil setup (see Tab. 3.1). The magnetic fields of the eight individual coils (blue) and the radial field of the MOT coils running at 56 A (dark blue) form the total field profile (black). An ideal square root shaped field profile is also shown (dashed red). The vertical lines depict the beginning and end of each Zeeman slower coils and the center of the MOT. The right figure shows the corresponding phase portrait obtained from a one dimensional trajectory simulation using Eq. 3.1 and a saturation parameter of $s = 5$. The horizontal gray line corresponds to the capture velocity of the MOT and the vertical gray lines to the capture radius and center of the MOT [93].

The drawings are updated versions from the PhD thesis of Jannis Joger [78], where details on the beam sizes and powers can be found.

3.4.1. The 399 nm laser

The first laser used for generating Yb$^+$ ions is a home-built grating-stabilized external-cavity diode laser (ECDL) near 399 nm, which is described in detail in Ref. [67]. It is used for the first step of photoionization as described in chapter 4. The setup of the beam is shown in Fig. 3.5. An optical isolator$^{20}$ (OI) protects the diode from back-reflections. A small fraction of the beam is split at a polarizing beam splitter (PBS) to go to a wavemeter for wavelength measurement and feedback as described

\[ \text{Thorlabs I0-5-405-LP} \]

Figure 3.5.: Sketch of the laser setup for the 399 nm beams.
3. Experimental Setup

in Sect. 3.6. The main beam is focused at a mechanical shutter\(^{21}\) (MS) that serves as a switch for the beam to enable/disable the creation of ions.

### 3.4.2. The 369 nm laser

The second laser used for trapping Yb\(^{+}\) ions is a Toptica DL Pro diode laser emitting light near a wavelength of 369 nm, used for the second step of ionization and Doppler cooling as described in chapter 4. The setup of the beam is shown in Fig. 3.6. To avoid multimode operation of the diode, two OIs\(^{22}\) are used. Two small fractions of beam power are split off, one to go to a home-built low-finesse cavity (described in [78]) for Pound-Drever-Hall stabilization \(^{[97]}\) (PDH) of the laser and one for the wavemeter.

The main beam is split into two paths, one is shifted by +205 MHz (detection beam) and the other one by +200 MHz (cooling beam) using acousto-optical modulators\(^{23}\) (AOM) that are also used for pulse-shaping. A fraction of the detection beam can be utilized for optical pumping with circularly polarized light at the experimental setup (\(\sigma\)-pumping), as described in Sect. 4.2, but is typically blocked. For optical pumping of \(^{171}\)Yb\(^{+}\) (see Sect. 4.4.1), an electro-optical modulator\(^{24}\) (EOM) can be used to modulate sidebands of 2.105 GHz onto the beam. The cooling and detection beam are overlapped to go through the same optical fiber. An additional MS can be used

\(^{21}\) Home-built, design and performance can be found in Ref. [67]

\(^{22}\) Thorlabs IO-3-375-GLB

\(^{23}\) Gooch & Housego 3200-1210

\(^{24}\) Qubig EO-T2100-3M equipped with a 2 W amplifier.

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**Figure 3.6.** Sketch of the laser setup for the 369 nm beams.
to reduce the amount of stray-light coming from switched-off AOMs during sensitive measurements.

3.4.3. The 935 nm laser

The third laser used for trapping Yb\(^+\) ions is also a Toptica DL Pro diode laser, emitting light near a wavelength of 935 nm, used to repump population from the \(2D_{3/2}\)-state back to the cooling cycle as described in chapter 4. The setup of the beam is shown in Fig. 3.7. A small amount of power is split at a PBS to go to the wavemeter, which we also use for frequency stabilization of the laser. The EOM\(^{25}\) is used to imprint sidebands at 3.07 GHz onto the main beam, which are useful when repumping the isotope \(^{171}\)Yb\(^+\) (see Sect. 4.4). For shutting the beam, we utilize an MS as well as an AOM\(^{26}\) at +80 MHz.

3.4.4. The 638 nm laser

Another laser used for trapping Yb\(^+\) ions is an ECDL emitting at a wavelength near 638 nm in the same design as the 399 nm laser described in detail in Ref. [67]. It is used to repump population back from the \(2F_{7/2}\) state as described in chapter 4. The setup of the beam is shown in Fig. 3.8. An external OI\(^{27}\) protects the diode from back-reflections. A small fraction of power is split to go to the wavemeter for monitoring and control of the wavelength (see Sect. 3.6). The main beam (re-repumper) goes to the experiment, where it is overlapped with the repumper beam. The MS can be used for switching the beams off as desired. Optionally, a fiber-coupled EOM\(^{28}\) can be implemented and used for fast and precise frequency scans and to bridge the hyperfine

\(^{25}\) Qubig EO-T3070-3M equipped with a 10 W amplifier
\(^{26}\) Gooch & Housego 3080-122
\(^{27}\) Thorlabs IO-3D-633-VLP
\(^{28}\) Jenoptik phase modulator PM785
3. Experimental Setup

3.4.5. The 329 nm laser

We use a Toptica TA-FHG PRO system, emitting light near a wavelength of 329 nm, to drive the $^{2}S_{1/2} \rightarrow ^{2}P_{3/2}$ (D2) transition in Yb$^+$ for optically pumping the ion into the $^{2}F_{7/2}$ state as it is used in chapter 6 and 7. The exact procedure is described in Sect. 4.2. We plan to use the laser for driving Raman transitions between the Yb$^+$ ground state Zeeman levels in the future [98]. The setup as it was used in this work is shown in Fig. 3.9. The 329 nm beam is derived from a frequency quadrupled laser at 1316 nm. The beam at 1316 nm gets first amplified by a tapered amplifier (TA) and is then sent through two frequency doubling cavities. After the first doubling, a part of the light is used for frequency stabilization to a fixed, temperature stabilized
3.5. Atom laser setups

reference cavity (described in [98]). A fiber-coupled EOM\(^{29}\) generates sidebands with a frequency between 0.1-3.0 GHz which are used to offset the laser’s carrier frequency with respect to the cavity mode. An AOM\(^{30}\) in double pass is used for pulse shaping and frequency scanning. Both rf signals to drive the EOM and AOM are derived from a dual channel microwave source\(^{31}\) that gets an external 10 MHz reference for enhanced frequency stability.

### 3.5. Atom laser setups

In this section we briefly describe the laser setups used for trapping and cooling \(^6\)Li atoms in our experiment. The drawings of the beams at 671 nm wavelength are adapted and updated versions of the setup shown in the PhD thesis of Jannis Joger [78]. As in the ion laser setups, lens distances are not to scale and focal lengths are given in mm. All fibers are single-mode polarization-maintaining and depicted as three loops. Couplers are not shown for simplicity.

#### 3.5.1. The 671 nm D1 laser

We use an interference-filter stabilized Radiant Dyes NarrowDiode diode laser, emitting at a wavelength near 671 nm, to drive the \(^2S_{1/2} \rightarrow \(^2P_{1/2}\) (D1) transition in \(^6\)Li for optical pumping as it is presented in Sect. 5.1.2. The setup of the beam is show in Fig. 3.10. We use an OI\(^{32}\) to ensure stable single mode operation of the diode. A fraction of the beam is split at the OI to go to the wavemeter for monitoring and control of the wavelength. We use a MS to shut off the whole beam for straylight sensitive applications. An AOM\(^{33}\) shifts the frequency by \(2 \times 114\) MHz to bridge the 228 MHz hyperfine splitting of the electronic ground state in \(^6\)Li. A second AOM\(^{34}\) is used for fast switching of the beam. Before going into the fiber towards the experiment, the beam is overlapped with one of the imaging beams coming from the \(^6\)Li D2 laser as described in the following subsection. We ensure the same polarization of the two beams by using the reflected light from a PBS.

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\(^{29}\) Jenoptik phase modulator PM635

\(^{30}\) Gooch & Housego 3200-1210

\(^{31}\) WindFreak SynthHD

\(^{32}\) Linos FI-680-5SV

\(^{33}\) Gooch & Housego 3100-125

\(^{34}\) Gooch & Housego 3100-125
3. Experimental Setup

Figure 3.10.: Sketch of the laser setup for the 671 nm D1 beams.

3.5.2. The 671 nm D2 laser

For cooling and trapping of $^6$Li, we use the 671 nm $^2S_{1/2} \rightarrow ^2P_{3/2}$ (D2) transition as it is explained in Sect. 5.1. Due to the rather high saturation intensity [99], a comparably large amount of laser power is required. Thus, we use a tapered amplifier (TA) system (Toptica SYST TA PRO 670), delivering around 200 mW of output power at the desired wavelength.

The optical setup has grown over the years and is therefore the most complex when compared to the other laser setups in our experiment, as shown in Fig. 3.11. Within the Laser housing, an ECDL serves as the master oscillator. A fraction of the beam is split off at a beam sampler and is guided to the wavemeter for monitoring of the wavelength. The amplified beam is guided through an AOM$^{35}$ running at 228 MHz to bridge the hyperfine splitting of the $^2S_{1/2}$ ground state. The frequency shifted component (repumper) contains around 1/3 of the total power and gets re-overlapped with the main beam (Doppler) at PBS1. A small amount of power is split off and used for locking of the laser and high field imaging. The remaining beam is sent through an AOM$^{36}$, shifting the laser frequency by -114 MHz. Thus, three branches of the original amplified beam have been created that will be described in the following.

- The shifted light is used for trapping the atoms in the magneto-optical trap (MOT) and deceleration in a Zeeman slower (ZSL), as described in Sect. 3.3.5. The AOM is optimized for maximum diffraction efficiency since as much light as possible is desired for trapping and cooling of the atoms. The frequency is set

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$^{35}$ Gooch & Housego 3200-125
$^{36}$ Gooch & Housego 3100-125
such that the MOT is detuned by -34 MHz from the atomic resonance. The light used in the ZSL branch gets an additional shift of -70 MHz via another AOM to avoid scattering of photons on the atoms trapped already in the MOT.

- The unshifted light is sent to another AOM, where the first diffraction order is shifted by 80 MHz to be on resonance with the D2 transition for absorption imaging.

The first order beam is split into a branch for imaging in the MOT region (imaging fiber) and a branch for imaging within the ion trap (upper imaging fiber).

The zeroth order beam is guided through another 80 MHz AOM of the same type and used to create a set of four near resonant additional MOT beams (upper MOT fibers) that are used for a second MOT within the ion trap, as explained in Sect. 5.2.

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37 Gooch & Housego 3080-125
38 Gooch & Housego 3080-122
3. Experimental Setup

- The small fraction of light created at PBS1 is used for laser stabilization and high field imaging. It is guided through an AOM\(^{39}\) operated at around 200 MHz in double pass configuration that can be tuned by ±10 MHz. The shifted beam is guided to the cavity for locking the ECDL similar as the 369 nm laser. Therefore, the AOM can be used to quickly shift the lock point on a very short timescale, e.g., for creating a compressed MOT (see Sect. 5.1.1) and fine-tuning of the absorption imaging resonance condition (see Sect. 5.1.3).

A second fraction is sent to a \(^6\)Li spectroscopy cell, which is used to lock the cavity to compensate for temperature drifts. The cell setup is described in Sect. 3.7.

A third fraction is used to generate light detuned by the 2×200 MHz plus another 2×350 MHz by using an additional AOM\(^{40}\) that can be tuned over a range of ±10 MHz. The light is used for imaging at high magnetic fields within the ion trap and thus overlapped with the upper imaging beam.

3.5.3. The 1070 nm dipole trap laser

The beam path of the 1070 nm dipole trap laser\(^{41}\) (IPG) used for dipole trapping of \(^6\)Li (see Sect. 5.2) was designed to be short and to contain as little components as possible, as high powers on the order of 100 – 200 W are required for creating a sufficiently deep optical trap for \(^6\)Li (for details on the dipole trapping, see Sect. 5.2). The design allows for stable operation and avoids losses due to imperfect coatings while keeping the cleaning effort low. The complete laser setup fits inside of a safety enclosure around the experiment to avoid light leaking into the laboratory. A sketch of the setup is shown in Fig. 3.12. The beam exits the fiber head of the IPG with a diameter of 7.5 mm. It is held by two lens tube mounts\(^{42}\) on solid bases. For alignment, we use a \(\lambda/2\) wave plate\(^{43}\) in combination with a Brewster window\(^{44}\) that guides vertically polarized light to a beam dump\(^{45}\). The beam is demagnified using an 8:1 telescope that consists of \(f = 200\) mm and \(f = -25\) mm lenses\(^{46}\), such that

\(^{39}\) Gooch & Housego 3200-125
\(^{40}\) Gooch & Housego 3350-125
\(^{41}\) IPG YLR-200-WC 200 W Ytterbium Fiber Laser
\(^{42}\) Thorlabs SM1TC
\(^{43}\) LENS Optics W2Z20-1064 HP
\(^{44}\) Altechna 2-HCBTFF-1064-2040
\(^{45}\) Altechna 10BD01
\(^{46}\) LENS Optics Fused Silica lenses, anti-reflection coating for 1070 nm
the collimated beam fits through the aperture of the AOM\textsuperscript{47}. The AOM is mounted on a solid four-axis tilt alignment stage\textsuperscript{48} and equipped with a passive cooling body. It can be used to smoothly reduce the power of the beam during evaporative cooling (see Sect. 5.2.2). Due to the potentially large power in the 0th order, it is guided to another beam dump using a D-shaped mirror. Both beam dumps are equipped with temperature sensors that are connected to the interlock of the laser and shut it down when the temperature exceeds 70 °C. A second telescope magnifies the beam back to its original size to reduce the intensity on the following optical elements. Both telescopes are built in lens tubes to prevent dust exposure. Each lens tube is fixed to the optical table using two lens tube mounts on solid bases. A PBS can be used to overlap a 935 nm beam for pre-alignment of the dipole trap on the ion, as described in Sect. 5.2.3. Behind the first and last mirror\textsuperscript{49}, large infrared photodiodes pick up the leaking light to monitor potential power loss due to misalignment as described in Sect. A.4. The beam gets elevated on the height of the ion trap and is focused through the end caps using $f = 400$ mm lenses under an angle of 5.0° to the ion trap axis. The mirrors depicted in blue are in piezo actuated mirror-mounts\textsuperscript{50} to fine-adjust the beam position within the ion trap. A second $\lambda/2$ wave plate turns the polarization of the return beam by 90° to prevent a standing wave pattern in the ion trap. After the return path through the ion trap, the beam gets dumped in a third, water-cooled beam dump\textsuperscript{51}.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure3.12.png}
\caption{Sketch of the laser setup for the 1070 nm beams.}
\end{figure}

\textsuperscript{47} Gooch & Housego 3110-191
\textsuperscript{48} Newport New Focus 9071
\textsuperscript{49} LENS Optics Fused Silica mirrors for high power, coated for 1030-1090 nm
\textsuperscript{50} Radiant Dyes MDI-H-1” piezo version
\textsuperscript{51} Altechna 10BDWC01-2 mounted in two AST OPTICS AST1262 80 mm tube mounts
3. Experimental Setup

3.6. Wavelength measurement and feedback

We monitor the wavelengths of all laser systems besides the 1070 nm dipole trap laser and the 671 nm Li D2 laser on a commercial wavelength meter\(^\text{52}\). The wavelength is read out within the experimental control software and can be used as an input for software regulation. For the 638 nm and 399 nm laser, the regulation loops are set to control the piezo voltage of the respective external gratings of the diode lasers via an analog output\(^\text{53}\) whose voltage gets amplified with a piezo amplifier\(^\text{54}\). In case of the 935 nm and 671 nm D1 systems, the analog voltage is amplified by the electronics of the manufacturer but also applied at the piezo of the ECDL grating.

For the 369 nm laser, the feedback is applied at the piezo of one of the cavity mirrors, since the laser is locked to the cavity. The piezo voltage of the second cavity mirror can be set at the same control computer with a stable but slow high voltage source\(^\text{55}\). Since the 671 nm laser is locked indirectly to a spectroscopy cell as described in Sect. 3.7, no wavelength monitoring is required.

For the 329 nm laser, which is locked to a temperature stabilized cavity, typically no automatized feedback is desired and required. Drifts in wavelength can be adjusted by hand via the frequency of the frequency-offset-lock as it is described in chapter 7.2 and Refs. [98, 100].

3.7. Lithium spectroscopy cell

To ensure wavelength-stable operation of the \(^6\)Li D2 laser, we use two coupled lock mechanisms. The D2 laser itself is locked via the PDH technique to the transmission signal of a Gaussian mode from a reference cavity\(^\text{78}\). Due to temperature fluctuations of the cavity, the mode and thus the wavelength of the laser may shift by a few MHz, immediately influencing the loading performance and the absorption imaging resonance-condition for the \(^6\)Li atoms. Therefore, we employ a spectroscopy cell filled with the \(^6\)Li isotope\(^\text{56}\), heated to 330 °C. We employ Doppler-free saturated absorption spectroscopy\(^\text{101}\) to derive an error signal that is fed back to the piezo of the

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\(^{52}\) HighFinesse WS7-30  
\(^{53}\) National Instruments PCI-6723  
\(^{54}\) TEM Messtechnik miniPiA  
\(^{55}\) iseog EBS 8030  
\(^{56}\) Made available by Prof. Jook Walraven
cavity mirror, thus locking the cavity to the spectroscopy cell via the PDH technique. The cell-setup is depicted in Fig. 3.13. The AOM\textsuperscript{57} is operated at 330 MHz and is required to compensate for the 400 MHz shift of the previous double-passed 200 MHz AOM employed for the frequency-offset-lock (see Sect. 3.5.2) and thus shifts the laser frequency on resonance. A beam sampler is used to split the beam in probe and pump beams that are guided counter propagating under a small angle through a home-built spectroscopy cell. The transmitted probe beam is focused on a photodiode (PD) used for deriving the error signal.

3.8. Optical setup around the experiment

Flexible optical access to the two trapping stages formed by the MOT and the ion trap is provided by three CF63 viewports, five CF16 viewports and the two inverted viewports as described in Sect. 3.1.

3.8.1. Lower part

On the height of the MOT, only the 671 nm lasers are used for trapping (D2), optical pumping (D1) and imaging (D2), as depicted in Fig. 3.14. The MOT beam is magnified to around 1 cm beam diameter immediately after the optical fiber. It is split into equal components by a PBS to create the axial and the vertical beam. The axial beam passes a quarter-wave plate before and after the vacuum chamber to create the correct circular polarization for both primary and retro-reflected beam. The vertical MOT beam also passes a quarter-wave plate and enters the vacuum chamber from below (path only partially shown). It gets reflected to the radial direction by the mirror inside the

\textsuperscript{57} Gooch & Housego 3350-125
3. Experimental Setup

Figure 3.14.: Sketch of the optical setup around the vacuum chamber at the height of the MOT stage, shown from below. The sketch shows an updated version of the setup presented in [78].

chamber. It exits the chamber on the vacuum-pump side of the setup where it passes another quarter-wave plate and gets retro-reflected.

The Zeeman slower beam passes a magnification stage and two mirrors, which allow for focusing and aligning it onto the atomic oven. The combined imaging (D2) and optical pumping (D1) beam passes the chamber under a small angle to allow for absorption imaging on a CCD camera\(^5^8\) (Stingray).

3.8.2. Upper part

In the optical setup at the height of the ion trap axis, all lasers used for trapping, cooling and imaging of both atoms and ions are present. A sketch of the setup is shown in Fig. 3.15. For simplicity, the dipole trap beams which enter and exit the trap axially through the end caps under an angle of 5.0° w.r.t. the ion trap axis are not shown (see Fig. 3.12). The 935 nm repumper and 638 nm re-repumper beams are overlapped at a PBS and enter the ion trap through the left end cap, focused on the ions. From

\(^{58}\) Allied Vision Stingray F-033
the other side, the 399 nm photoionization beam and the optional 369 nm $\sigma$—pumping beam are overlapped at a PBS and enter the ion trap axially from the right, also focused onto the ions. The 671 nm axial imaging beam is superimposed at a dichroic mirror\textsuperscript{59} and is used for absorption imaging of ultracold atoms within the ion trap onto another Stingray CCD camera. Due to the presence of ion lasers and potential scattered light from the dipole trap beams, a bandpass filter\textsuperscript{60} mounted directly in front of the camera protects the CCD. Under 45° two 329 nm Raman beams (due to their future purpose), are focused onto the ions. During the experiments presented in this thesis, only one of them was used. On the lower side of the sketch, the 369 nm cooling beam enters the chamber under 45° as well as the two 671 nm upper MOT beams, which are retro-reflected on the upper part of the drawing, to create the desired MOT configuration.

\textsuperscript{59} Edmund Optics 69-204 600 nm dichroic shortpass filter
\textsuperscript{60} Thorlabs FB670-10
3. Experimental Setup

3.8.3. Combined imaging system

Fluorescence imaging of the ion and absorption imaging of the ultracold atoms within the ion trap as well as the upper MOT stage requires a flexible imaging system. A sketch of the setup is shown in Fig. 3.16. For completeness, the path of the vertical/radial MOT beam is shown as well.

Fluorescence light of the trapped ions (1) is collected with a high numerical aperture \( (N.A = 0.61) \) aspheric \( f = 32 \text{ mm lens} \) (2), guided to a mirror (3) and imaged with the help of two \( f = 200 \text{ mm lense} \) (4), a dichroic mirror (5), a color filter (6) and an adjustable aperture (7) onto the photomultiplier tube (8) and a CCD camera (9) simultaneously using a beam splitter (10). The aperture is placed into the imaging plane to enhance the signal-to-noise ratio by spatial restrictions. The detection efficiency of the ion objective can be computed by multiplying the individual transmissions/reflections of the optical elements at the fluorescence wavelength of 369 nm times the numerical aperture of the imaging lens and the quantum efficiency of the photomultiplier, leading to around \( \eta_{\text{obj}} \lesssim 0.00044 \).

The high field absorption imaging of the ultracold atoms within the ion trap is done with an imaging beam coming through the lower viewport. The atoms are imaged onto another Stingray CCD camera (11) using a \( f = 35 \text{ mm aspheric lens} \) (12) and a color filter (13) for stray-light protection. The vertical upper MOT beams are formed by two counterpropagating beams guided through the upper and lower viewport. The upper beam gets collimated at the atoms position by an additional \( f = 50 \text{ mm lens} \) (13). A motorized mirror (14) is used to switch between upper MOT operation and high field absorption imaging.

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61 Thorlabs AL4532-A  
62 Thorlabs BB2-E02  
63 Thorlabs LA1979-A  
64 Thorlabs DMLP550  
65 Thorlabs FGUV11-UV  
66 Owis SP 40  
67 Sens-Tech P25PC  
68 Andor Zyla 5.5  
69 Edmund Optics 46-705 UV beam splitter plate 70T/30T  
70 Edmund Optics 49-663  
71 Thorlabs FB670-10  
72 Thorlabs LA1255-A  
73 Using a TTL triggered Arduino Mega 2560 microcontroller with a connected ULN2003 stepper motor shield to steer a 28-BYJ48 stepper motor from 0 – 45°.
3.9. Computer control system

The experiment is controlled via two computers, both running a C++ based control program, developed mainly by Prof. Kilian Singer and the group of Prof. Ferdinand Schmidt-Kaler, enabling the flexible implementation of hardware and experimental sequence structures.

One of the two computers is dedicated for wavelength monitoring and feedback as described in Sect. 3.6 and the control of the static ion trap voltages, as they are not changed within the experimental sequences. The computer is also connected to webcams that monitor the cavity modes and the MOT.

The second computer is connected via Ethernet to an FPGA-based combined digital-to-analog (DAC)/TTL control box, developed in the Group of Prof. Ferdinand Schmidt-Kaler. Its analog and digital outputs are connected to all elements of the experiment that need to be controlled within timed sequences, e.g., the analog current programming inputs of the power supplies and the switches for the AOMs and EOMs. The

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74 http://quantumtechnology.info
75 http://quantenbit.de
data acquired from measurements is stored on a network drive within the lab that is accessible from both computers via gigabit Ethernet for flexible accessibility.

The stored data is mirrored every night on another hard drive and uploaded by the end of each week to a drive outside of the lab as a backup.

### 3.10. Microwave setup

To excite the 12.6 GHz hyperfine transitions in $^{171}\text{Yb}^+$ [102], we use a Rohde & Schwarz SMB100A signal generator that provides 18 dBm at 12.6 GHz. The signal generator is not switched off to avoid fluctuations due to warm-up of the device. We mix the signal with the output of an arbitrary waveform generator. The waveform generator is used to switch the signal, tune the frequency to the desired hyperfine transition and program pulsetrains for microwave qubit operations as they are presented in Sect. 4.4. In addition, an absorptive switch can be used to ensure a proper switch off for sensitive applications by attenuating the signal by at least 80 dB. The signal is amplified with an air-cooled 10 W amplifier and irradiated into the experimental setup from below using an SMA-to-waveguide adapter. All cables carrying the unmixed and mixed 12.6 GHz signals are semi-rigid and kept as short as possible to prevent mechanical instabilities that may cause impedance fluctuations and reflections.

### 3.11. High current switching

All central coils besides the axial compensation and the upper MOT coil are equipped with a circuit for fast switching. The axial compensation coils are connected to a bipolar power supply which can actively stop the current by applying voltage of opposite sign when required. At no point of the experimental sequence both MOT coils need to be switched off fast, since the MOT is slowly transferred to the set of Feshbach coils in anti-Helmholtz configuration. For the Feshbach and radial compensation coils, the situation is different. They are used to form a magnetic trap from which absorption

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76 Mini-Circuits Mixer ZX05-153MH-S+
77 VFG 150, developed in the group of Prof. Wunderlich [103]
78 Meuro SPST120180A8
79 Microwave Amplifiers Ltd. AM53-12.4-12.8-40-40
80 Flann 18094-SF40
81 Mini-Circuits 086 and 141 series
images are taken after release, thus fast switching is required to ensure that the fields are off during the imaging.

Two types of switches were constructed, both based on the idea of stopping the current flow from the power supply using transistors and of dissipating the energy stored in the magnetic field quickly by using a circuit with a differential resistance in parallel to the coil. To limit the induction voltage spikes when switching off the current source, we use either transient voltage suppressor diodes (TVS) or varistors, which both limit the voltage to be close to their breakdown voltage until the current has stopped flowing. In a simple model, this can be described by the differential equation

\[ L_{\text{coil}} \dot{I} + R_{\text{coil}} I + U_D(I) = 0, \]  

(3.3)

where \( L_{\text{coil}} \) and \( R_{\text{coil}} \) is the inductance and resistance of the coil, \( I \) is the time-dependent current and \( U_D \) is the voltage drop across the TVS diode or varistor that is used to dissipate the energy. For an ideal diode, the Shockley equation \cite{104}

\[ I(U_D) = I_S \left( e^{\frac{U_D}{nU_T}} - 1 \right), \]  

(3.4)

implicitly describes the voltage drop \( U_D \) at the TVS diode with \( I_S \) the reverse bias saturation current, \( n \approx 1-2 \) the ideality factor and \( U_T \) the threshold voltage. Inversion leads to

\[ U_D = nU_T \ln \left( \frac{I_D + I_S}{I_S} \right). \]  

(3.5)

Combined with Eq. 3.3, the equation can be solved numerically to estimate the requirements on \( U_D \) for reaching a desired switching speed. A typical solution for switching off a current of \( I(0) = 320 \, \text{A} \) is shown in Fig. 3.17. For the solution, we set \( R_{\text{coil}} = 10.6 \, \text{m\Omega} \), \( L_{\text{coil}} = 1 \, \text{mH} \), \( n = 1.5 \), \( I_S = 1 \, \text{mA} \) and \( U_T = 40 \, \text{V} \) (red), 80 V (blue), 120 V (green), corresponding to the approximate values for one of the Feshbach coils. For all three breakthrough voltages shown, the current damps out in less than 0.5 ms.

For the set of radial compensation coils, the switch is based on an IGBT\textsuperscript{82} and a commercially available IGBT driver board\textsuperscript{83}. The role of the IGBT is to shut down the flowing current on demand. The energy stored in the magnetic field then leads to a sudden build-up of an induction voltage that can discharge across a varistor\textsuperscript{84} and the

\textsuperscript{82} Semikron SKM75GB12T4
\textsuperscript{83} Semikron SKHI 10/12 R
\textsuperscript{84} Epcos S20K35
3. Experimental Setup

![Graph](image)

**Figure 3.17.** Theoretical damping of the current in an ideal inductor when biased in a loop along with a resistor and a TVS diode with breakthrough voltage 40 V (red), 80 V (blue) and 120 V (green) according to Eq. 3.3.

coil resistance. When designing the switch, it is important that the reverse breakdown voltage of the IGBT is higher than the breakdown voltage of the varistor to not break the IGBT or the power supply. The power supply itself is protected from induction voltage spikes by two parallel high current diodes\(^\text{85}\), mounted on an active air-cooled heat sink along with the IGBT. A schematic of the switch is shown in Fig. 3.18 (left).

![Diagram](image)

**Figure 3.18.** Schematic of the current switch for the radial compensation coil (left) and the upper Feshbach coil (right). The working mechanisms are similar, although due to the difference in inductance and maximum currents, the used elements for switching are different, as explained in the text. The coils are drawn as an ideal inductor and a resistor.

\(^\text{85}\) ST STTH10002TV2
3.11. High current switching

For the upper Feshbach coil (ufc) a similar circuit is used. Instead of the IGBT, ten parallel high current MOSFETs of the same type as for the lower Feshbach coil shut down the current on demand. The MOSFETs are driven by a commercially available driver board\textsuperscript{86}. When switching to non-conducting, the energy stored in the coil is dumped in a set of three parallel branches of five TVS diodes\textsuperscript{87} in series, two parallel high power diodes\textsuperscript{88} and the resistance of the coil. An additional stack of six parallel low forward voltages diodes\textsuperscript{89} mounted on a large air cooler protects the power supply from induction voltage spikes, as shown in Fig. 3.18 (right).

The switching circuit of the lower Feshbach coil (lfc) is inspired by a design of Prof. Selim Jochim’s group in Heidelberg [105]. Due to the necessity of having large homogeneous magnetic fields for evaporative cooling of the $^6$Li atoms, the direction of the lower coil current can be switched such that the pair of Feshbach coils not only can be operated in anti-Helmholtz configuration to create a quadrupole field but also in Helmholtz configuration to create a large homogeneous field in vertical direction. Heart of the switch is the H-bridge driver IC Intersil HIP4081a, that ensures fast switching of a stack of four times ten parallel high current MOSFETs\textsuperscript{90} mounted on a huge copper construction for heat dissipation and easy connection of the large diameter wires to the coils. The circuit diagram for the connection of the H-bridge driver can be found in the appendix, see Fig. A.14. For electrical insulation but thermal contact between the massive copper parts, a special gel mat\textsuperscript{91} was used instead of heat sink grease, to withstand potential mechanical stress due to the weight of the parts. The H-bridge driver serves both as a switch for the direction of current but also as a complete current switch, both controlled via TTL inputs. A schematic of the circuit is shown in Fig. 3.19. The H-bridge driver either opens the gates $V_{GH1}$ and $V_{GL2}$ and closes $V_{GH2}$ and $V_{GL1}$ or vice versa, to guide the current in the two possible directions through the coil in normal operation. When switched to non-conducting, all gates close and the energy stored in the coil is dissipated in a similar way as in the case of the upper Feshbach coil. Due to the two possible directions of the current through the coil, two pairs of diodes ($D_3$, $D_4$) serve as a bridge rectifier for the TVS stack.

For the lower MOT coil, the switch is very similar to the one for the lower Feshbach

\textsuperscript{86} Texas Instruments ISO5851EVM
\textsuperscript{87} Bourns SMLJ8.0A
\textsuperscript{88} IXYS DSEI2x101-06A
\textsuperscript{89} ST STTH200W06TV1
\textsuperscript{90} Infineon IRFB3077PbF
\textsuperscript{91} Fischer Elektronik Gel 10
3. Experimental Setup

Figure 3.19.: Schematic of the current switch for lower Feshbach coil. The gates of the MOSFETs are controlled by an H-bridge driver IC (see appendix, Fig. A.14) as described in the text. The coil is drawn as a perfect inductor $L_{\text{LFC}}$ and resistor $R_{\text{LFC}}$.

The only difference in circuit design is the reduced number of required MOSFETs ($4 \times 2$ in parallel) due to the lower currents and the lack of the diode stacks, since no fast switching is required. The only purpose of the switch is to change the MOT coil configuration from anti-Helmholtz to Helmholtz to support the Feshbach coils in producing large homogeneous magnetic fields during evaporative cooling, see 5.2.2.
In this chapter we present the typical measurements performed on trapped ions in our experiment. First, we discuss the relevant energy levels and transitions used for trapping, cooling and imaging of the ions. We present and analyze an electron shelving technique to read out the Zeeman sublevel of the electronic ground state in the Yb$^+$ isotopes without nuclear spin. Using the isotope $^{174}$Yb$^+$, we analyze the detection efficiency of our imaging system. We present the hyperfine qubit in the electronic ground state of $^{171}$Yb$^+$, including the schemes for state preparation and state readout. Knowledge of the detection efficiency of our imaging system allows us to analyze the possibility of projective measurements of the hyperfine qubit in our experiment. We use the qubit to measure and calibrate the large magnetic fields produced by the coils in our experiment. Furthermore, we perform vacuum quality measurements by analyzing the frequency of ion crystal melting events. This is done by tracking the location of non-fluorescing impurity ions in a linear crystal over time. Finally, we present a full set of tools to analyze and compensate excess micromotion and measure the heating rate in our ion trap setup using a set of techniques. The results we find are of crucial importance to judge the atom-ion collision energies achievable in our experiment.
4. Trapped ions

4.1. Loading, cooling and imaging of trapped Yb$^+$ ions

In order to load Yb$^+$ ions into the trap, the Yb oven is operated at a current of typically 3.0 to 3.5 A, dissipating a power of less than 1.4 W. This leads to a small flux of neutral Yb atoms into the ion trapping region where they are isotope-selectively excited by light at a wavelength of 399 nm, resonant with the $^1S_0 \rightarrow ^1P_1$ transition of the respective isotope [106, 107]. From the $^1P_1$ state the atoms are ionized by the 369 nm Doppler cooling beams and subsequently cooled to the center of the trap. The cooling laser is typically red-detuned by about 10 MHz from the $\Gamma = 2\pi \cdot 19.72(22)$ MHz [108] wide $^2S_{1/2} \rightarrow ^2P_{1/2}$ cooling transition of the ion. On average, every 200$^{th}$ photon scattered [79] leads to the population of the meta-stable $^2D_{3/2}$ state with a lifetime of $\tau = 52(1)$ ms [109], from which the 935 nm repumper beam transfers the ion back into the cooling cycle, as depicted in Fig. 4.2. Thus, the ions are continuously cooled and form a Coulomb crystal that can be observed on the camera and the PMT signal by collecting the 369 nm fluorescence photons. An example of such a crystal is shown in Fig. 4.1. The distance between the ions depends on the strength of the axial confinement and the number of ions [82] and is on the order of tens of micrometers.

![Figure 4.1:](image)

**Figure 4.1.:** False color CCD image of a linear seven-ion Coulomb crystal within our trap. The tight radial confinement leads to a linear shape along the ion trap axis.

Once the desired number of ions is reached, the ionization process can be stopped by mechanically shutting the 399 nm beam. Within a sequence, the fluorescence signal detected with the PMT can be used for automatized loading.

From time to time an ion is loaded into a larger orbit where less cooler and repumper light is present. Thus, it can happen that even after a few minutes of closing the photoionization beam an additional ion cools into the crystal. To prevent such a situation, we are able to lower the radial confinement for a period of a few milliseconds.
4.1. Loading, cooling and imaging of trapped Yb\textsuperscript{+} ions

to expel the ions with a large orbit from the ion trap. By carefully choosing the amplitude of the low radial confinement, it is also possible to eject single ions from the crystal. The method is especially handy if a dark ion appears within an ion crystal. This might happen due to off-resonant loading of the wrong isotope or after a chemical reaction with a background-gas molecule, leading to trapped molecular ions. As these ions are not Doppler-cooled and less tightly confined due to their higher mass, they are more likely to be ejected from the lowered trapping potential.

Dark ions also appear occasionally due to collisional quenching to the very stable low-lying \( ^2F_{7/2} \) state. Thus, a laser at 638 nm is utilized to pump the population back into the cooling cycle, as shown in Fig. 4.2.

![Figure 4.2: Simplified level scheme of Yb\textsuperscript{+} showing the transitions at 369 nm, 935 nm and 638 nm relevant for Doppler cooling a trapped ion. Additionally shown is the D2 transition near 329 nm that can be used for electron shelving to the metastable \( ^2F_{7/2} \) state as described in Sect. 4.2. Dashed arrows indicate the relevant decay processes for cooling and shelving. The hyperfine structure in case of \( ^{171}\text{Yb}^+ \) is not shown. Details about lifetimes and branching ratios can be found in the table.](image)
4.2. State preparation and shelving of $^{174}\text{Yb}^+$

In order to measure spin-dependent atom-ion collision processes, methods for spin detection and preparation are required. For initialization of the $^{174}\text{Yb}^+$ ion in a Zeeman level of the $^2S_{1/2}$ ground state, we apply a pulse of resonant circularly polarized light on the 369 nm cooling transition along the trap axis. A small magnetic bias field pointing either parallel or anti-parallel along the trap axis is used to prepare either of the two Zeeman states. We measure the optical pumping efficiency by comparing the fluorescence during the optical pumping pulses for the correct $\sigma$-polarization and the fluorescence for linear polarization with the case where no ion is present. From these measurements we obtain an optical pumping efficiency of $98.5(6)$ % for the $|^{2}S_{1/2}, m_J = 1/2\rangle = |\uparrow\rangle$ state and $97.8(7)$ % for the $|^{2}S_{1/2}, m_J = -1/2\rangle = |\downarrow\rangle$ state.

![Figure 4.3.](image.png)

**Figure 4.3.:** Probability for finding an ion in the bright state versus duration of the 329 nm shelving pulse. When initially prepared in the $|\downarrow\rangle$ state (red) the ion remains unshelved with a probability of $28(3)$ %, whereas in the case of $|\uparrow\rangle$ (black) the ion is only shelved off-resonantly. The data is shown along with an analytic model that involves all relevant levels.

To detect the spin state, we state-selectively shelve the ion into the long-lived $^2F_{7/2}$ state. We therefore apply a homogeneous magnetic field of 72.5 mT to separate the $^2S_{1/2} \rightarrow ^2P_{3/2}$ transitions by 680 MHz and irradiate a shelving pulse resonant with the $|\downarrow\rangle \rightarrow |^2P_{3/2}, m_J = -3/2\rangle$ transition, allowing for a decay channel via $^2D_{5/2}$ to the $^2F_{7/2}$ state with a probability of $72(3)$ % [81, 111, 112]. We measure the probability for finding the ion being still in the $^2S_{1/2}$ ground state by switching off the magnetic field after the shelving and subsequent detection of the fluorescence during Doppler
4.3. Detection efficiency of the imaging system

We determine the detection efficiency \( \eta_{\text{obj}} \) of the PMT imaging system experimentally using a single \(^{174}\text{Yb}^+\) ion. First, we analyze the fluorescence decay after the 935 nm repumper beam is switched off. Due to the fast dynamic of the decay, the data was obtained using a 100 \( \mu \)s PMT-bin that is shifted in steps of 100 ns with respect to the point where the repumper beam is switched off. The signal follows the form

\[
N_{\text{det},PD}(t) = S_0 + \frac{\eta_{\text{obj}}}{B_{PD}} e^{-t/\tau_{PD}},
\]

(4.1)

where \( B_{PD} = 0.00501(15) \) is the branching ratio of the \(^2P_{1/2} \rightarrow ^2D_{3/2}\) transition [79], \( \tau_{PD} \) is the decay time of the process and \( S_0 \) is the number of background photons within one time bin (100 \( \mu \)s). Alternatively, we can observe the reverse process. We prepare the ion in the \(^2D_{3/2}\) state by switching off the repumper for a time much larger than \( \tau_{PD} \) and observe the fluorescence of the ion after switching the repumper beam back on again. The obtained signal is of the form

\[
N_{\text{det},DS}(t) = S_0 + \frac{\eta_{\text{obj}}}{B_{PD}} \left( 1 - e^{-t/\tau_{DS}} \right),
\]

(4.2)

where \( \tau_{DS} \) is the time it takes the repumper to pump the population back into the bright cooling cycle. The obtained data of both methods along with a combined fit is shown in Fig. 4.4. The low number of photons requires a large number of averages, thus 12000 individual runs were taken. From the fit we obtain a detection efficiency of \( \eta_{\text{obj}} = 3.68(12) \cdot 10^{-4} \). This is a bit less than the theoretical upper limit of \( 4.4 \cdot 10^{-4} \).
4. Trapped ions

![Figure 4.4](image-url)

Figure 4.4.: Observation of the fluorescence of a single $^{171}\text{Yb}^+$ ion turning dark due to a switched off repumper (blue) and turning bright after switching the repumper back on (gray). The data was fit using a combined fit according to Eqs. 4.1–4.2, leading to the solid curves.

computed in Sect. 3.8.3, obtained from the datasheets of the optical elements and the reduced numerical aperture due to the presence of the ion trap.

From the fitted decay time $\tau_{PD} = 8.71(41) \mu$s, we are also able to extract the saturation parameter $s_{369}$ of the detection beam. Knowing that on average every $1/B_{PD} \approx 200^{th}$ photon scatters to the $^2D_{3/2}$ state, we deduce the resonant scattering rate [115] in our experiment to be

$$\Gamma_{\text{exp}} = \frac{1}{\tau_{PD} B_{PD}} = \frac{\Gamma_0}{2} \frac{s_{369}}{s_{369} + 1},$$

with the natural linewidth $\Gamma_0 = 2\pi \cdot 19.72(22)$ MHz [108]. Solving for the saturation parameter, we get $s_{369} = 0.587(53)$, which we will use in Sect. 4.4.5 to estimate the average photon number scattered during the state detection of $^{171}\text{Yb}^+$.

4.4. The hyperfine qubit in $^{171}\text{Yb}^+$

In addition to the normal cooling scheme, the isotope $^{171}\text{Yb}^+$ requires a few more transitions to be bridged due to its nuclear spin of $1/2$. This leads to a hyperfine splitting of around 12.6 GHz [102] in the electronic ground state, where the two hyperfine states with $m_F = 0$ form a first-order magnetic field-insensitive microwave qubit [79]. Also
4.4. The hyperfine qubit in $^{171}$Yb$^+$

![Figure 4.5](image)

**Figure 4.5.** Simplified level scheme of $^{171}$Yb$^+$. It shows the relevant transitions at 369 nm for cooling/detection and optical pumping to the $F = 0$ hyperfine ground state using an EOM (see Sect. 3.4.2). The hyperfine splittings of the repumper and re-repumper transitions are bridged using EOMs and taken from Ref. [79] and [112, 116], respectively.

the $^2P_{1/2}$ state shows a significant splitting of 2.105 GHz, as it is depicted in the level scheme in Fig. 4.5. The ion is cooled on the $^2S_{1/2}, F = 1 \rightarrow ^2P_{1/2}, F = 0$ transition. Off-resonant coupling of the 369 nm cooling laser to the $^2P_{1/2}, F = 1$ states can lead to a population of the $F = 0$ hyperfine ground state. Therefore, the 12.6 GHz transition is bridged by irradiation of resonant microwaves as described in Sect. 3.10. The hyperfine splittings of the $D$ states are bridged by modulating sidebands at 3.07 GHz on the 935 nm laser beam with a resonant EOM (see Sect. 3.4.3) to pump population from all $^2D_{3/2}$ states back to the Doppler cooling cycle [79]. The hyperfine splitting of the 638 nm re-repumper transition can be bridged using a fiber-coupled EOM as mentioned in Sect. 3.4.4. The dashed gray arrows indicate the population and depopulation of the $D$ states within the cooling/detection cycle. The $^2D_{3/2}, F = 2$ state gets only rarely populated by off-resonant excitation of the $^2P_{1/2}, F = 1$ state during cooling/detection. Only during optical pumping a significant effect of the 3.07 GHz EOM can be observed.

While during Doppler cooling the hyperfine ground state splitting seems more as an
obstacle, the $|F = 0, m_F = 0\rangle$ and $|1, 0\rangle$ states can serve as a first-order magnetic field-insensitive microwave qubit [79] as we present in the following subsections.

4.4.1. State preparation

To initialize the microwave qubit in a defined state, we add sidebands at 2.105 GHz using a resonant EOM as described in Sect. 3.4.2 to optically pump population via the $^2P_{1/2}, F = 1$ state to the $F = 0$ ground state while the microwave radiation at 12.6 GHz is switched off. For typical laser and EOM powers, this can be achieved in less than 100 $\mu$s. To prepare one of the $m_F$ states in the $F = 1$ ground state manifold, we apply a subsequent microwave rapid adiabatic passage (RAP) [117] or a $\pi$-pulse resonant with the respective $\Delta m_F$ transition.

4.4.2. State detection

To detect the hyperfine state of the ion, we apply a pulse of light resonant with the 369 nm cooling transition together with light resonant with the 935 nm repumper transition and collect the fluorescence. In the case of $F = 1$, the ion scatters photons until it eventually gets off-resonantly excited to the $^2P_{1/2}, F = 1$ state from which it can decay to the $F = 0$ hyperfine ground state. Thus, the number of collectable fluorescence photons that are scattered during detection is limited, as we will discuss in Sect. 4.4.5. The detection scheme does not allow for the direct distinction of the $m_F$ sublevels in the $F = 1$ manifold as due to the broad linewidth of the cooling transitions all three sublevels will scatter photons in a low magnetic field. To distinguish, one first has to swap the population $p_{m_F}$ of the desired $m_F$ sublevel with the $F = 0$ ground state by a resonant RAP or $\pi$-pulse and apply the detection pulse, as it is used for the analysis of the hyperfine states. The obtained signal is then proportional to $1 - p_{m_F}$.

4.4.3. Microwave frequency scan

We determine the transition frequency of the respective hyperfine ground state transitions by preparing an ion in the $F = 0$ state via optical pumping as described in 4.4.1. We apply a microwave pulse at a certain frequency $f_{mw}$ for a fixed time $T_{mw} = 3$ ms, much larger than the expected Rabi period, to eventually flip the spin when close to resonance. For each frequency setting, we detect the state of the ion and repeat
4.4. The hyperfine qubit in $^{171}$Yb$^+$

the measurement for 50–100 times to obtain satisfying statistics. After each state
detection the ion is Doppler cooled for 5 ms. A full spectrum of all three transitions
using the preparation and detection as described is shown in Fig. 4.6 (left) in red,
showing very sharp peaks at three positions as well as small broad peaks, possibly due
to leaking cooling light. The spectrum in blue was taken by scanning the frequency of
the microwave source while all cooling lasers were switched on. Thus, it shows significant
broadening and Stark shift due to the presence of the laser fields, indicating that
efficient Doppler cooling is possible on all three transitions at a slightly red shifted
microwave frequency. The narrow peak of the $\Delta m_F = +1$ transition is shown on the
right. The Zeeman shift of 7.3 MHz translates to a magnetic bias field of 5.2 G and
can be used to probe small magnetic fields of all coils. For larger fields, it is more
convenient to use the weak quadratic Zeeman effect of the $\Delta m_F = 0$ transition as we
present it in Sect. 4.5.

![Figure 4.6: Full spectrum of the three hyperfine transitions in the electronic ground state of $^{171}$Yb$^+$ (left) for the preparation and detection as mentioned in the text (red) and while Doppler cooling (blue). The plot on the right shows only the narrow peak of the $\Delta m_F = +1$ transition.](image)

4.4.4. Manipulation of the qubit

Having the resonant transition frequencies of the hyperfine ground state at hand al-
 lows us to, e.g., coherently drive Rabi oscillations to optimize the microwave coupling
strength and to perform Ramsey-experiments to check the coherence times for esti-
mating the magnetic field stability.

To drive a Rabi oscillation, we prepare the ion’s electronic ground state in $F = 0$ via
optical pumping, followed by a microwave pulse of gradually increased length $T_{mw}$ at
the determined transition frequency for the respective transition. After the pulse, we
detect the state and Doppler cool the ion again for 5 ms. An exemplary signal for
a Rabi oscillation on the $\Delta m_F = +1$ transition is shown in Fig. 4.7 (left). Due to
magnetic field noise, the signal decays within 2.7(3) ms. In contrast, the first-order
magnetic field-insensitive $\Delta m_F = 0$ transition survives much longer (right) and no
decay is visible on the timescale shown. Both signals were obtained by averaging over

![Figure 4.7.](image)

**Figure 4.7.** Rabi oscillations between the hyperfine ground states $F = 0 \leftrightarrow F = 1$,
$m_F = 1$ (left) and $m_F = 0$ (right), along with a fit according to Eq. 4.4 (solid blue
lines).

250 individual measurements and fit with the theoretical prediction taken from [118],

$$S(t) = A_0 e^{-t/\tau} \left( \sin^2 \left( \frac{\Omega_R t}{2} \right) - \frac{1}{2} \right) + S_\infty,$$

(4.4)

where the exponentially decaying envelope takes the decoherence into account, $S_\infty$ is
the equilibrium brightness of the signal and $S_\infty - A_0$ the signal background. From
the fit we obtain the Rabi frequency $\Omega_R$ and thus the pulse lengths to drive $\pi$ and
$\pi/2$-pulses, $T_\pi = 2 \cdot T_{\pi/2} = \frac{2\pi}{2\Omega_R}$, for inverting the population or creating a super-
position between the two respective hyperfine states. For the transitions shown, it is
$\Omega_R(\Delta m_F = 0) = 2\pi \cdot 4.43(1)$ kHz $= \Omega_R(\Delta m_F = +1)$. These values can be tuned by
increasing the microwave source power and by proper positioning of the microwave
horn to increase the intensity of the microwave field and improve the polarization at
the position of the ion. Typically, achievable Rabi frequencies in our experiment are
about an order of magnitude higher than the ones shown.

Having the correct resonant pulse widths at hand, one can perform a Ramsey-experiment [119] to determine the coherence time of the respective transition within
the laboratory environment for potential improvements on, e.g., the magnetic field
stability. Being sensitive to the detuning of the pulses to the real transition frequency,
4.4. The hyperfine qubit in $^{171}\text{Yb}^+$

we use a Ramsey-experiment to probe frequency shifts due to static magnetic fields, as we will present in Sect. 4.9.2, where also the sequence is explained in detail. Using a spin echo-technique [120], we also use a Ramsey experiment as an interferometer to probe for example the ac-Stark effect of the involved levels for alignment purposes, as we will present in Sect. 5.2.3.

4.4.5. Detection limits of the $^{171}\text{Yb}^+$ hyperfine qubit

In this section we analyze the limiting factors for state detection of the hyperfine ground state in $^{171}\text{Yb}^+$. While for the previous measurements the distinguishability between bright ($F = 1$) and dark ($F = 0$) within a state detection was of less importance due to the large number of averages, it is of critical importance for quantum information applications to be able to perform high fidelity single shot readouts of the quantum state, so called projective measurements. Therefore, the signal of the bright state must always be significantly higher than the signal of the dark state. In our detection scheme this means that the number of photons scattered and detected before the bright ion falls into the $F = 0$ state must be always more than the number of background photons. The number of collectable photons for an ion in the $F = 1$ state is limited by two factors. One of them is the intrinsic detection efficiency of our objective, $\eta_{\text{obj}}$, as measured in Sect. 4.3, and the other is the total number of photons that are scattered during a detection pulse, limited by the off-resonant coupling of the detection laser to the $^2P_{1/2}, F = 1$ state, which is shifted to the blue by the hyperfine splitting $\Delta_{\text{hfs}} = \frac{2\pi}{1049(13)} \text{GHz}$ [121].

We can estimate the total number of scattered detection photons $N_{\text{tot}}$ via the off-resonant scattering rate [115]

$$\Gamma(\Delta) = \frac{\Gamma_0}{2} \frac{s_{369}}{1 + 4(\Delta/\Gamma_0)^2 + s_{369}},$$

(4.5)

where $\Delta$ is the detuning from resonance. Using the saturation parameter of the detection beam $s_{369}$ as determined in Sect. 4.3, we estimate that on average it takes $N_{369} = 3\Gamma(0)/\Gamma(\Delta_{\text{hfs}}) = 8.61(34) \cdot 10^4$ photons before the state gets off-resonantly excited, followed by a decay to the $F = 0$ ground state. The decay time of the whole process is given by $\tau_{\text{flu}} = 3/\Gamma(\Delta_{\text{hfs}}) = 3.76(36) \text{ms}$, where the factor of three

$^1$ Note that this estimation does not take into account the time the population may spend in the $^2D_{3/2}$ state, which can be safely neglected due to the fast repumping dynamics given by $\tau_{\text{DS}} = 0.80(5) \mu\text{s}$ as determined in Sect. 4.3.
4. Trapped ions

in photon number and fluorescence time is due to the Clebsch-Gordan coefficients of
the decay process. Thus, we expect at most \( \eta_{\text{obj}} N_{369} = 32(2) \) photons (on average) to
be detected for an ion prepared in the \( F = 1 \) state.

In the limit of \( s_{369} \to 0 \), a maximum number of \( 1.37(8) \cdot 10^5 \) photons can be scattered
before a transition to the dark state occurs, as it is shown in Fig. 4.8 (left), while
the detection time diverges as shown in the right. Thus, we conclude that lowering

the saturation of the detection beam can only lead to mild improvements in the to-
tal number of scattered photons while dramatically increasing the required detection
time.

![Figure 4.8](image1)

**Figure 4.8.** Average photon number scattered before the ion undergoes a transition to
the \( F = 0 \) electronic ground state (left) and the time it takes versus saturation parameter
of the detection beam (right).

![Figure 4.9](image2)

**Figure 4.9.** Average number of detected photons versus length of the detection time bin
of the PMT for the bright (blue) and dark (gray) state (left). During the detection, the
bright state gets depopulated to the dark state, indicated by the exponential reduction
in slope. The data was fit as explained in the text. A histogram showing the statistical
frequency of the number of detected photons for the dark (gray) and bright (blue) state
at a bin time of \( t_{\text{bin}} = 2 \) ms is shown in the right.
4.4. The hyperfine qubit in $^{171}\text{Yb}^+$

To verify the estimated decay time $\tau_{\text{fluo}}$ of the bright state during detection within our experiment, we measure the average photon number within a detection bin versus the detection bin size $t_{\text{bin}}$ for the ion prepared in both hyperfine states. The results are shown in Fig. 4.9 (left). When prepared in the dark ($F = 0$) hyperfine ground state (gray), the average number of photons increases linearly in time due to ambient light and stray light from the detection laser, whereas in the case of the bright ($F = 1$) state, the slope starts much steeper and decreases exponentially (blue). The data was fit using a combined model including a linear function $N_{\text{avg},d}(t_{\text{bin}}) = \gamma_{\text{bg}} t_{\text{bin}}$ for the dark state (black line) and $N_{\text{avg},b}(t) = \gamma_{\text{bg}} t_{\text{bin}} + N_b \left(1 - e^{-t_{\text{bin}}/\tau_{\text{exp}}} \right)$ for the bright state (blue line). For the photon number difference between dark and bright state we obtain $N_b = 5.6(2)$ and for the time scale of the depopulation $\tau_{\text{exp}} = 2.4(1)$ ms in rough agreement with the expected value of $\tau_{\text{det}} = 3.76(36)$ ms. Although the average photon number difference seems to be easily detectable, the spread of detected photons in the single shot measurements is large, as it can be seen in Fig. 4.9 (right). The histograms show 500 single shot measurements for a detection time bin of $t_{\text{bin}} = 2$ ms for the ion prepared in the dark (gray) and bright (blue) state. From the histograms, we can deduce a photon number threshold that minimizes the detection errors. The threshold is chosen to minimize the percentage of events $\epsilon_b$ where the ion was prepared in $F = 1$ but scatters less than $N_{\text{th}}$ photons and the percentage of events $\epsilon_d$ where the ion was in $F = 0$ but scatters $\geq N_{\text{th}}$ photons. For the given histogram a threshold of two photons minimizes these to $\epsilon_d = 11.0\%$ and $\epsilon_b = 26.4\%$. From measurements at slightly lower or higher detection bin lengths, we do not detect a significant improvement.

We conclude that we are currently not able to perform projective measurements on the two qubit states. A large increase in detection efficiency would be required to decrease the detection errors. Improving the imaging optics and a redesign of the compensation electrodes close to the imaging lens may lead to an improvement of a factor of two, which is still not sufficient. A workaround could be the implementation of a shelving laser at 411 nm, that can be used to transfer the population of the $F = 1$ hyperfine ground state via the $F = 2$ manifold of the $^2D_{5/2}$ state to the metastable $^2F_{7/2}$ state. Detection of the population in $F = 0$ can then be performed by observing the fluorescence during normal Doppler cooling without the 638 nm re-repumper beams. Note that this technique can also be used to detect the spin state of the Zeeman ground state levels in $^{174}\text{Yb}^+$ as, e.g., in Ref. [45]. Although these techniques are not accessible in our setup yet, we are still able to detect the average population of each spin state in $^{171}\text{Yb}^+$, which we will use in chapter 6.
4.5. Probing magnetic fields

We can use the Zeeman splitting of the $|F = 0, m_F = 0 \rangle \rightarrow |1, \pm 1 \rangle$ transitions of the $^{171}\text{Yb}^+$ ground state to measure and calibrate small magnetic fields produced by the MOT coils and the two sets of compensation coils. The first-order magnetic field-insensitive $|0, 0 \rangle \rightarrow |1, 0 \rangle$ transition can be utilized to measure the large magnetic fields of the pair of Feshbach coils. Knowledge of the correct fields is beneficial during the evaporative cooling process of the $^6\text{Li}$ atoms and for high field imaging (see Sect. 5.2.2 and 5.2.1). Thus, we measure the shifted transition frequencies of the $\Delta m_F = 0$ transition versus various high current settings. The second order Zeeman effect of the insensitive transition is given by $\Delta f_0 = B^2 \cdot 310.8 \text{ Hz}/\text{G}^2$ for $B$ the absolute magnetic field [79]. We measure the shift of the transition over a broad range of coil currents, first varying both, $I_{ufc}$ and $I_{lfc}$, simultaneously. To create a relatively homogeneous field, we first fix the relation $I_{lfc} = 1.5 \cdot I_{ufc}$, as the upper coil, according to the coil simulation, creates a magnetic field which is approximately 1.5 times stronger at the position of the ion than the lower coil when given the same current. The data is shown in Fig. 4.10 (left). The inset shows the behavior of the frequency shift when we fix the lower coil current to the maximum value and scan the upper current. All data was fit using the function

$$ \Delta f_0 = (I_{ufc}b_{ufc} + I_{lfc}b_{lfc})^2 310.8 \text{ Hz}/\text{G}^2, \quad (4.6) $$

were the $b_{\text{coil}}$ parameters are the vertical magnetic fields produced per ampere of the respective coil at the position of the ion. The fit (dark blue) matches the data within errors and leads to $b_{lfc} = 1.00(3) \text{ G/A}$ and $b_{ufc} = 1.68(4) \text{ G/A}$, in qualitative agreement with the simulated factor of 1.5. The density plot in Fig. 4.10 (right) shows the achievable vertical magnetic fields when using the parameters found from the fit, leading to a field of $858(12) \text{ G}$ when setting both currents to the maximum value of 320 A.

4.6. Vacuum quality measurements

Typically, collisions with the background gas lead to a sudden melting and recooling of the ion crystal, which is hard to observe in real time on the PMT signal or the camera due to the long exposure times, averaging out the fast recooling fluorescence signal. Since these collisions are of Langevin type [75], they can in principle serve as direct
4.6. Vacuum quality measurements

Figure 4.10.: Frequency shift of the $\Delta m_F = 0$ microwave transition in the electronic ground state of $^{171}\text{Yb}^+$ versus applied currents on the lower and upper Feshbach coils (left). The data (blue) was fit according to Eq. 4.6 (dark blue line). From the fit we extract the achievable vertical magnetic field on the ion position for different sets of currents as shown on the right.

measure of the background gas pressure at the position of the ions due to the direct density dependence of the Langevin rate. To detect the individual Langevin collisions one can utilize the fact that occasionally the ions leave the cooling cycle by populating the meta-stable $^2F_{7/2}$ state and therefore appear as a gap in the ion crystal image on the camera. This enables tracking of the position of this gap after each background gas collision [122]. To have the same effect, it is also possible to load an impurity ion into the ion crystal by tuning the wavelength of the 399 nm first step ionization laser towards the resonance of another isotope of Yb. This has the disadvantage that ions of the impurity isotope are only sympathetically cooled into the coulomb crystal and may thus orbit around it for minutes before they appear as a gap.

To estimate the background gas pressure, a crystal of around five ions is loaded and cooled without using the 638 nm re-repumper. To enhance the chance for one of the ions to populate the low lying $^2F_{7/2}$ state or to undergo a chemical reaction to turn dark, the 369 nm cooling transition is oversaturated by operating the responsible AOM at higher power as usual. Once one of the ions has turned dark, the power is reduced to a level where the ions are at the edge of being visible on the camera image and a series of images is recorded over 10-20 minutes. Since the crystal is linear, it is sufficient to record only a few lines of the CCD-chip, thus keeping the amount of data small. By averaging over the pixels containing an individual ion, the data can be easily converted into the digital information ‘bright’ when the fluorescence level is above a set threshold or ‘dark’ when the fluorescence level is below, creating a vector for each image with a Boolean entry for each ion, e.g., $\vec{b}_i = (1, 1, 1, 0, 1)$ for a dark ion at position four. A set of raw and processed example data for a 5-ion crystal is
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Figure 4.11: Observed and processed ion positions of a 5-ion crystal containing a dark ion over a time span of 10 minutes. The camera image data (left) was digitized to the binary structure (right), containing only the information whether the ion at the respective position is dark or bright.

shown in Fig. 4.11. To determine a collision event, each pairs of consecutive vectors are compared to each other by multiplication,

\[ \vec{b}_i \cdot \vec{b}_{i+1} = \begin{cases} N_{\text{ions}} - 1 & \text{no difference in positions,} \\ N_{\text{ions}} - 2 & \text{position of dark ion changed.} \end{cases} \] (4.7)

From the total number of position jumps \( N_{\text{jump}} \) one can estimate the Langevin rate \( \gamma_L \) via

\[ \gamma_L = \frac{1}{p_{\text{obs.}} \cdot T_{\text{aq.}} \cdot N_{\text{ions}}} \frac{N_{\text{jump}}}{T_{\text{aq.}} \cdot (N_{\text{ions}} - 1)}, \] (4.8)

where \( T_{\text{aq.}} \) is the total acquisition time. The prefactor \( p_{\text{obs.}} = (N_{\text{ions}} - 1)/N_{\text{ions}} \) corrects for the fact that the position of the dark ion may be the same after recooling. Using the ideal gas law \( p_{bg} = \rho_{bg} k_B T_{bg} \), one can estimate the background gas pressure \( p_{bg} \) by eliminating the density \( \rho_{bg} \) via the Langevin rate \( \gamma_L = 2\pi \rho_{bg} \sqrt{C_{4, bg}/\mu_{bg}} \), where the reduced mass \( \mu_{bg} \) derives from the mass of the trapped ion and the average mass of the background gas, assumed to be mainly air (\( \text{N}_2 \) and \( \text{O}_2 \)). The \( C_4 \)-parameter for a background gas collision is on the order of \( C_{4, bg} \approx 2.65 \cdot 10^{-57} \text{ J m}^4 \) and can be derived from the static polarizabilities of the background gas molecules [123, 124]. The temperature of the background gas \( T_{bg} \) is given by the temperature of the main vacuum.
chamber, approximately 24°C in normal operation. A typical value for the observed hopping rate is 1.2(1) per minute (58(3) events for a recording time of 47.5 min), leading to an estimated background gas pressure of $p_{bg} \leq 1.3(2) \cdot 10^{-10}$ mbar, in rough agreement with the displayed value on the ion getter pump controller of the main chamber (1 – 2 $\cdot 10^{-10}$ mbar) and the ion gauge (0.5 – 1.0 $\cdot 10^{-10}$ mbar). The presented method therefore provides a precise and sensitive estimation of the pressure at the ion position and can be performed as a service measurement to check the vacuum quality before the potential usage of the titanium sublimation pump and without switching on the usually quite contaminated filament of the ion gauge. Also, it allows us to assess whether the lifetime of the trapped atoms, which are always lost in a background gas collision, is limited by vacuum or by other technical issues.

### 4.7. Trap frequency measurements

To characterize the Paul trap, we measure the secular trap frequencies by applying an oscillating electric field with a very small amplitude on either one of the four compensation rods (see Fig. 3.3 (b)) for the radial and on one of the end caps (see Fig. 3.3 (a)) for the axial trap frequencies. To not disturb the dc compensation and trapping voltages, the field is coupled in via capacitors. For convenience the field is generated by mixing down$^2$ the output of two channels of a microwave generator$^3$, since it can be remote controlled easily via a serial interface. When the irradiated electric field’s frequency approaches the secular frequency, the ion’s secular motion is excited coherently, even when Doppler cooled. The excitation can be observed on the camera image, where the ion appears blurry once the radiofrequency source is resonant with the secular trap frequency. For an adequately small photomultiplier aperture, the excitation can also be observed as a rapid drop in fluorescence. Typically, the values for the secular trap frequencies can be determined to around 100 Hz precision (limited due to power broadening). For higher precision, the amplitude of the irradiated electric field needed to be further reduced, which would result in oscillation amplitudes that cannot be detected anymore on both camera and PMT signal.

For a set of end cap voltages $\{V_L, V_R\} = \{15.0, 15.4\}$ V, we measure the axial trap frequency to be $\omega_z = 2\pi \cdot 40.8(1)$ kHz. According to Eqs. 2.3–2.5, the dc coefficient $u_{dc}$ is then given by $u_{dc} = 1.185(5) \cdot 10^5$ Vm$^{-2}$.

$^2$ Mini-Circuits ZX05-153+

$^3$ Windfreak SynthHD
4. Trapped ions

For a perfectly symmetric ion trap, both radial trap frequencies should be degenerate but this leads to inefficient cooling of the ion, since the cooling laser couples only to the horizontal motion of the ion. Thus, the vertical motion is not cooled which can lead to ion loss. To prevent this effect, we shift the rf-ground blades to a nonzero value by applying a small analogue voltage $V_{\text{ofst}}$ that breaks the symmetry of the radial pseudopotential by adding a dc-quadrupole potential, enhancing the confinement in one direction and weakening it in the other radial direction. Thus, the radial dc Mathieu parameters $a_1$ and $a_2$ as introduced in Eq. 2.5 are slightly modified, proportional to the applied offset voltage,

$$a_{1/2} = -\frac{2e (u_{\text{dc}} \pm (V_{\text{ofst}} - V_{\text{ofst}}^{(0)}) g_{\text{ofst}})}{m_{\text{ion}} \Omega_{\text{rf}}^2}, \quad (4.9)$$

where $V_{\text{ofst}}^{(0)}$ takes into account for a potential geometric asymmetry and $g_{\text{ofst}}$ is a geometry factor. A nonzero angle between the cooling laser beam and the directions of radial normal motion then leads to a coupling to all modes of motion and thus to efficient cooling [125, 126]. The voltage is applied via a resistive 1:10 voltage divider and low passed to prevent rf pickup. A measurement of both radial trap frequencies versus $V_{\text{ofst}}$ is shown in Fig. 4.12 (left). Interestingly, in our case the trap frequencies do not cross, leading to the assumption that our rf blade pairs are not mounted exactly under $90^\circ$ with respect to each other, as it is in the case of, e.g., micro traps [127]. Also the two pairs of compensation electrodes may lead to this effect, modifying the curvature of the rf field in the vertical direction. At the point where the crossing is expected, the trap frequencies cannot be measured using the presented method, since at this point one of the two radial normal modes is not coupling to the cooling laser. The data was fit using the approximation $\omega_i \approx \frac{1}{2} \Omega_{\text{rf}} \sqrt{a_i + \frac{1}{2} q_i^2}$ with the modified $a_i$ from Eq. 4.9 and $q_i$ as defined in Eq. 2.5. From the fit we obtain $V_{\text{ofst}}^{(0)} = -1.15(12)$ V and $g_{\text{ofst}} = 7.62(14) \cdot 10^4$ m$^{-2}$. In addition, we are able to extract the rf gradient $u_{\text{rf}} = 2.06(6) \cdot 10^7$ Vm$^{-2}$ from the $q_i$.

For a fixed value of $V_{\text{ofst}} = -5$ V, the lower radial trap frequency was measured for several trap drive amplitudes as shown in Fig. 4.12 (right). The trap drive amplitude is controlled via the set point input $V_{\text{set}}$ of a PID loop that sets and stabilizes the trap drive amplitude. A schematic and description of the PID setup can be found in the next section (see Fig. 4.13). The data was fit using the approximation $\omega_i \approx \frac{1}{2} \Omega_{\text{rf}} \sqrt{a_{1/2} + \frac{1}{2} q_i^2}$ with the modified $a_i$ from Eq. 4.9 and filling in the found values for $g_{\text{ofst}}$, $V_{\text{ofst}}^{(0)}$, leaving $u_{\text{rf}} = \alpha_{\text{rf}} (V_{\text{set}} - V_{\text{set}}^{(0)})$ as free parameters, matching perfectly to the data. From the
4.8. Magnification of the imaging system

Knowledge of the magnification of our imaging system is of importance to estimate the radial excess micromotion in the horizontal plane and a potential axial rf field gradient (see Sect. 4.9.1 and 4.9.3). We determine the magnification $M_{\text{obj}}$ by trapping a two ion crystal to define two points on the camera chip. We fit two Gaussian functions to obtain the distance of the two ion images on the CCD chip $d_{\text{ccd},2} = 29.2(6) \text{ px} = 190(4) \mu \text{m}$ using the known pixel size $\Delta \text{px} = 6.5 \mu \text{m}$ of the camera\textsuperscript{4}. We repeat the procedure for a three ion crystal and obtain $d_{\text{eq},3} = 24.7(2) \text{ px} = 160(1) \mu \text{m}$. Knowing the axial trap frequency from the previous section, we can solve for the axial inter-ion spacing $d_{\text{eq},2}$ and $d_{\text{eq},3}$ of a two and three ion crystal from the equilibrium conditions between

\textsuperscript{4} Andor Zyla 5.2
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harmonic axial confinement and Coulomb force

\[ m_{\text{ion}}\omega_z^2d_{\text{eq},2} = \frac{e^2}{4\pi\varepsilon_0d_{\text{eq},2}^2}, \quad (4.10) \]

\[ m_{\text{ion}}\omega_z^2d_{\text{eq},3} = \frac{e^2}{4\pi\varepsilon_0d_{\text{eq},3}^2} + \frac{e^2}{4\pi\varepsilon_0(2d_{\text{eq},3})^2}, \quad (4.11) \]

leading to \( d_{\text{eq},2} = 28.97(5) \mu m \) and \( d_{\text{eq},3} = 24.77(4) \mu m \) for \(^{174}\text{Yb}^+\) and \( \omega_z = 2\pi \cdot 40.8(1) \text{kHz} \). From this we obtain a magnification of \( M_{\text{obj}} = d_{\text{ccd},i}/d_{\text{eq},i} = 6.5(1) \) for both \( i = 2, 3 \).

4.9. Micromotion detection and compensation

As discussed in Sect. 2.2.2, imperfections in a real ion trap can lead to substantial amounts of excess micromotion in addition to the intrinsic micromotion [72] that can lead to micromotion-induced heating in the atom-ion collisions [50]. In this section we present the employed micromotion detection techniques in our experiment and derive upper limits for the corresponding parameters and energies for each case as they were used in the numerical simulations in chapter 2.

4.9.1. Radial micromotion detection by ion position tracking

As shown in Sect. 2.2.2, a radial stray field component \( E_{\text{rad},i} \) leads not only to excess micromotion but also a shift in equilibrium position as given in Eqs. 2.9–2.10. In the horizontal direction, defined by the elementary vector \( \hat{e}_h = \frac{1}{\sqrt{2}} (\hat{e}_x + \hat{e}_y) \), this can be detected by tracking the ion position for different radial trap frequencies, shifting the ion position by

\[ r^{(0)}_h \approx \frac{1}{\sqrt{2}} \frac{e}{m_{\text{ion}}} \left( \frac{E_{\text{rad},x}}{\omega_x^2} + \frac{E_{\text{rad},y}}{\omega_y^2} \right). \quad (4.12) \]

The expression can be simplified for degenerate trap frequencies \( \omega_h = \omega_x = \omega_y \) to \( r^{(0)}_h \approx \frac{eE_{\text{rad},h}}{m_{\text{ion}}\omega_h^2} \). Tracking of the ion position then immediately allows for determination of the horizontal stray field component \( E_{\text{rad},h} \) but also an estimation of the additional
4.9. Micromotion detection and compensation

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**Figure 4.13.:** Sketch of the PID loop to stabilize and set the trap amplitude. The radiofrequency amplitude set within the control software acts as the set point for a PID loop that attenuates the trap drive via a voltage variable attenuator (Mini-Circuits ZX73-2500). The SIM900 PID controller measures a dc signal that is derived from the amplified trap drive voltage output of the helical resonator via a capacitive divider and a rectifier circuit.

Micromotion energy caused by the stray field according to Eq. 2.10,

\[
E_{\text{emm},h} \approx \frac{4}{m_{\text{ion}}} \left( \frac{q_{h} e E_{\text{rad},h} \Omega_{rf}}{8 \omega_{h}} \right)
\]

\[
\approx \frac{1}{2m_{\text{ion}}} \left( \frac{e E_{\text{rad},h}}{\omega_{h}} \right),
\]

where the assumption \( q_{h} = q_{x} = q_{y} \) and \( a_{h} = a_{x} = a_{y}, |a_{h}| \ll \frac{1}{2} q_{h}^{2} \) was used. To measure the shift on the ion, we extract the ion’s horizontal position from averaging over five images at each radial trap frequency setting and fitting a Gaussian function. Example data for the determination of the ion position for a given trapping field is shown in Fig. 4.14 (right). The radial trap frequency is controlled by shifting the set point of the SIM900 PID controller, effectively varying the amplitude of the trap drive, as it is shown in Fig. 4.13. From the ion positions on the camera chip and the measured magnification \( M_{\text{obj}} = 6.5(1) \) of the objective as defined in Sect. 4.8, the shift of the ion position within the ion trap with respect to the radial confinement can be determined. A measurement of the ion position versus the radial trapping frequency \( \omega_{x} \) is shown in Fig. 4.14 (left). The data was fit according to Eq. 4.12 under the assumption \( \omega_{x} \approx \omega_{y} \). From the fit we obtain an electric field of \( E_{\text{rad},h} = 0.50(5) \text{ V/m} \), pushing the ion to a region with a non-vanishing rf amplitude, thus leading to the excess micromotion energy \( E_{\text{emm},h} = k_{B} \cdot 1.03(21) \text{ mK} \) as given in Eq. 2.10. Unfortunately, the micromotion in the horizontal direction cannot be compensated by a dc electric field in the current trap design since the compensation electrodes’ electric field in horizontal direction is shielded by the rf blades of the ion trap, demanding for additional pairs.
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![Graph showing horizontal ion position vs. secular frequency](image1)

**Figure 4.14.**: Horizontal shift of the ion position within the trap versus radial secular frequency (left) along with a fit function according to Eq. 4.12. For low radial confinement, the ion’s equilibrium position changes due to the presence of radial dc electric fields. Shown in the right is the projected signal a single ion produces on the camera, along with a Gaussian fit to determine its position on the camera chip. The inset shows the full camera image.

...of compensation electrodes in the horizontal plane of the trap.

In order to prevent large horizontal dc stray electric fields from surface charges and accumulation of background gas molecules on the trap electrodes, the ion trap is occasionally operated at a higher rf frequency and amplitude over night to evaporate charged background gas molecules and lithium atoms from the electrode surface. To bake the pair of ground blades, rf and ground can be swapped. The baking procedure is typically performed when the excess micromotion energy in the horizontal direction is larger than $k_B \cdot 2 \text{ mK}$.

### 4.9.2. Vertical micromotion detection by Ramsey microwave spectroscopy

In the vertical direction the micromotion caused by a stray electric field cannot be detected by using the camera image, since the direction of the shift is along the imaging path. Thus, a movement of the ion mainly leads to a tiny shift out of the imaging plane, which is hard to detect and calibrate for. A much more reliable and precise method to detect and compensate the vertical micromotion is to make use of the magnetic-field sensitive $\Delta m_F = +1$ hyperfine ground state transition of the $^{171}\text{Yb}^+$ isotope. In a vertical magnetic field gradient of $g_v = 13.4 \text{ G/cm}$ we perform microwave Ramsey spectroscopy, subsequently for a high and a low trap drive amplitude, corresponding to a high $\omega_{h,>}$ and a low $\omega_{h,<}$ radial trap frequency. An electric stray field $E_{\text{rad,v}}$...
4.9. Micromotion detection and compensation

in the vertical direction then leads to a vertical shift in positions $\Delta r_{v}$ between the two settings. The shift in positions translates into a position dependent transition frequency of the $^2S_{1/2} F = 0, m_F = 0 \rightarrow F = 1, m_F = 1$ ($\Delta m_F = +1$) transition, given by

$$\Delta f_{mw} = g_e \frac{\mu_B}{2\pi \hbar} \Delta r_v, \quad (4.15)$$

with the difference in vertical position of

$$\Delta r_v \approx \frac{eE_{rad,v}}{m_{ion}} \left( \frac{1}{\omega_{h,>}^2} - \frac{1}{\omega_{h,<}^2} \right), \quad (4.16)$$

derived from Eq. 2.9 under the assumption of degenerate radial confinement. The experimental sequence works as follows. First, we determine the resonance frequency $f_{\Delta m_F=+1}$ of the $\Delta m_F = +1$ transition as described in Sect. 4.4.3. We detune the microwave source around $\Delta f_{\text{ofst}} \approx 15 - 20$ kHz to the blue side to ensure a Ramsey signal at around this detuning frequency. To measure the Ramsey signal, we prepare the ion in its $F = 0$ hyperfine ground state via optical pumping (see Sect. 4.4.1) and apply a $\pi/2$ pulse at the detuned microwave frequency. After an evolution time of $t_{\text{ram}}$, we repeat the $\pi/2$ pulse and detect the spin state of the ion (see Sect. 4.4.2). We scan the evolution time $t_{\text{ram}}$ to obtain a Ramsey fringe signal. For each point of $t_{\text{ram}}$, we repeat the measurement 50 times for both high and low trap frequency settings. Typical data is shown in Fig. 4.15 for $\omega_{h,<} = 2\pi \cdot 98.6(1)$ kHz and $\omega_{h,>} = 205(1)$ kHz. The plot on the left shows a case where the micromotion is miscompensated, thus leading to a large shift in position between the two trap frequency settings and therefore a large difference in the Ramsey fringe frequencies, $f_{\text{ram,>} - f_{\text{ram,<}} = \Delta f_{mw}}$, whereas the right shows a perfectly compensated case. In case of a miscompensation, we apply a symmetric voltage difference between the upper and lower pair of compensation electrodes, $\Delta V_v = V_{\text{up}} - V_{\text{down}}$, $V_{\text{up}} = -V_{\text{down}} = \Delta V_v/2$. We repeat the measurements of Fig. 4.15 for different voltages to compensate the micromotion down to the detection limit of the method. A full set of compensation measurements is shown in Fig. 4.16. The data was fit according to Eqs. 4.15–4.16 using a simple linear model. For optimal compensation, we find $\Delta V_v = 67.82(16)$ V on the vertical electrodes. The uncertainty translates to an uncertainty of the vertical electric field component to $E_{\text{rad,v}} = 48.2(1)$ mV/m and an average kinetic energy of $E_{\text{emm,v}} = k_B \cdot 10(1) \mu$K, according to Eq. 2.10. Typically, the compensation drifts from day to day less than 1 V, corresponding to an upper limit of $E_{\text{emm,v}} < k_B \cdot 0.38 \mu$K and $E_{\text{rad,v}} < 0.3$ V/m for a
4. Trapped ions

Figure 4.15.: Ramsey fringes of the $\Delta m_F = +1$ hyperfine ground state transition of a single $^{171}$Yb$^+$ ion for a strong (blue) and weak (gray) radial confinement in a vertical magnetic field gradient. For bad micromotion compensation in the vertical direction, the position shift of the ion caused by a vertical stray electric field leads to a difference in resonance frequency, thus causing a frequency difference of the fringes (left). For perfect compensation (right) the difference is zero. The data was fit with a decaying cosine function (solid lines).

measurement day after a single compensation run in the morning.

4.9.3. Axial and quadrature micromotion detection by observation of line broadening

To determine the axial micromotion, we observe the line broadening of the $935$ nm $^2D_{3/2} \rightarrow ^3D_{5/2}[3/2]_{1/2}$ repumper transition in $^{174}$Yb$^+$. Therefore, we align the $935$ nm beam along the trap axis to exclude line broadening from the radial micromotion. We lower the power of the beam to avoid power broadening of the transition. Due to a non-vanishing magnetic field and the thermal motion of the ion, the observed linewidth $\Gamma_{\text{mm}}$ may still be broadened when compared to the natural linewidth $\Gamma_{\text{nat}} = 2\pi \cdot 4.2$ MHz [110]. The line shape for a transition with the presence of micromotion is given by [72]

$$\Gamma_{\text{mm}}(\Delta_{935}) = c \cdot \sum_{n=-\infty}^{\infty} J_n (\beta_{\text{mm}})^2 \frac{\Gamma_{\text{nat}}^2}{(\Delta_{935} - n\Omega_{\text{rf}})^2 + \Gamma_{\text{nat}}^2}, \quad (4.17)$$

where $c$ is a constant, $J_n (\beta_{\text{mm}})$ is the $n^{\text{th}}$ Bessel function evaluated at a modulation index of $\beta_{\text{mm}} = k_{935} z_{\text{mm}}$ with the axial micromotion amplitude $z_{\text{mm}}$ and $k_{935} = 2\pi/935 \text{nm}$ the wavevector of the repumper beam. The trap drive frequency during these measurements was set to $\Omega_{\text{rf}} = 2\pi \cdot 1.8420$ MHz. We observe the fluorescence of
4.9. Micromotion detection and compensation

a laser cooled $^{174}\text{Yb}^+$ ion while scanning the detuning $\Delta_{935}$ of the repumper beam at different axial ion positions. We change the axial ion position by unbalancing the end cap voltages. At each axial ion position, we take a spectrum of the repumper transition for a high and a low rf amplitude, set by the PID loop set point $V_{\text{set,}>}$ = 0.5 V and $V_{\text{set,<}}$ = 0.35 V respectively. This changes the modulation index by a factor of around 1.4 from one to another setting, since the axial oscillating field amplitude $E_{\text{ax}}$ due to rf pickup is proportional to the rf amplitude set by the value of $V_{\text{set}}$. Two example spectra for two different ion positions are shown in Fig. 4.17. For both high (gray) and low (blue) rf amplitudes, the line shapes for the shifted ion (left) are broadened with respect to the unshifted ion (right). We repeat the measurement at ion camera positions between -550 and 450 pixels. The resulting electric field amplitudes from the fit for the higher rf amplitude $V_{\text{set,}>}$ = 0.5 V is shown in Fig. 4.18. The data was fit using a square root function,

$$E_{ax}(x) = \sqrt{u_{rf,z}^2 (x - x_0)^2 + E_{ax,0}^2},$$

(4.18)

where the field $E_{ax,0}$ is a potential offset field due to rf pickup of the end cap electrodes and $x_0$ the minimum position on the camera chip. The parameter $u_{rf,z}$ is the axial electric field gradient in V/m per pixel. The fit is shown in dark blue along with a worst case estimation of $E_{ax,0}$ = 20 V/m (dashed blue). For ion positions close to the center, the effect of the sidebands cannot be observed due to the broad linewidth of the transition employed, as it is shown in Fig. 4.19 (left). The curves show the theoretical

Figure 4.16.: Vertical compensation voltage versus frequency difference of the microwave transition for two different trap frequency settings.
4. Trapped ions

Figure 4.17: Spectra of the repumper transition in $^{174}$Yb$^+$ for different axial ion positions and high (gray) and low (blue) rf amplitudes. The spectra on the left were taken at end cap voltages of $(V_L, V_R) = (26.1, 10.8)$ V, leading to an axial position shift of $-350$ px with respect to the settings $(V_L, V_R) = (15.0, 15.4)$ V used for the spectra on the right. The data is shown along with fits according to Eq. 4.17 (solid lines).

Figure 4.18: Amplitude of the oscillating axial rf field component versus position of the ion on the camera obtained from the line shapes of the 935 nm repumper spectrum (blue points). Also shown is a fit of the data (solid blue) as well as a worst case estimate for a potential residual oscillating electric field amplitude (dashed blue).
4.9. Micromotion detection and compensation

line shapes for \( E_{ax} = 0 \text{ V/m} \) (light green) and \( E_{ax} = 20 \text{ V/m} \) (dark green), which are hard to distinguish. At larger electric fields, where the sidebands become visible, a difference of 20 V/m in \( E_{ax} \) is easier to detect since not only the central height of the peak changes but also the position of the sidebands, as it is shown for \( E_{ax} = 220 \text{ V/m} \) (light blue), 210 V/m (dashed blue) and 200 V/m (blue). Thus, we assume the error \( \Delta E_{ax} \approx 20 \text{ V/m} \) in the center of the trap and \( \Delta E_{ax} \approx 10 \text{ V/m} \) on the outer regions at \( V_{set,>} = 0.5 \text{ V} \). Note that employing a transition with much narrower linewidth, e.g., the 22 Hz wide \( ^2S_{1/2} \rightarrow ^2D_{5/2} \) clock transition at 411 nm [81] can lower this limit significantly, since then all sidebands can be resolved. The theoretical line broadening for such a narrow transition is shown in Fig. 4.19 (right), where even for \( E_{ax} = 5 \text{ V/m} \) (dashed green) a clear difference from \( E_{ax} = 0 \text{ V/m} \) can be observed.

![Graphs showing line shapes for different axial electric field amplitudes](image)

**Figure 4.19.** Theoretical line broadening of the repumper transition in \(^{174}\text{Yb}^+\) for different axial electric field amplitudes (left). For \( E_{ax} = 0 \text{ V/m} \) (light green) and 20 V/m (dark green) the difference is only slightly visible in the center of the peak. For 200 V/m (light blue), 210 V/m (dashed blue) and 220 V/m (dark blue), a clear broadening is observable. On the right the line broadening for a hypothetical transition with a linewidth of 50 kHz is shown. Here, it is easily possible to resolve the difference between \( E_{ax} = 0 \text{ V/m} \) (light green) and 5 V/m (dashed). For 20 V/m (dark green) also the second sidebands become visible.

From the worst case fit in Fig. 4.18, we estimate the residual axial oscillating electric field at the trapping center for typical trapping conditions \( (V_{set} = 0.35 \text{ V/m}) \) to be \( E_{ax,0} = \Delta E_{ax} \frac{V_{set, <}}{V_{set, >}} \leq 14 \text{ V/m} \). From the fit we also obtain the axial electric field gradient \( u_{rf,z} = 0.35(1) \text{ Vm}^{-1} \text{ px}^{-1} \). Together with the pixel size of the camera \( \Delta px = 6.5 \mu\text{m} \) and the measured magnification of the objective \( M_{obj} = 6.5(1) \), we know that one pixel corresponds to 6.5(1) \( \mu\text{m} \) in reality and obtain \( u_{rf,z} = 3.5(4) \cdot 10^5 \text{ Vm}^{-2} = 7.0(7) \cdot 10^5 \text{ m}^{-2} \cdot V_{set} \). According to Eq. 2.5, this translates to a non-vanishing axial \( q \)-parameter of \( q_z = 5.9(6) \cdot 10^{-3} \cdot V_{set} \), thus we expect \( q_z = 2.1(2) \cdot 10^{-3} \) for the usually used trap amplitude setpoint of \( V_{set} = 0.35 \text{ V} \).
4. Trapped ions

To estimate the level of phase micromotion we repeated the measurement at the point of optimal radial and axial compensation. To couple to apparent phase micromotion, we aligned the desaturated repumper beam under $45^\circ$ with respect to the trap axis, but could not detect any broadening of the spectrum. Thus, we can only give an upper limit as in the axial case by setting the amplitude of the phase micromotion field as given in Eq. 2.14 equal to the worst case estimate of the axial field,

$$E_{ax,0} = \frac{1}{4e} q_e m_{ion} \delta \phi_{rf} \Omega_{rf}^2 R_{trap}, \quad (4.19)$$

and solve for $\delta \phi_{rf}$. Given the typically used trapping parameters, we obtain $\delta \phi_{rf} \lesssim 0.65$ mrad. As mentioned in Sect. 2.8, this should be an overestimation by at least one order of magnitude. Also here, the use of a narrow linewidth transition would enable a much lower detection limit.

4.10. Heating rate measurement

Due to occurring charge transfer in the excited electronic states, the ion needs to be prepared in its electronic ground state before the atom cloud is shuttled into the ion trap [80]. To estimate the heating of the ion during the loading and shuttling time of the atom cloud, we utilize the ground state hyperfine transitions of $^{171}$Yb$^+$. In order to resolve motional sidebands on the magnetic field sensitive $\Delta m_F = \pm 1$ microwave transitions, we run the MOT coils at 30 A producing a vertical magnetic field gradient of $g_v = 0.22$ T/m and a bias field of $B_{ver} = 1.1$ mT at the position of the ion. The magnetic field gradient creates a state-dependent force, leading to an effective Lamb-Dicke parameter of $\eta_{eff} \approx 1/\sqrt{2} \mu_B g_v \sigma_{rad}/(\hbar \omega_{rad}) = 5.2 \times 10^{-4}$ [128], where $\sigma_{rad} = 19$ nm is the size of the radial harmonic oscillator ground state wave function. To obtain the position of the sidebands we take a microwave spectrum around the $\Delta m_F = +1$ transition by preparing the ion in the $F = 0$ ground state followed by a 5 ms microwave pulse and state-selective fluorescence detection. A coarse spectrum showing both blue and red sidebands of the two radial trap frequencies is shown in Fig. 4.20 (left). For the carrier transition we obtain a Rabi frequency of $\Omega_+ = 2\pi \cdot 36.4(1)$ kHz. To estimate the heating rate, we drive Rabi oscillations on the red sideband of the lower trap frequency as shown in Fig. 4.20 (right) immediately after Doppler cooling and optical pumping (blue) and after a wait time of 500 ms (red). Also shown is a Rabi oscillation on the carrier transition (gray). Assuming a thermal distribution $p(n)$ with mean vibrational quantum number $\bar{n}$, we fit the
4.11. Conclusions and outlook

In this chapter we have presented the two commonly used isotopes of Yb$^+$ in our experiment. We have described the loading and cooling procedure as well as state preparation and state readout for both isotopes, including the hyperfine ground states of $^{171}$Yb$^+$. 

\[ P(t) = \sum_n p(n) \frac{\Omega_n^2}{\Omega_n^2 + \Delta^2} \left( \frac{1}{2} - \frac{1}{2} \cos \left( \sqrt{\Omega_n^2 + \Delta^2} \cdot t \right) e^{-t/\tau} \right), \tag{4.20} \]

with $\Omega_n = \eta_{\text{eff}} \sqrt{n} \Omega_+$ the vibrational quantum number-dependent Rabi frequencies of the red sideband in the Lamb-Dicke limit. We use $\Delta = 2\pi \cdot 0.35 \text{ kHz}$ as the detuning of the microwave with respect to the red sideband to take the asymptotic behavior into account and $\tau = 0.5 \text{ ms}$ corresponding to the coherence time of the oscillations. The fits suggest an ion temperature of 4 mK and a heating rate of less than 4 mK/s. More precise heating rate and temperature measurements are planned utilizing the 329 nm D2 laser as a Raman-system [98]. Due to the narrow linewidth also a 411 nm shelving laser could be used as mentioned in Sect. 4.9.3.

**Figure 4.20.** Microwave frequency scan around the $\Delta m_F = +1$ transition in the $^{171}$Yb$^+$ hyperfine ground state at a magnetic field of 1.1 mT (left). Due to the presence of a magnetic field gradient, both red and blue sidebands of the two radial trap frequencies are resolved. Pulse width scans (right) on the carrier (gray) and the red sideband after Doppler cooling (blue). The red data corresponds to an additional wait time of 500 ms, to probe ion heating. Note that the carrier data corresponds to the upper time axis, while the sideband data corresponds to the lower axis. The sideband data are fit according to Eq. 4.20.
4. Trapped ions

Furthermore, we have determined the detection efficiency of our imaging system using the $^{174}$Yb$^+$ isotope. Using this knowledge, we have analyzed the possibility of a projective measurement on the hyperfine ground states of $^{171}$Yb$^+$. We have found that in our current setup, this cannot be achieved even with dramatic optimization of the imaging system. Thus, the implementation of a 411 nm shelving laser seems to be a possible solution and is planned in the near future.

Using the hyperfine transitions in $^{171}$Yb$^+$, we have calibrated the magnetic fields of the two Feshbach coils at the position of the ion to be used for atom trapping, demonstrating the benefit of using a single ion as a precise probe to measure electromagnetic fields.

To estimate the vacuum quality, we have presented a method to analyze the hopping rate of a dark ion within a Doppler cooled ion string, leading to a comparable value as the ion pump and ion gauge readings.

In addition, we have demonstrated a set of methods to compensate micromotion in all directions and approximated the heating rate of the ion. We found that to reach the quantum regime, both, methods and compensation, have to be improved, for example by the implementation of the aforementioned 411 nm laser and the addition of horizontal compensation electrodes.
In this chapter we present the typical procedure to cool and trap $^6$Li atoms in the different stages of our experiment for preparing an ultracold atomic sample for atom-ion experiments. Starting from the loading of a MOT, we describe the optical pumping into a magnetic trap, followed by magnetic transport into the ion trap. Further, we analyze the loading into the crossed optical dipole trap and present the first results on evaporative cooling, which we analyze using high-field absorption imaging. Finally, we present a technique for precise alignment of the dipole trap laser beams within the ion trap by using a single Yb$^+$ ion. Note that the atom-ion experiments performed in chapter 6 were carried out using only the magnetic trap overlapped with the ion, as the dipole trap beams were not built up yet at that point.

5.1. Trapping and cooling

5.1.1. Slowing and MOT

We magneto-optically trap a cloud of $^6$Li in a quadrupole field formed by the pair of MOT coils running at 56 A, generating a vertical field gradient of approximately 44 G/cm. The MOT is loaded from a Zeeman-slowed atomic beam under an angle of
5. Trapped atoms

48° with respect to the ion trap axis. Since the MOT position is below the center of the vacuum chamber, we push the center of the quadrupole field down by approximately 14 mm with the help of the Feshbach coils running in Helmholtz configuration at $I_{ufc} = 32.5 \text{ A}$ and $I_{lfc} = 20.5 \text{ A}$ for the upper and lower coil, respectively. Horizontally we shift the field minimum by approximately 6–8 mm to be below the mirror where the two retroreflected MOT beams form the mirror MOT. We achieve that by running the radial compensation coils at $I_{rad} = 19.5 \text{ A}$ each.

The atoms get slowed down and cooled into the MOT using laser light red detuned\(^1\) from the D2 line in $^6\text{Li}$, as shown in the reduced level scheme in Fig. 5.1 (left). Due to the large branching ratio \cite{99} for decaying back into the $F = 1/2$ hyperfine ground state, we use around 1/3 of the total laser power to saturate the repumper transition (dashed red extension of the arrows). Typically, we use around 15 mW total power in the Zeeman slower beam and 75 mW total power in the MOT beams.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{level_scheme.png}
\caption{Reduced level scheme of $^6\text{Li}$. The energy splittings are not to scale. The Zeeman splittings of the $^2S_{1/2}$ state are shown in a magnetic field range of 0–200 G, whereas the splittings of the $^2P_{3/2}$ state are only shown from 0–5 G.}
\end{figure}

\footnote{The detuning from the $^2S_{1/2}, F = 3/2 \rightarrow ^2P_{3/2}, F = 5/2$ transition is $-104 \text{ MHz}$ for the Zeeman slower beam and $-34 \text{ MHz}$ for the MOT beams.}
Having the Zeeman slower and the relevant laser beams switched on, we load approximately $50 \cdot 10^6$ atoms within 3 s at a temperature close to the Doppler temperature $T_D = 141 \mu K$ [99], when the $^6$Li oven runs at 400 $^\circ$C. Due to the slow switching times of the MOT coils, the atom number was determined using the collected fluorescence light during loading [93]. While observing the fluorescence, all beams and the magnetic field minimum position were fine-tuned to optimize the loading rate and total number of atoms. Due to the restricted space, we had to remove the camera such that we are not able to directly quantify the fluorescence of the MOT anymore.

After the loading, we block the atomic beam using the mechanical shutter and transfer the atoms in a quadrupole field formed only by the Feshbach coils. This is done by controlled ramping down of $I_{\text{MOT}}$ while ramping up $I_{\text{ufc}}$ to 83.5 A and $I_{\text{lfc}}$ to -27.5 A within 70 ms, involving a polarity switch of the lower coil using the switch described in Sect. 3.11. To increase the density of the atomic cloud, we compress the MOT by ramping the detuning of the MOT beams from -34 MHz to -17 MHz and reducing the total power to less than a mW within 3 ms.

### 5.1.2. Magnetic trap

To load a magnetic trap from the compressed MOT, we initialize atoms in the $F = 1/2$ hyperfine ground state by switching off the repumper light for 100 $\mu$s, followed by a 150 $\mu$s optical pumping pulse using $\sigma^+$ light resonant with the D1 transition as depicted in Fig. 5.1. This leads to population of the low-field-seeking $F = 3/2, m_F = 3/2$ hyperfine ground state. Due to the quadrupole field, not all atoms get resonantly pumped and not all atoms experience the right polarization. Thus, to enhance the number of successfully pumped atoms, we temporarily displace the quadrupole field minimum towards the propagation direction of the optical pumping beam by applying $I_{ax} = 8$ A at the axial compensation coils during the laser pulse.

### 5.1.3. Absorption imaging and time-of-flight sequence

Having the atoms magnetically trapped in a quadrupole field formed by the fast Feshbach coils, we are able to perform time-of-flight absorption imaging to determine the atom number, size and temperature of the atomic cloud. Therefore, we switch off the Feshbach coils and the radial compensation coils using the switches described in Sect. 3.11. Due to the finite switching time of the switches and eddy currents in
5. Trapped atoms

the vacuum chamber, the magnetic fields have vanished completely only after around 1.5 ms. After that we take absorption images using the D2 imaging beam going through the same fiber as the D1 optical pumping beam as described in Sect. 3.8.1. During the absorption images we apply a bias field, using the axial compensation coils at 5 A, to ensure a defined polarization. We determine the atom number following Ref. [129] from the obtained CCD images.

A typical absorption image of the initial magnetic trap is shown in Fig. 5.2 (left), where also the mirror of the MOT can be seen in the top left corner. We fit both, horizontal (h) and vertical (v) width $\sigma_{h/v}$ of the cloud, assuming Gaussian profiles and scan the expansion times $t_{\text{tof}}$ after switching the magnetic fields to obtain a time-of-flight signal. From the amplitude of the Gaussian profiles we obtain the atom number $N_{\text{atoms}}$. We fit the temporal evolution of the widths according to the expected free expansion,

$$
\sigma_{h/v}(t_{\text{tof}}) = \sqrt{\sigma_{0,h/v}^2 + \frac{k_B T_{h/v}}{m_{\text{Li}}} t_{\text{tof}}^2},
$$

(5.1)

to obtain the initial horizontal and vertical cloud sizes $\sigma_{0,h/v}$ and temperatures $T_{h/v}$. A typical time-of-flight expansion signal after the initial magnetic trap is shown in Fig. 5.2 (right). From the fits we obtain $61(9) \cdot 10^6$ atoms at a temperature of $T_v = 127(6) \mu\text{K}$ ($T_h = 43(1) \mu\text{K}$), which is lower than the Doppler temperature. We expect this to be caused by the mirror close by, leading to a quick loss of the atoms with large

**Figure 5.2.:** Absorption image signal after a 1.5 ms time-of-flight (left) averaged over ten measurements and time-of-flight signal (right) for a cloud of $^6\text{Li}$ atoms after the magnetic trap stage. The data was fit according to Eq. 5.1 and shows a faster expansion in the vertical (black) than in the horizontal (blue) direction.
5.1. Trapping and cooling

orbits, especially in the horizontal direction (blue data).

5.1.4. Magnetic transport

To shuttle the magnetically trapped atoms adiabatically to the location of the ions, we first ramp down the current of the radial compensation coils while ramping up the gradient of the trapping field by increasing the currents in the Feshbach coils to compress the magnetically trapped cloud. To ensure smooth acceleration, deceleration and compression of the cloud, the current ramps were designed following a polynomial function with vanishing first and second derivative at the start and end of the ramps,

\[ I(s) = I_0 + (I_1 - I_0) \left( 10s^3 - 15s^4 + 6s^5 \right) , \quad \text{with } s = t/T_{\text{hor}} . \quad (5.2) \]

Here, \( I(s) \) is the respective coil current ramped from \( I_0 \) to \( I_1 \) within \( T_{\text{hor}} \). For the vertical transport, we design the potential minimum to follow this polynomial form while we maintain the gradient at a maximum level, limited by the maximum design currents of the Feshbach coils (\( I_{\text{max}} = 320 \text{ A} \)) to ensure a maximally compressed cloud. This minimizes losses that occur when entering the ion trap due to the geometrical constrains given by the compensation rods and blade electrodes.

To check the adiabaticity of the horizontal and vertical transport we performed Monte-Carlo trajectory simulations as well as measurements of the atom number and temperature after transporting the cloud back to the initial magnetic trap. We found \( T_{\text{hor}} = 70 \text{ ms} \) and \( T_{\text{ver}} = 50 \text{ ms} \) to be optimal.

To measure size and position of the magnetically trapped atomic cloud within the ion trap, we make use of position-dependent ion loss rates due to charge transfer reactions with the atoms as described in our previous work [80]. We found approximately \( 7 \times 10^6 \) atoms at a temperature of \( 0.6(2) \text{ mK} \) in a cloud of size \( \sigma_h \cdot \sigma_v = 0.47(4) \text{ mm} \cdot 0.41(4) \text{ mm} \), trapped in a quadrupole field with an axial gradient of \( 280 \text{ G/cm} \). In the meantime, we were able to fine-tune the loading and transport of the magnetic trap to obtain \( 20 - 30 \times 10^6 \) atoms within the ion trap.
5. Trapped atoms

5.2. The crossed optical dipole trap

Unfortunately, the atom temperatures are still far above the s-wave limit for the combination $^6$Li/Yb$^+$, demanding for further steps of cooling. Therefore, we employ the broad Feshbach resonance near 832 G [91] between the two $m_F = \pm 1/2$ sublevels of the $F = 1/2$ hyperfine ground state manifold for forced evaporative cooling as it is typically done in other $^6$Li experiments, achieving, e.g., degenerate Fermi-gases [130] or even the formation of bosonic $^6$Li$_2$ molecules [131] followed by their Bose-Einstein condensation [64].

To achieve the high homogeneous magnetic fields required for forced evaporative cooling of $^6$Li, we need to switch off the magnetic trap first and transfer the atomic cloud into a crossed optical dipole trap using a 1070 nm high-power fiber laser as explained in Sect. 3.5.3. As the magnetically trapped atoms are in the wrong states for forced evaporative cooling, another optical pumping pulse is required. Therefore, we employ a second MOT stage that not only prepares the correct mixture of states to employ the broad Feshbach resonance but also cools the atomic cloud further from 0.6(2) mK towards the Doppler temperature $T_D = 141$ $\mu$K of $^6$Li, and compresses the cloud to increase the geometric overlap with the shallow crossed optical dipole trap. By switching off the repumper part in the MOT beams, we achieve nearly equal optical pumping into the $F = 1/2$ hyperfine ground state manifold. The configuration of the second MOT beams is described in Sect. 3.8.2. The sequence is sketched and described in Fig. 5.5, where also optional evaporative cooling is shown, which will be explained in Sect. 5.2.2.

From the second MOT we capture the atomic cloud by switching on the crossed optical dipole trap laser beams as shown in Fig. 5.3. When both focal points of the trapping beams are overlapped properly, they create an additional optical potential which can be computed using Ref. [132]. In the center the potential leads to a harmonic confinement with approximate trap frequencies of $\{\omega_v, \omega_a, \omega_h\} = 2\pi \cdot P_{\text{dip}} \times \{1541, 135, 1535\}$ Hz/W and a depth of $V_{\text{dip}}(0)/k_B = P_{\text{dip}} \times 46 \mu$K/W when assuming a crossing angle of 10°, a computed Rayleigh length of 4.0 mm and a waist of 37 $\mu$m for each beam. This limits the overlap with the second MOT volume and thus the loading efficiency of the dipole trap.
Figure 5.3.: Sketch of the ion trap electrodes including the two dipole trap beams that are sent through the 2 mm holes in the end caps and overlapped in the center (top). The plot below shows a magnified version of the overlapped beams. The overlapped region is much smaller than the individual Rayleigh length $R_R = 4.0 \text{ mm}$ of each beam.

5.2.1. High-field imaging

We image the atomic cloud after dipole trapping in a large homogeneous magnetic field to avoid acceleration and distortion due to fast switching of the fields after evaporation. In addition, due to the closed imaging transitions at large fields, the determination of atom numbers is more reliable than in the low field regime and allows us to measure the amount of atoms in each spin state independently. The imaging beam is sent either through the end cap or from below the ion trap, as it is described in Sect. 3.8 to observe the time-of-flight expansion in all three directions.

To reliably image the cloud in a large magnetic field, it is of importance to not only be on resonance with the imaging beam on the respective imaging transition as shown in Fig. 5.1 (right) but also to compensate for magnetic field gradients and gravitation, in order to keep track of the expanding cloud on the imaging CCD. While we can adjust the resonance condition via an AOM, compensation of gradients requires the fine adjustment of the Feshbach coil currents. To do so, we use a reasonable guess from the coil simulations, and track the center of mass of the expanding cloud in time-of-flight measurements. In case of a movement, we compensate by slightly adjusting one of the Feshbach coil currents until the fitted center of mass is standing still within a time-of-flight measurement. For the first ($|1\rangle = |m_J = -1/2, m_I = 1\rangle$) and second ($|2\rangle = |m_J = -1/2, m_I = 0\rangle$) lowest hyperfine ground state we find $I_{ufc}^{(1)} = 278 \text{ A}$. 
$I^{(1)}_{\text{lfc}} = 320 \, \text{A}$ and $I^{(2)}_{\text{lfc}} = 245 \, \text{A}$, $I^{(2)}_{\text{ufc}} = 320 \, \text{A}$.

Due to the imperfect Helmholtz configuration of the Feshbach coils, there is still a magnetic field curvature present, leading to an additional confinement in the vertical and axial (w.r.t. the ion trap) direction and anti-confinement in the horizontal radial direction after switching off the optical dipole trap. We attempt to reduce this curvature by adding a much more homogeneous field produced by the MOT coils in Helmholtz configuration. For a current of $I_{\text{MOT}} = 35 \, \text{A}$, we need to reduce the currents in the Feshbach coils to $I^{(1)}_{\text{ufc}} = 169.8 \, \text{A}$, $I^{(1)}_{\text{lfc}} = 259.5 \, \text{A}$ and $I^{(2)}_{\text{ufc}} = 155.0 \, \text{A}$, $I^{(2)}_{\text{lfc}} = 228.5 \, \text{A}$ to remain resonant with the absorption imaging beam, reducing the driven expansion of the cloud dramatically.

A model for the expansion of the fitted widths of the clouds in the residual magnetic field curvature can be obtained from Liouville’s equation [133] and reads

$$
\sigma_{v,a}(t_{\text{tof}}) = \sqrt{\cos^2 (\omega_{v,a} t_{\text{tof}}) \sigma^2_{0,v,a} + \frac{k_B T}{m_{\text{Li}}} \frac{\sin^2 (\omega_{v,a} t_{\text{tof}})}{\omega^2_{v,a}}},
$$

(5.3)

for the confining vertical ($v$) and axial ($a$) direction and

$$
\sigma_{h}(t_{\text{tof}}) = \sqrt{\cosh^2 (\omega_h t_{\text{tof}}) \sigma^2_{0,h} + \frac{k_B T}{m_{\text{Li}}} \frac{\sinh^2 (\omega_h t_{\text{tof}})}{\omega^2_{h}}},
$$

(5.4)

for the anti-confining horizontal radial ($h$) direction. The given frequencies $\omega_{v,a,h}$ describe the strength of the magnetic field curvature that leads to expansion or revival of the cloud assuming purely harmonic (anti-) confinement by the potential,

$$
V(q) = \pm \frac{1}{2} m_{\text{Li}} \omega^2 q^2 = \frac{1}{2} \mu \frac{\partial^2 B}{\partial q^2} q^2,
$$

(5.5)

where $q \in \{v,a,h\}$ stands symbolic for the coordinate, $\mu$ is the magnetic moment of the atom and $B$ is the absolute magnetic field at the center of the trap. Following Maxwell’s equations, we assume $\omega^2_v = \omega^2_h + \omega^2_a$. A typical series of images after evaporative cooling (described in the following Sect. 5.2.2) is shown in Fig. 5.4 (top) for both, axial (first row) vertical (second row) absorption imaging. The temporal evolution of the fitted widths is also shown (bottom) for vertical (left) and axial (right) absorption imaging. To obtain the temperature $T$, the initial widths $\sigma_{0,v,a,h}$ and the frequency describing the (anti-) confinement, the data was fit (solid lines) using a combined model according to Eq. 5.3 and 5.4. The vertical (blue) data shows a
5.2. The crossed optical dipole trap

The crossed optical dipole trap is used for high-field imaging of an atomic cloud from the axial direction (first row) and the vertical direction (second row). The fitted widths of the clouds are shown in the figures below. The temporal evolution of the widths was fit using the models of Eq. 5.3 and 5.4, respectively, leading to a temperature of $4.8(8) \mu K$ and an initial cloud size of $\sigma_{0,\{v,a,h\}} = \{12(1), 224(5), 25(1)\} \mu m$.

![Series of TOF images](image)

**Figure 5.4.** Series of TOF images (top) for high-field imaging of an atomic cloud from the axial direction (first row) and the vertical direction (second row). The fitted widths of the clouds are shown in the figures below. The temporal evolution of the widths was fit using the models of Eq. 5.3 and 5.4, respectively, leading to a temperature of $4.8(8) \mu K$ and an initial cloud size of $\sigma_{0,\{v,a,h\}} = \{12(1), 224(5), 25(1)\} \mu m$.

revival, corresponding to a magnetic confinement whereas the horizontal (red) and axial (purple) data shows a clear expansion. Due to the combined fit model, the small errors on the blue data cause rather large deviations of the red fit from the red data in the case of vertical absorption imaging (left). From the fit we obtain $\omega_{\{v,a,h\}} = 2\pi \cdot \{129(1), 38(15), 123(5)\} \text{Hz}$, $T = 4.8(8) \mu K$ and an initial cloud size of $\sigma_{0,\{v,a,h\}} = \{12(1), 224(5), 25(1)\} \mu m$.

5.2.2. Evaporative cooling

To achieve an ultracold and dense cloud of $^6$Li, we rely on forced evaporative cooling of the atomic cloud close to the Feshbach resonance near 832 G [91] within the dipole trap. Using the presented high-field imaging technique, we are able to characterize and optimize the evaporative cooling process in our system in terms of atom number, temperature and phase-space density.

To initiate evaporative cooling of the dipole trapped cloud, we ramp down the magnetic quadrupole potential that was forming the magnetic trap/second MOT and invert the
5. Trapped atoms

polarity of the lower Feshbach coil and the lower MOT coil. To achieve a rather homogeneous vertical magnetic field across the cloud, we set the MOT coils and the Feshbach coils (both pairs now in Helmholtz configuration) to run at $I_{\text{MOT}} = 35 \, \text{A}$, $I_{\text{ufc}} = 164 \, \text{A}$ and $I_{\text{lfc}} = 250 \, \text{A}$ corresponding to a magnetic field of approximately 780 G. This leads to a scattering length of around 6000 Bohr radii [134] between the two trapped states and allows for rapid re-thermalization during evaporation. Note that using also the MOT coils to produce the large magnetic field is not only advantageous for the enhanced field homogeneity but also leads to a much lower current in the lower Feshbach coil, allowing for evaporation times on the order of seconds. To evaporate the hot atoms, we ramp down the dipole trap laser power from 100 W in four linear ramps as shown in Fig. 5.5. After the four steps we keep the final power setting $P_{\text{dip}}$ for another 49 ms while switching the Feshbach coils to the high-field imaging currents, followed by a variable time-of-flight time $t_{\text{tof}}$ in which the dipole trap beams

Figure 5.5.: Sketch of the dipole trapping and evaporative cooling sequence. The sequence starts with the coil settings from the magnetic trap. The second MOT beams (671 nm) cool down atoms from the magnetic trap for 0.2 ms (red) before the dipole trap beams are switched on (light brown). The atoms are further cooled into the dipole trap potential, followed by an optical pumping (o.p.) pulse, where the repumper fraction of the beam is switched off to prepare the atoms in the $F = 1/2$ ground state manifold. For evaporative cooling, we apply a five step sequence where the dipole trap power gets reduced to a few mW. To increase the magnetic field, we run the MOT coils (blue) in Helmholtz configuration in addition to the Feshbach coils (dark red, dark green). The evaporation is followed by state-selective high-field absorption imaging (a.i.) at the currents required for the respective nuclear spin state to be resonant with the a.i. light.
are switched off. From the absorption images we extract the initial size of the atomic cloud and the atom numbers as shown in Fig. 5.6 for different final dipole trap powers $P_{\text{dip}}$. The initial cloud size (left) in the vertical direction (blue) depends weakly on the final dipole trap power when compared to the axial (purple) and the horizontal (red) sizes which reduce by an order of magnitude due to the cooling process. The atom numbers (right) reduce dramatically for low dipole trap powers as the trap depth reaches less than 10 $\mu$K for powers below 0.2 W.

![Figure 5.6: Fitted initial cloud sizes (left) and atom numbers (right) from a series of evaporative cooling experiments using different final dipole trap beam powers $P_{\text{dip}}$. The axial (purple) and horizontal (red) cloud size changes rather dramatically over the different laser powers, while vertically (blue) the dependence is rather flat. Due to the evaporation process, the atom number for low final laser powers is more than an order of magnitude lower than for high powers.](image)

From the time-of-flight scans we obtain cloud temperatures which we can combine with the initial cloud sizes and atom numbers to obtain the peak phase space density (PSD) of the cloud,

$$\rho_{\text{PSD}} = n_{\text{at}} \lambda_{\text{dB}}^3$$

$$= \frac{N_{\text{Atoms}}}{(2\pi)^{3/2}\sigma_{0,h}\sigma_{0,v}\sigma_{0,a}} \left( \frac{2\pi \hbar^2}{m_{\text{Li}}k_B T} \right)^{3/2},$$

which is an important measure of achievability for Bose-Einstein condensation [135, 136, 137]. For phase space densities on the order of one or higher, the thermal de Broglie wavelength $\lambda_{\text{dB}}$ is in the same range as the interatomic distance, thus the wavefunctions of the individual atoms begin to overlap, which is a necessary requirement for the production of a BEC.

The achieved temperatures and phase space densities for the different final dipole trap beam powers are shown in Fig. 5.7. The temperature (left) clearly shows that we
are able to prepare an atomic sample well below a $\mu$K. Due to the errors of the five values (widths, atom number, temperature), used to compute the phase space density (right), there is a rather large uncertainty in the maximum achievable value. We see that with the current evaporation technique, initial temperature and atom numbers we are able to reach a peak PSD of $\rho_{PSD} = 0.36(17)$ at $n_{at} = 70(26) \cdot 10^{15} \text{ m}^{-3}$ and $T = 0.17(3) \mu$K for the lowest final dipole trap laser power used in the scan. Note that this density is one order of magnitude higher than the one we achieve within the magnetic trap ($49(15) \cdot 10^{14} \text{ m}^{-3}$), thus increasing the Langevin rate for atom-ion collisions by a factor of $\sim 14$. The efficiency of evaporation $\eta_{evap}$ is typically quantified by the relation $\eta_{evap} = \frac{-d \log \rho_{PSD}}{d \log N_{at}}$ [138]. From a fit we find $\eta_{evap} = 3.2(2)$, meaning that we gain 3.2 orders of magnitude in phase space density by losing one order of magnitude in atom number $N_{at}$. Although the achieved peak PSD is not high enough to achieve Bose-Einstein condensation of $^6\text{Li}_2$ molecules [64], the ultracold and dense sample should be usable for sympathetic cooling of the ions as discussed in chapter 2 and for reaching the $s$-wave limit of atom-ion collisions.

To achieve even higher phase space densities, the evaporation ramp could potentially be fine-tuned to lose less atoms during the process. Another option is to increase the initial atom number captured from the second MOT by increasing the dipole trapping region. Therefor, one modulates the dipole trap AOM frequency to shake the overlapping beams, such that on time average, the overlapping region of the beams becomes larger. This method has recently been implemented in our experiment and will be presented in Ref. [98]. A third option is to reduce the minimum achievable temperature by reducing the anti-confinement of the atoms in the horizontal region to enable lower final dipole trap powers. This could be achieved by, e.g., using an additional axial far-detuned laser beam that is overlapped with the atoms or a redesign
5.2. The crossed optical dipole trap

of the coil setup to reduce the second derivatives of the magnetic field at the atomic cloud positions.

5.2.3. Alignment process

To let the small ultracold atomic cloud interact with an equally small crystal of trapped ions, the dipole trap beams have to cross exactly at the position of the ions. The very limited space on the upper breadboards around the experiment impedes the aligning process of the beams, which is crucial due to the high intensities within the ion trap and the potential damage the dipole trap beams can cause to the end cap electrodes.

For pre-alignment of the dipole trap beam we first measured the focal length of the first 400 mm lens. Using a collimated beam of 1070 nm light, we therefore measured the beam diameters at several positions behind the lens using the knife-edge technique [139]. From this we obtain a focal length of 409(1) mm at 1070 nm wavelength, a beam waist of 48(10) µm in the focus and a Rayleigh length of 5(1) mm (in approximate agreement with the computed values in Sect. 5.2), allowing us for a precise positioning of the four dipole trapping lenses.

To ensure the dipole trap beam is pointing exactly at the ion’s position, it was overlapped with the 935 nm repumper laser of the ion as depicted in Fig. 3.12. To ensure a sufficient overlap, we measured both 935 nm and 1070 nm beam profiles and evaluated their peak positions using a CCD camera directly after the overlapping cube and directly after the first dipole trap lens (see Fig. 3.12). We iteratively optimized their overlap, ensuring a deviation of less than 10 µm in relative peak positions. For further pre-alignment the ion fluorescence was optimized using the last mirror before the dipole trap beam enters the vacuum chamber, ensuring the ion is in the center of the beam. By desaturating the 935 nm repumper transition, also the return beam can be pre-aligned that way.

As the radial position of the focal point of the dipole trap beam is extremely sensitive to the settings of the steering mirrors, we employed piezo actuated mirror mounts to correct for small daily drifts of the beam pointing. To optimize the positioning, we use an $^{171}$Yb$^+$ ion as a tool and maximize the differential AC Stark shift on the magnetic field insensitive hyperfine ground state transition $|F = 0, m_F = 0\rangle \rightarrow |F = 1, m_F = 0\rangle$ in $^{171}$Yb$^+$ by employing a Ramsey experiment [119]. Therefore, we prepare the ion in the $|0, 0\rangle$ state by optical pumping (see Sect. 4.4.1), followed by a $\pi/2$ pulse to create
5. Trapped atoms

a coherent superposition $|\psi(0)\rangle = \frac{1}{\sqrt{2}} (|0,0\rangle + |1,0\rangle)$. During the Ramsey wait time $t_{\text{wait}} = 9$ ms we switch on the dipole trap beams that shift both states according to Ref. [132] by

$$
\Delta E_{|F,0\rangle} = -\frac{3\pi c^2}{2} \sum_{J', F', m'_F} \left( \frac{|c_{F,J', F', m'_F, P}|^2}{\omega_{F,J'}^3} \left( \frac{\Gamma_{J'}}{\omega_{F,J'} - \omega_{\text{dip}}} + \frac{\Gamma_{J'}}{\omega_{F,J'} + \omega_{\text{dip}}} \right) I_{\text{dip}}(\vec{r}) \right),
$$

(5.8)

where $c$ is the speed of light, $\omega_{F,J'} \approx 2\pi c / \lambda_{F,J'}$ the transition frequency of the closest dipole-allowed transitions (labeled here with $J'$) plus/minus the respective hyperfine splitting frequency, depending on $F$ and $F'$ the hyperfine quantum number of the ground and excited state of the dipole transitions. In the case of $^{171}\text{Yb}^+$, we have to take into account the D1 transition ($J' = 1/2$) near $\lambda_{1/2} = 369$ nm with the natural linewidth $\Gamma_{1/2} = 2\pi \cdot 19.7$ MHz and the D2 transition ($J' = 3/2$) near $\lambda_{3/2} = 329$ nm with $\Gamma_{3/2} = 2\pi \cdot 25.9$ MHz (see Fig. 4.2). Further, $\omega_{\text{dip}} = 2\pi c / 1070$ nm is the angular frequency of the 1070 nm dipole trap beam and $c_{F,J', F', m'_F, P}$ the polarization ($P$) dependent Clebsch-Gordan coefficients of the transition from the $^2S_{1/2} |F,0\rangle$ state to the respective excited state.

For both states, the computed energy shift is very similar, regardless whether linear or $\pi$ polarized light is used. Mainly the splitting between the two hyperfine ground states $\omega_{\text{MW}} \approx 2\pi \cdot 12.6$ GHz causes a slight difference, leading to the accumulation of a relative phase difference $\phi_{\text{ac}}$ in the superposition state,

$$
|\psi(t_{\text{wait}})\rangle = \frac{1}{\sqrt{2}} \left( |0,0\rangle + e^{-i\phi_{\text{ac}}} |1,1\rangle \right),
$$

(5.9)

with $\phi_{\text{ac}} = (\Delta E_{|1,0\rangle} - \Delta E_{|0,0\rangle}) t_{\text{wait}} / \hbar$.

(5.10)

The phase difference is given by $\phi_{\text{ac}} \approx 4.18 - 4.32 \cdot 10^{-9} \frac{m^2}{\text{W} \cdot \text{s}} I_{\text{dip}}(\vec{r}) t_{\text{wait}}$, where the lower value is for linear and the higher value for $\pi$ polarized light. For the used intensities of around $I_{\text{dip}} \approx 2 \cdot 25$ W/ $(\pi \cdot (50 \mu \text{m})^2)$ and $t_{\text{wait}} = 9$ ms, we expect phase shifts on the order of tens of degrees. To detect the phase shift, we apply a $\pi$-pulse followed by another wait time $t_{\text{wait}}$ without the dipole trap beams switched on and finally another $\pi/2$ pulse followed by state detection of the ion as explained in Sect. 4.4.2.

Instead of scanning the second wait time, we scan the phase of the second $\pi/2$ pulse to obtain Ramsey fringes [119, 140], as it is shown in Fig. 5.8 (left) as red data. As a

\[ This is known as a spin echo sequence [120], used to prevent dephasing of the superposition state, for example due to residual slow magnetic field noise. \]
5.3. Conclusions and outlook

In this chapter we have presented all stages for the production of an optically trapped ultracold and dense cloud of $^6$Li atoms at the position of the ions. We have described the required optical pumping methods and imaging techniques for both, low and high field.

For the optical dipole trap, we have modeled the behavior of the atoms during a time-of-flight sequence within a non-vanishing magnetic (anti-)confinement. Using these results, we have presented and analyzed a first attempt of evaporative cooling.
5. Trapped atoms

in our setup. We achieved a peak density that is about a factor of 14 higher than in the magnetic trap, used for our first atom-ion experiments [58, 80]. With atom temperatures of less than a µK, the atomic cloud should be suitable for the observation of sympathetic cooling of the ion and for reaching the s-wave regime of ultracold atom-ion collisions. For the observation of a molecular BEC and the study of collisions of its interactions with the trapped ions, the peak phase space density of $\rho_{PSD} = 0.36(17)$ is not sufficient. We have presented ideas to increase the atom number and to reduce the magnetic anti-confinement to reach colder temperatures by spatially modulating the trapping volume and the use of an additional axial trapping beam. Furthermore, a blue MOT [141], utilizing the narrow 323 nm $^2S_{1/2} \rightarrow ^3P_{3/2}$ transition, or a gray molasses cooling scheme [142] and optimized optical pumping could lead to a much higher initial phase space density, even before the magnetic transport. Unfortunately, the latter two require a much faster control over the magnetic fields that cannot be achieved with the current setup.

Further, we have described and discussed the alignment procedure of the optical dipole trap and presented a method to ensure precise positioning of the beams using the differential AC Stark effect on the hyperfine ground states of a single $^{171}\text{Yb}^+$ ion to ensure a perfect overlap of the atomic cloud with the trapped ion.
Dynamics of a single ion-spin impurity in a spin-polarized atomic bath

We report on observations of spin dynamics in single Yb$^+$ ions immersed in a cold cloud of spin-polarized $^6$Li atoms. This species combination has been proposed to be the most suitable system to reach the quantum regime in atom-ion experiments. For $^{174}$Yb$^+$, we find that the atomic bath polarizes the spin of the ion by 93(4)\% after a few Langevin collisions, pointing to strong spin-exchange rates. For the hyperfine ground states of $^{171}$Yb$^+$, we also find strong rates towards spin polarization. However, relaxation towards the $F = 0$ ground state occurs after 7.7(1.5) Langevin collisions.

We investigate spin impurity atoms as possible source of apparent spin-relaxation leading us to interpret the observed spin-relaxation rates as an upper limit. Using \textit{ab initio} electronic structure and quantum scattering calculations, we explain the observed rates and analyze their implications for the possible observation of Feshbach resonances between atoms and ions once the quantum regime is reached.

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6. Dynamics of a single ion-spin impurity in a spin-polarized atomic bath

6.1. Introduction

For ion-atom mixtures to be used in quantum technology applications - in which quantum information will be stored in the internal states of the ions and atoms - it is required that spin-changing collision rates are small [143]. In a recent experiment Ratschbacher et al. [45] showed very fast spin dynamics in Yb$^+$ interacting with Rb atoms. Besides fast spin-exchange - which conserves the total spin of the collision partners - strong spin-nonconserving rates known as spin-relaxation were observed. Very recently, spin-dynamics were also measured in Sr$^+/\text{Rb}$ [47]. Tscherbul et al. [46] calculated that an exceptionally large second-order spin-orbit coupling in Yb$^+/\text{Rb}$ provides a mechanism for the observed spin-relaxation rates. For Yb$^+/\text{Li}$ the second-order spin-orbit coupling is expected to be much smaller [46]. A detailed knowledge about the spin-dependence in cold atom-ion collisions gives insight into the possibilities of finding magneto-molecular (Feshbach) resonances between the atoms and ions [26, 56, 57, 59]. These play a pivotal role in neutral atomic systems for tuning the atom-atom interactions and find widespread application in studying atomic quantum many-body systems [7, 26]. In ion-atom mixtures, their existence has been predicted [56, 59], but they have not been observed so far since the required low temperatures have not been reached. These considerations make an experimental study of the spin-dynamics in Yb$^+/\text{Li}$ of key interest.

In this chapter, we investigate the spin dynamics of single trapped Yb$^+$ ions in a cold, spin-polarized bath of $^6\text{Li}$ atoms. We prepare specific (pseudo-) spin states in the ion by optical pumping and microwave pulses. Electron shelving and fluorescence detection allow us to determine the spin state after interacting with the atomic cloud. For $^{174}\text{Yb}^+$ we find that the cloud of atoms polarizes the spin of the ion by $93(4)\%$. Our results indicate a very large spin-exchange rate of $1.03(12) \cdot \gamma_L$, whereas spin-relaxation rates are estimated to be $\leq 0.08(4) \cdot \gamma_L$. Here, $\gamma_L = 2\pi \rho_{\text{Li}} \sqrt{C_4/\mu} = 22(7) \text{ s}^{-1}$ is the Langevin collision rate, with $\rho_{\text{Li}}$ the density of Li atoms at the location of the ion, $C_4$ is proportional to the polarizability of the atom and $\mu$ is the reduced mass. For the $^{171}\text{Yb}^+$ isotope, we prepare all four hyperfine ground states and measure all decay rates. As in $^{174}\text{Yb}^+$, we find strong rates towards spin polarization. However, relaxation from the $m_F = 1$ state towards the $F = 0$ ground state occurs at a rate of $0.13(3) \cdot \gamma_L$. All relevant energy levels of both Yb$^+$ isotopes can be seen in Fig. 6.1. We combine ab initio quantum scattering calculations with the measured spin dynamics and infer a large difference between the singlet and triplet scattering lengths in Yb$^+/^6\text{Li}$, which will be beneficial for the observation of Feshbach
6.2. Experiment

6.2.1. Setup

The experimental setup has been described in detail in chapter 3 and details on ion and atom trapping have been given in chapters 4 and 5, respectively. In short, a cloud of magnetically trapped $^6$Li atoms in the $^2S_{1/2} \, |F = 3/2, m_F = 3/2\rangle$ electronic ground state is prepared 2.1 cm below the ion. The atoms are transported towards the ion by adiabatically changing the magnetic field minimum position to a position 150 $\mu$m below the ion, where the $\sim 400$ $\mu$m wide cloud interacts with the ion for a period of time $t_{\text{int}}$. Afterwards, the atoms are transported back, released from the trap and imaged on a CCD camera. Approximately $7 \cdot 10^6$ atoms interact with the trapped ion at a peak density of $49(15) \cdot 10^{14}$ m$^{-3}$ and a temperature of $T_a = 0.6(2)$ mK.

Figure 6.1.: Energy levels and relevant transitions in $^{174}$Yb$^+$ and $^{171}$Yb$^+$. More detailed levels and the references for the lifetimes and branching ratios are given in Fig. 4.2 and Fig. 4.5.

resonances. Our electronic structure calculations also confirm that spin-nonconserving relaxation rates due to second-order spin-orbit coupling should be smaller than for Yb$^+$/Rb [46].
The energy of the ion is composed of its micromotion in the Paul trap and its secular energy. Before the experiment, we measured and compensated the ion’s excess micromotion in all three dimensions as described in chapter 4 and Ref. [80]. We estimate a residual excess micromotion energy of \( \approx 2 \) mK per direction. We employ microwave sideband spectroscopy on a single \(^{171}\)Yb\(^{+}\) ion [128, 144] and infer an ion temperature in the secular motion of \( \approx 4 \) mK after Doppler cooling and a heating rate of less than \( 4 \) mK/s. The combined energy of the ion is \( E_{\text{Yb}}/k_B \leq 20 \) mK during the experiments. Due to the large mass ratio \( m_i/m_a \), however, the collision energy \( E_{\text{col}} = \frac{\mu}{m_{\text{Yb}}} E_{\text{Yb}} + \frac{\mu}{m_{\text{Li}}} E_{\text{Li}} \approx k_B \cdot 1 \) mK is dominated by the energy of the atoms.

During the interaction, the ion experiences a magnetic field of 0.42 mT caused by the magnetic trap. The energy splitting of the ion’s magnetic sublevels is therefore kept small, allowing for spin-exchange. Following each experimental run, control measurements are performed to verify the conservation of the ionic spin in the sequence when no atoms are loaded.

### 6.2.2. Spin preparation and spin detection

The isotope \(^{174}\)Yb\(^{+}\) has no hyperfine structure. Therefore, the spin is encoded in two magnetic sublevels \( |\uparrow\rangle = |m_J = 1/2\rangle \) and \( |\downarrow\rangle = |m_J = -1/2\rangle \) of the \(^2\)S\(_{1/2}\) electronic ground state. We prepare the spin state by applying an optical pumping pulse of circularly polarized light resonant with the 369 nm \(^2\)S\(_{1/2}\) \(\rightarrow\) \(^2\)P\(_{1/2}\) cooling transition. To detect the spin state, we shelve \( |\downarrow\rangle \) to the extremely long-lived \(^2\)F\(_{7/2}\) state. For this, we use a laser at 329 nm that couples the electronic ground state to the \(^2\)P\(_{3/2}\) state, from which the ion cascades down to the \(^2\)F\(_{7/2}\) state via the \(^2\)D\(_{5/2}\) state with a probability of 72(3)\% [81, 111, 112] as depicted in Fig. 6.1 (left). A magnetic field of 72.5 mT shifts the \( |\uparrow\rangle \) state far out of resonance such that its shelving probability is reduced to 9(1)\%. We detect the unshelved population by fluorescence imaging on the 369 nm cooling transition after switching off the magnetic field. For further details on both preparation and shelving, see Sect. 4.2.

To study the dynamics of the \(^{171}\)Yb\(^{+}\) hyperfine states, we initialize the ion in \( F = 0 \) via optical pumping [79] and apply a microwave pulse (rapid adiabatic passage) to prepare one of the three \( F = 1 \) sublevels before the interaction with the atoms. After the interaction, we measure the population in the \( F = 1 \) state by state-selective fluorescence imaging to obtain a signal proportional to \( \sum_{m_F} p_{1,m_F} = 1 - p_{0,0} \) as depicted in Fig. 6.1 (right). To analyze the population in each of the magnetic sublevels,
6.3. Results

6.3.1. $^{174}\text{Yb}^+$

We scan the atom-ion interaction time $t_{int}$ in units of the inverse Langevin rate $1/\gamma_L$ for $^{174}\text{Yb}^+$ initially prepared in one of the two spin states. The results are shown in Fig. 6.2. When the ion is initialized in $|\downarrow\rangle$ (red discs), around one Langevin collision is sufficient to flip its spin. In contrast, when initialized in the $|\uparrow\rangle$ state (green squares), the ion keeps its initial polarization. We fit the data to a two-level rate equation model [45],

$$P_{b,\uparrow}(t_{int}) = (P^0_{b,\uparrow} - P^\infty_b) e^{-\gamma_{eq}t_{int}} + P^\infty_b,$$
$$P_{b,\downarrow}(t_{int}) = (P^\infty_b - P^0_{b,\downarrow}) (1 - e^{-\gamma_{eq}t_{int}}) + P^0_{b,\downarrow},$$

where 

we invert $p_{|1,m_F\rangle}$ with $p_{|0,0\rangle}$ by applying a second microwave pulse before detection to get a signal proportional to $1 - p_{|1,m_F\rangle}$. 

Figure 6.2.: Probability for finding the $^{174}\text{Yb}^+$ ion in the bright state versus interaction time in units of the inverse Langevin rate. The gray bars indicate the minimum (for $|\downarrow\rangle$) and maximum (for $|\uparrow\rangle$) probabilities to find the ion in a bright state and their error range when no atoms are loaded, indicating the limits of the employed preparation and shelving techniques. The dashed lines are obtained from a combined two-level rate equation fit (Eq. 6.1). The inset shows the obtained spin flip rates of the two Zeeman sublevels in units of Langevin rates.
where \( P_{b,m_J}^0 \) are the probabilities to find an ion prepared in \( |m_J\rangle \) to be in the bright state when no atoms were loaded (lower and upper gray bars in the plot), resembling the limits of our optical pumping and shelving technique. \( P_b^\infty \) is the equilibrium probability to appear bright after interaction with the atomic cloud. For the equilibration rate we obtain \( \gamma_{\text{eq}} = 1.1(1) \cdot \gamma_L \). In the two-level model \( \gamma_{\text{eq}} = \gamma_+ + \gamma_- \), with \( \gamma_{\pm} \) the rates for \( \Delta m_J = \pm 1 \) transitions of the Zeeman state respectively. From the control measurements (without atoms) we get \( P_{b,\downarrow}^0 = 0.34(2) \) and \( P_{b,\uparrow}^0 = 0.90(2) \). Together with the equilibrium probability \( P_b^\infty = 0.86(1) \) we obtain the equilibrium polarization of the ion \( p^\infty_\uparrow = (P_b^\infty - P_{b,\downarrow}^0)/(P_{b,\downarrow}^0 - P_{b,\uparrow}^0) = 0.93(4) \) as well as \( \gamma_+ = 1.03(12) \cdot \gamma_L \) and \( \gamma_- = 0.08(4) \cdot \gamma_L \) from the relation \( p^\infty_\uparrow = \gamma_+ / (\gamma_+ + \gamma_-) \).

### 6.3.2. \(^{171}\text{Yb}^+\)

![Figure 6.3:](image)

**Figure 6.3.** Collision-induced population transfer in the \(^{171}\text{Yb}^+\) hyperfine ground state after the preparation of \( |1, -1\rangle \) (row (a)), \( |1, 0\rangle \) (row (b)) and \( |1, 1\rangle \) (row (c)). The first column shows the decay of the initially prepared state in the \( F = 1 \) manifold and the second column the build up of population in the \( F = 0 \) ground state. The other two columns show the population dynamics of the two remaining states in \( F = 1 \). The lines are obtained from a combined fit model assuming the rates for \( \Delta m_F = -1 \) within the \( F = 1 \) manifold to be zero (solid) or allowing for all decay channels (dashed). The interaction time is given in units of the inverse Langevin rate.

The data obtained in the determination of population in the hyperfine states of \(^{171}\text{Yb}^+\)
was fitted by the solutions of the four-level coupled rate equations

\[
\begin{bmatrix}
\dot{p}_{(0,0)} \\
\dot{p}_{(1,-1)} \\
\dot{p}_{(1,0)} \\
\dot{p}_{(1,1)}
\end{bmatrix} =
\begin{bmatrix}
0 & \Gamma_{-1} & \Gamma_0 & \Gamma_1 \\
0 & -\Gamma_{-1} - \gamma_{-1,0} & \gamma_{0,-1} & 0 \\
0 & \gamma_{-1,0} & -\Gamma_0 - \gamma_{0,1} - \gamma_{0,-1} & \gamma_{1,0} \\
0 & 0 & \gamma_{0,1} & -\Gamma_1 - \gamma_{1,0}
\end{bmatrix}
\begin{bmatrix}
p_{(0,0)} \\
p_{(1,-1)} \\
p_{(1,0)} \\
p_{(1,1)}
\end{bmatrix}, \quad (6.2)
\]

where the dot denotes the time derivative, \(\Gamma_{mF}\) denote the rates from \(|1, m_F\rangle\) to \(|0, 0\rangle\) and \(\gamma_{mF,m_F'}\) denote the rates from \(|1, m_F\rangle\) to \(|1, m_F'\rangle\). Note that we assumed the \(\Delta m_F = \pm 2\) rates to be zero and that transitions changing the total angular momentum by \(\Delta F = 1\) are energetically forbidden due to the 12.6 GHz hyperfine splitting. To obtain analytic solutions of Eq. 6.2, we need to set the spin-nonconserving \(\Delta m_F = -1\) rates \(\gamma_{0,-1}\) and \(\gamma_{1,0}\) to be zero, since there was no clear evidence for these events in the experimental data, as shown in the twelve relevant plots in Fig. 6.3. To obtain upper bounds on these two rates, we take the fitted curves (solid lines) as an initial guess and numerically minimize the mean quadratic distance of the full numerical solutions of Eq. 6.2 to the experimental data. The optimized solutions are shown as dashed lines and deviate only slightly from the initial guess.

The resulting rates are shown in Fig. 6.4. While the transition rates \(\gamma_{mF,m_F'}\) for \(\Delta m_F = m_F' - m_F = 1\) within the \(F = 1\) manifold are both approximately equal to \(\gamma_{-1,0} = 0.44(11) \cdot \gamma_L \approx \gamma_{0,1} = 0.44(8) \cdot \gamma_L\), the rates \(\Gamma_{mF}\) changing the total angular momentum by \(\Delta F = -1\) decrease with increasing \(m_F\) in the \(F = 1\) manifold from \(\Gamma_{-1} = 0.57(8) \cdot \gamma_L\) via \(\Gamma_0 = 0.21(7) \cdot \gamma_L\) to \(\Gamma_1 = 0.13(3) \cdot \gamma_L\). Note that the decay \(\Gamma_1\) does not conserve the total spin of the atom-ion system. The rates changing only \(m_F\) by \(-1\) are hardly detectable in our experiment due to the dominating rates \(\Gamma_0\) and \(\Gamma_{-1}\).

### 6.3.3. Purity of atomic spin

The observed spin-nonconserving rates \(\gamma_{-}\) and \(\Gamma_1\) could be due to second-order spin-orbit coupling which was recently suggested as a source of spin-relaxation [46]. However, another possibility is that atomic spin impurities within the gas cause sporadic collisions that appear as spin non-conserving. In particular, we expect the presence of atoms in the low-field seeking \(|3/2, 1/2\rangle\) state (see Fig. 5.1) due to imperfect optical pumping. When such impurity atoms collide with a spin-polarized ion, spin-allowed transitions such as \(|3/2, 1/2\rangle_{\text{atom}} |1, 1\rangle_{\text{ion}} \rightarrow |3/2, 3/2\rangle_{\text{atom}} |0, 0\rangle_{\text{ion}}\) may occur.
Dynamics of a single ion-spin impurity in a spin-polarized atomic bath

Figure 6.4.: Measured transition rates between the $^{171}$Yb$^{+} 2S_{1/2}$ hyperfine ground states in units of the Langevin rate $\gamma_L$. The $\Delta m_F = +1$ processes (dark red) dominate the dynamics, whereas the $\Delta m_F = -1$ transitions (dashed, black) can hardly be detected. The $\Delta F = -1$ transitions are shown in blue.

that cannot be distinguished from spin-relaxation caused by majority atoms. In this subsection, we study the spin purity of the atomic cloud.

The spin of the atoms in the magnetic trap is polarized by applying a 150 $\mu$s $\sigma^+$-polarized optical pumping pulse at the D1 transition while applying an additional magnetic field of 1.0 mT along the beam direction. Due to magnetic field inhomogeneities not every atom is in the correct magnetic field to be pumped resonantly to the desired $|F = 3/2, m_F = 3/2\rangle$ ground state. To estimate the purity of the magnetically trapped $^6$Li cloud in the $|3/2, 3/2\rangle$ state, we perform a Stern-Gerlach experiment. We abruptly displace the trap minimum radially by approximately 6 mm in less than a millisecond while keeping the gradient constant at $g_r = 0.22$ T/m. To image the accelerating cloud, we switch off the trapping field after a variable time $t_{SG}$. We wait 1 ms for the magnetic fields to settle and take an absorption image. A series of projected absorption images for different times $t_{SG}$ is shown in Fig. 6.5. The main part of the cloud moves out of the imaging region within 8 ms whereas a second fraction leaves the region at around 14 ms. We identify the fast fraction with atoms in the $|3/2, 3/2\rangle$ state and the slow fraction with atoms in the $|3/2, 1/2\rangle$ state due to the different accelerations caused by the difference in magnetic moment. The fraction in the $|3/2, 3/2\rangle$ state reappears three more times due to the faster oscillation period, whereas the return of the atoms in $|1/2, 1/2\rangle$ can only be observed once at 50–60 ms within the scanned time window. The data is shown along with the idealized single particle trajectories for $|3/2, 3/2\rangle$ (red) and $|3/2, 1/2\rangle$ (black), matching the observed
6.3. Results

Figure 6.5.: Series of projected absorption images for different Stern-Gerlach acceleration times $t_{SG}$. The data is shown along with the expected single atom trajectories for the $|3/2, 1/2\rangle$ state (black) and the $|3/2, 3/2\rangle$ state (red) for an instantaneous shift of the magnetic field.

return behavior of the fractions. Small deviations are due to the finite switching time of the magnetic field as well as the waiting time before absorption imaging. For a quantitative description of the fractions, the camera position was adjusted to observe the visible separation of the cloud at $t_{SG} = 11.5\,\text{ms}$. At that time, the atoms in the $|3/2, 1/2\rangle$ state have separated from the main fraction in the $|3/2, 3/2\rangle$ state caused by the difference in magnetic moment, in agreement with simulations. To make sure we image both fractions equally well, we scanned the imaging laser frequency $\pm 10\,\text{MHz}$ around the resonance and average over the results. In order to obtain the fraction of $|3/2, 1/2\rangle$ atoms, we project the images along the vertical axes, as it is shown in Fig. 6.6. The atoms in the $|3/2, 1/2\rangle$ state (left peak) did not pass the trap minimum at around 6 mm yet whereas the atoms in the $|3/2, 3/2\rangle$ state have reached their turning point at around 12 mm and show a long tail lagging behind, in agreement with simulations. Due to the lack of a suitable model, we fit the data with the sum of three Gaussian distributions (red), one for the $|3/2, 1/2\rangle$ state and two for the $|3/2, 3/2\rangle$ state to model the tail of the distribution (red, dashed). By comparing the peak integrals, we obtain a fraction of $\widetilde{N}_{|3/2,1/2\rangle} = N_{|3/2,1/2\rangle}/N_{\text{tot}} = 24(1)\%$ of the atoms being in the undesired state.

Due to the difference in magnetic moment, the spatial distribution for the $|3/2, 1/2\rangle$ state is expected to be broader than for the $|3/2, 3/2\rangle$ state. Thus, the possibility to find an impurity atom at the ion’s position, given by $\widetilde{\rho}_{|3/2,1/2\rangle} = \rho_{|3/2,1/2\rangle}/\rho_{\text{tot}}$, is
6. Dynamics of a single ion-spin impurity in a spin-polarized atomic bath

Figure 6.6.: Absorption image (left) and the projection on the horizontal axis (right) for a Stern-Gerlach acceleration time of $t_{SG} = 11.5$ ms. The weaker peak corresponds to the signal of the impurity atoms in the undesired $|3/2, 1/2\rangle$ state lagging behind the atoms in $|3/2, 3/2\rangle$ (bigger peak). Note that the x-axis points in the direction of acceleration. The data is shown along with a heuristic fit model as described in the text.

Reduced with respect to the fraction $\tilde{N}_{3/2,1/2}$. To estimate this ratio, we assume both fractions of the cloud to have the same initial size and temperature before they are loaded into the magnetic trap, justified by their origin from a compressed magneto-optical trap (cMOT). When transferring the atoms from the cMOT to the magnetic trap both temperature and size of the clouds change, depending on their magnetic moment which is proportional to their $m_F$ quantum number at low magnetic fields. Using realistic parameters obtained from the experiment, we simulate this transfer to the magnetic trap followed by a combined compression and transport to the interaction zone within 135 ms. The temporal evolution of the cloud sizes is shown in Fig. 6.7. While the cloud size in $|3/2, 3/2\rangle$ remains almost unchanged, the impurity fraction initially expands because of its weaker trapping potential. Thus, we obtain a fractional density of $\tilde{\rho}_{3/2,1/2} \leq 10\%$ at the position of the ion. Due to the increased cloud size, we assume to lose a large fraction of the impurity atoms during the magnetic transport by collisions with the ion trap electrodes such that the actual density fraction is expected to be lower than in the simulation. Furthermore, spin-exchange with majority atoms occurs, leading to the loss of the impurity atoms [145]. We justify these assumptions by performing the same Stern-Gerlach experiment as described above, but on the atoms that return after the interaction time, where we cannot observe an impurity spin signal anymore. However, since we cannot rule out the presence of some impurity atoms at the location of the ion, we treat the measured spin-nonconserving rates $\gamma_-$ and $\Gamma_1$ as an upper limit.
Figure 6.7.: Simulated evolution of the horizontal \((x, y)\) and vertical \((z)\) cloud sizes of \(|3/2, 3/2\rangle\) (solid) and \(|3/2, 1/2\rangle\) (dashed) for loading the magnetic trap from a compressed MOT (0–15 ms) followed by a compressing transport to the interaction zone (the cloud is moved in the \(x\)-direction during the time-interval 15–85 ms, and in the \(z\)-direction during the time-interval 85–135 ms). For more details, see Ref. [80].

6.4. Theory

The work presented in this section was realized in collaboration with Dr. Michal Tomza, who did numerical simulations on the spin-exchange rates and the spin-relaxation to compare with the experimental results and the potential observation of Feshbach resonances. A more detailed description can be found in Ref. [58], where also the plots within this section originate from.

6.4.1. Spin-exchange

We explain the measured spin-exchange rates by solving a quantum model of cold atom-ion collisions based on the \textit{ab initio} coupled-channel description of our system as it was used in Refs. [59, 146]. To match the experimental conditions, we use \(^{6}\text{Li}\) in the spin polarized \(|3/2, 3/2\rangle\) state and \(\text{Yb}^+\) in the state of interest as initial conditions and a magnetic field of \(B_z = 0.42\) mT. For the exit channels, we allow all potential states,

\[
|\text{i}_{\text{Yb}^+, m_{\text{i,Yb}^+}}\rangle|s_{\text{Yb}^+, m_{\text{s,Yb}^+}}\rangle|\text{i}_{\text{Li}, m_{\text{i,Li}}}\rangle|s_{\text{Li}, m_{\text{s,Li}}}\rangle|l, m_l\rangle,
\]
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where \( m_j \) is the projection of angular momentum \( j \) on the space-fixed \( z \)-axis, and assuming the projection of the total angular momentum \( M_{\text{tot}} = m_{f,Yb^+} + m_{f,\text{Li}} + m_l = m_{i,Yb^+} + m_{s,Yb^+} + m_{i,\text{Li}} + m_{s,\text{Li}} + m_l \) to be conserved.

We solve the coupled-channel scattering problem to obtain the spin-exchange rates for all relevant input states to all participating output states. Exemplary results for two different ion input states are shown in Fig. 6.8. Technical details on the computation can be found in Ref. [58]. To match the results (dashed and solid lines) with to the experimentally obtained rates (red squares), we use \( a_T = -a_S = R_4 \) as triplet (T) and singlet (S) scattering lengths, where \( R_4 = \sqrt{2\mu C_4/\hbar^2} \) is the characteristic length scale of the atom-ion interaction potential. As already assumed in the experiment, the simulations show that transitions with \( \Delta m_F = +2 \) are negligible. The simulations show an increase of the rates that reduce the \( F \) quantum numbers at collision energies lower than \( k_B \cdot 0.1 \text{ mK} \), releasing the hyperfine energy of either the atom’s or ion’s electronic state.

It has been shown that the spin-exchange rates depend on the difference between the singlet and triplet scattering phases [26]. Thus, we computed the total spin-exchange rates for three different sets of scattering lengths. An example is shown in Fig. 6.9. We find that even for collision energies of several hundred mK, the spin-exchange rates strongly depend on the difference between the scattering lengths [60, 61]. As in Fig. 6.8, matching the simulations to the measured data requires the scattering lengths to be large and of opposite sign, \( a_T = -a_S = R_4 \). As a consequence, broad magnetic
6.4. Theory

Feshbach resonances can be expected when the s-wave regime is reached [26, 59].

6.4.2. Magnetically tunable Feshbach resonances

To confirm the presence of large resonances at scattering lengths of $a_T = -a_S = R_4$, we compute the thermally averaged elastic and inelastic collision rates for experimentally achievable fields between 0–300 G. An example result for the energetically lowest entrance channel ($M_F = m_f,^{171}\text{Yb}^+ + m_f,^6\text{Li} = 0$) is shown in Fig. 6.10. For collision energies of $k_B \cdot 100\text{ nK}$, both thermally averaged (red) and energy resolved (blue) rates are almost the same due to the dominant contribution of s-waves. The scanned regime shows dominant resonances but is far off from experimentally realizable collision energies. For a collision energy of $k_B = 10\mu\text{K}$, which should be within reach after minor changes in our setup [62], still s-wave collisions are the dominant contribution and large resonances occur. Finally, for the collision energies that can be achieved in the current status of the experiment, the resonances are washed out by both the contribution of many partial waves and thermal averaging.
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Figure 6.10: Elastic scattering rates for $^{174}\text{Yb}^+/^6\text{Li}$ versus magnetic field for the lowest channel with $M_F = m_{f,Yb^+} + m_{f,\text{Li}} = 0$ at (a) $E_{\text{col}}/k_B = 100 \text{nK}$, (b) $10 \mu\text{K}$, and (c) $1 \text{mK}$. Blue dotted lines are energy-resolved rates and red solid lines are thermally averaged rates.

6.4.3. Spin-relaxation

The spin-nonconserving relaxation process can be described by the effective Hamiltonian [46, 147]

$$\hat{H}_{\text{dip}} = \left( -\frac{\alpha^2}{R^3} + \lambda_{\text{SO}}(R) \right) \left[ 3 \hat{s}_{\text{Yb}^+}^z \hat{s}_{\text{Li}}^z - \hat{s}_{\text{Yb}^+} \cdot \hat{s}_{\text{Li}} \right], \quad (6.3)$$

where $\hat{s}_{\text{Li}/\text{Yb}^+}$ are the electronic spins and $\alpha$ is the fine-structure constant. While the first term describes the short range direct magnetic dipole-dipole interaction, the second term dominates on long ranges and arises from second-order perturbation theory of the first-order spin-orbit couplings between the $a^3\Sigma^+$ and the $^3\Pi$ electronic states of the molecular system. In case of the Yb$^+/\text{Rb}$ system, this term seems to be the main source of the large spin-relaxation [45, 46]. The exact $R$-dependence of this second-order spin-orbit coupling is given by [147]

$$\lambda_{\text{SO}}(R) = \frac{2}{3} \frac{|\langle a^3\Sigma^+ | H_{\text{SO}} | b^3\Pi \rangle|^2}{V_{b^3\Pi}(R) - V_{a^3\Sigma^+}(R)}, \quad (6.4)$$
with \( \langle a^3\Sigma^+ | H_{SO} | b^3\Pi \rangle \) the matrix element of the spin-orbit coupling between the \( a^3\Sigma^+ \) and \( b^3\Pi \) electronic states and \( V_{b^3\Pi}(R) \) and \( V_{a^3\Sigma^+}(R) \) the potential energy curves of the \( a^3\Sigma^+ \) and \( b^3\Pi \) electronic states of the molecular system. Due to the large energy difference in the denominator, the contribution of higher \( ^3\Pi \) states is negligible. To compute the term, we used the molecular potentials obtained from Ref. [59] and wave functions obtained from ab initio electronic structure methods as discussed in Ref. [148] for the matrix elements.

![Figure 6.11: Second-order spin-orbit coupling coefficient \( \lambda_{SO}(R) \) for the Yb\(^+\)/Li system as a function of the atom-ion distance. The point and vertical line indicate the value for the equilibrium distance and the position of the classical turning point of the \( a^3\Sigma^+ \) electronic state, respectively. The inset shows the matrix elements of the spin-orbit coupling for the \( a^3\Sigma^+ \) and \( b^3\Pi \) electronic states of the Yb\(^+\)/Li system.](image)

In Fig. 6.11 both the complete second-order spin-orbit coupling coefficient \( \lambda_{SO}(R) \) (red) and the matrix element (red inset) can be found. To confirm the quality of the calculations, also the matrix element \( \langle b^3\Pi | H_{SO} | b^3\Pi \rangle \) is shown (black inset), reaching the experimental value of the spin-orbit splitting in neutral Yb [149] for the corresponding \( ^3P \) state. Both, matrix element and the second-order spin-orbit coupling, decrease exponentially at large distances. At the classical turning point of the \( a^3\Sigma^+ \) electronic state (vertical line) and the equilibrium distance (dot) the coupling coefficient is 14.2 cm\(^{-1}\) and 4.1 cm\(^{-1}\), about an order of magnitude smaller than for the Yb\(^+\)/Rb system [46, 150]. As already indicated by Ref. [46], this is mainly reasoned by the larger potential energy difference in the denominator of Eq. 6.4 in the case of Yb\(^+\)/Li, thus explaining the much smaller spin-relaxation rate in our system.
6. Dynamics of a single ion-spin impurity in a spin-polarized atomic bath

6.5. Conclusions

We have measured the spin dynamics of single trapped Yb$^+$ ions immersed in a cold cloud of spin-polarized $^6$Li atoms. We have observed very fast spin-exchange that occurs within a few Langevin collisions. For $^{174}$Yb$^+$, spin-relaxation rates are found to be a factor $\geq 13(7)$ smaller than spin-exchange rates. Spin impurity atoms in the atomic cloud may lead to apparent spin-relaxation, such that we interpret the observed relaxation rate as an upper limit. The observed ratio between spin-allowed and spin-nonconserving collisions is higher than those observed in Yb$^+$/Rb [45], where a ratio of 0.56(8) was measured for Rb atoms in the stretched $|F = 2, m_F = 2\rangle$ state. For Sr$^+$/Rb [47], both spin-exchange and spin-relaxation rates for Rb atoms prepared in the $|F = 1, m_F = -1\rangle$ state are lower than the rates observed in this work and have a lower ratio of 5.2(8). For $^{171}$Yb$^+$, we have measured the decay channels of all spin states within the ground state hyperfine manifold and observe both spin-exchange and spin-relaxation processes. We have compared our measured rates to predictions from \textit{ab initio} electronic structure and quantum scattering calculations and conclude that a large difference between singlet and triplet scattering lengths is responsible for the observed large spin-exchange rates, whereas small second-order spin-orbit coupling results in small spin-relaxation rates. These findings suggest good prospects for the observation of Feshbach resonances in the Yb$^+$/Li system.
In this chapter we report on spectroscopic results on the $^2S_{1/2} \rightarrow ^2P_{3/2}$ transition in single trapped Yb$^+$ ions. We measure the isotope shifts for all stable Yb$^+$ isotopes except $^{173}$Yb$^+$, as well as the hyperfine splitting of the $^2P_{3/2}$ state in $^{171}$Yb$^+$. Our results are in agreement with previous measurements but are a factor of 5–9 more precise. For the hyperfine constant $A \left(^2P_{3/2}\right) = 875.4(10)$ MHz our results also agree with previous measurements but deviate significantly from theoretical predictions. We present experimental results on the branching ratios for the decay of the $^2P_{3/2}$ state. We find branching fractions for the decay to the $^2D_{3/2}$ state and $^2D_{5/2}$ state of 0.17(1)% and 1.08(5)%, respectively, in rough agreement with theoretical predictions. Furthermore, we measured the isotope shifts of the $^2F_{7/2} \rightarrow ^1D_{5/2}$ transition and determine the hyperfine structure constant for the $^1D_{5/2}$ state in $^{171}$Yb$^+$ to be $A \left(^1D_{5/2}\right) = -107(6)$ MHz.

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7. Precision spectroscopy of the D2 line in Yb$^+$

7.1. Introduction

Laser-cooled ions in Paul traps form one of the most mature laboratory systems for performing optical metrology, precision measurements as well as quantum-computation and quantum-simulation [8, 151, 152, 153, 154]. The ion species Yb$^+$ is a particularly versatile system for many of these applications owing to its rich electronic structure with multiple meta-stable states [155, 156]. Furthermore, the hyperfine structure of $^{171}$Yb$^+$ provides a first-order magnetic field-insensitive qubit in the electronic ground state [79, 102, 157] that may be used in quantum information applications [158, 159].

While many transitions between low lying electronic states in Yb$^+$ have been studied with great precision [79, 81, 113, 116, 160, 161], there has been only one measurement of the isotope shifts in the $^2S_{1/2} \rightarrow ^2P_{3/2}$ (D2) transition as well as of the hyperfine splitting of the $^2P_{3/2}$ state [162] so far, which was performed in a hollow-cathode discharge lamp. Remarkably, the experimental result for the hyperfine splitting disagrees significantly with theoretical predictions [121, 163, 164, 165, 166]. Although there has been a lot of theoretical work on transition amplitudes for the decay of the $^2P_{3/2}$ state [111, 163, 164, 165, 167], there seems to be no experimental data available for the branching ratios of the decay of the $^2P_{3/2}$ state up until now.

Here, we present experimental results on the isotope shifts in the D2 transition, the hyperfine splitting of the $^2P_{3/2}$ state as well as on the branching ratios of its decay obtained from a single trapped and laser-cooled ion. Furthermore, we present measurements of the isotope shift in the $^2F_{7/2} \rightarrow ^1D_{5/2} [5/2]$ transition, as well as the hyperfine splitting in the $^1D_{5/2}[5/2]$ state in $^{171}$Yb$^+$. Single trapped ions are very well suited to perform such precision measurements, as both state preparation and detection can be performed with great accuracy while at the same time errors due to back-ground gas collisions are negligible. Using isotope-selective photoionization to load the Paul trap, we are able to conduct the experiments even with the rare isotope $^{168}$Yb$^+$ (0.13% abundance [149]) for which no previous data seems to exist.

7.2. Experimental setup

The experiments have been performed in the linear Paul trap described in chapter 3. We load a single Yb$^+$ ion into the trap by two-step photoionization with lasers at 399 nm wavelength for the resonant excitation of the $^1S_0 \rightarrow ^1P_1$ transition in neutral...
Yb and 369 nm wavelength for the excitation into the ionization continuum. Tuning the wavelength of the first step to the resonance of a specific isotope allows for isotope-selective loading of Yb$^+$ ions. Due to overlapping resonances [168], $^{170}\text{Yb}^+$ and $^{172}\text{Yb}^+$ cannot be loaded deterministically, but only in combination with $^{171}\text{Yb}^+$ and $^{173}\text{Yb}^+$, respectively. However, by temporarily lowering the trap drive amplitude we can expel the heavier isotopes from the trap and keep only the isotope $^{170}\text{Yb}^+$ or $^{172}\text{Yb}^+$, respectively.

![Figure 7.1:](image)

(a) Relevant electronic levels and transitions in Yb$^+$. We perform spectroscopic measurements on the $^2S_{1/2} \rightarrow ^2P_{3/2}$ (D2) transition near 329 nm wavelength. The $^2P_{3/2}$ state decays in $\tau = 6.15(9)$ ns [108] either back into the ground state or into one of the metastable states $^2D_{3/2}$ or $^2D_{5/2}$. While an ion which is initially in the states $^2S_{1/2}$ or $^2D_{3/2}$ scatters light during Doppler cooling (thin gray arrows), it will not scatter light when it is in the $^2D_{5/2}$ state. This allows for detection of a successful excitation of the $^2S_{1/2} \rightarrow ^2P_{3/2}$ transition as well as for measurement of the branching fractions of the $^2P_{3/2}$ decay. From the $^2D_{5/2}$ state the ion decays in $\tau = 7.2(3)$ ms [81] to either the ground state or the very long lived $^2F_{7/2}$ state ($\tau \approx 10$ yr [114]). We use the $^2F_{7/2} \rightarrow ^1D_{5/2}$ transition near 638 nm wavelength to depopulate the $^2F_{7/2}$ state. (b) Hyperfine structure of the $^2F_{7/2} \rightarrow ^1D_{5/2}$ and $^2S_{1/2} \rightarrow ^2P_{3/2}$ transitions in $^{171}\text{Yb}^+$. 

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Lasers near wavelengths of 369 nm and 935 nm are used to Doppler cool the ion on the \( ^2S_{1/2} \rightarrow ^2P_{1/2} \) transition and pump population trapped in the metastable \(^2D_{3/2}\) state back into the cooling cycle via excitation to the \(^3D_{3/2}\) state, as shown in Fig. 7.1a. We image the ion’s fluorescence at 369 nm wavelength to a photomultiplier tube (PMT) for detection.

For cooling of the isotope \(^{171}\text{Yb}^+\), which has a nuclear spin of \( I = 1/2 \) and accordingly hyperfine splittings of the electronic states, we use the closed transition \(|^2S_{1/2}, F = 1 \rangle \rightarrow |^2P_{1/2}, F = 0 \rangle\). However, due to off-resonant excitation of the \(|^2P_{1/2}, F = 1 \rangle\) state, the ion occasionally decays to the \(|^2S_{1/2}, F = 0 \rangle\) state. Microwave radiation at a frequency of 12.6 GHz couples the \( F = 0 \) and \( F = 1 \) ground states to ensure continuous cooling. To prepare the ion in the \(|^2S_{1/2}, F = 0 \rangle\) state, we excite the \(|^2S_{1/2}, F = 1 \rangle \rightarrow |^2P_{1/2}, F = 1 \rangle\) transition resonantly while the microwave radiation is switched off.

In addition to the lasers required for cooling and detection of the ion, we use light near the wavelengths of 329 nm and 638 nm to drive the transitions \(^2S_{1/2} \rightarrow ^2P_{3/2}\) and \(^2F_{7/2} \rightarrow ^1D_{5/2}\), respectively. We generate light at 329 nm wavelength with a frequency quadrupled, amplified diode laser. After the first doubling cavity, light at 658 nm wavelength is coupled into a high bandwidth fiber electro-optic modulator (EOM). Sidebands at frequencies of 0.1–3.0 GHz are modulated onto the light and used to stabilize the laser to an external reference cavity. Thus, the laser is stabilized to the fixed reference cavity with a variable frequency offset which is given by the modulation frequency of the EOM. The reference cavity consists of two mirrors with a reflectivity of \( R \approx 99\% \) glued to a 10 cm long Zerodur spacer in a temperature stabilized vacuum housing. The laser is frequency stabilized by the Pound-Drever-Hall technique [97].

For further frequency scanning and pulse shaping we use an acousto-optic modula-
tor (AOM) in double-pass configuration with a center frequency of 200 MHz and a bandwidth of 100 MHz. The signals for the AOM and the fiber EOM are generated by a two channel microwave generator, which is stabilized to a 10 MHz reference signal from a signal generator. A mechanical shutter prevents any light from reaching the ion if switched off. Light from the first doubling cavity is coupled to a commercial wavelength meter, allowing for a coarse absolute frequency determination of the frequency-quadrupled light with an accuracy of 60 MHz according to specification.

We generate light at 638 nm wavelength with a home-made ECDL. This laser is stabilized to the wavelength meter to compensate for frequency drifts and has a short-time frequency stability of better than 10 MHz. We switch the light with a mechanical shutter. The light is coupled to a fiber EOM which allows for modulating sidebands in order to drive transitions between multiple hyperfine states in the case of $^{171}$Yb$^+$, and guided to the experiment. The part of the setup relevant for the spectroscopy is shown in Fig. 3.9 and 3.8.

7.3. Results

7.3.1. Isotope shifts and hyperfine splitting

In case of the isotopes without nuclear spin, we measure the resonance frequency of the D2 transition by applying laser pulses with a width of 5 $\mu$s and a saturation parameter $s \approx 1$ to the ion. From the $^2P_{3/2}$ state, there is a probability of about 1% for the ion to decay to the metastable state $^2D_{5/2}$ ($\tau = 7.2$ ms) from where it decays with 83% probability [81] to the long-lived $^2F_{7/2}$ state. An ion in either of these states does not scatter light during Doppler cooling. On resonance, about 50% of the population decays to the dark $^2D_{5/2}$ state in 5 $\mu$s. To detect whether the ion is in one of the dark states, we image the ion’s fluorescence to a PMT for 4 ms during Doppler cooling, allowing for almost perfect state detection. We scan the laser over the atomic resonance in steps of 2 MHz by tuning the drive frequency of the AOM ($\nu_{\text{aom}}$). We compensate for the frequency-dependence of the diffraction efficiency in the AOM by supplying appropriate radio-frequency power at each frequency. After the detection, we pump the ion back into the cooling cycle by exciting the $^2F_{7/2} \rightarrow ^1D [5/2]_{5/2}$ transition. A post-selection measurement is performed before each spectroscopy pulse in order to check if the ion was successfully pumped out of the $^2F_{7/2}$ state. The measurement data for a single scan of the transition in $^{174}$Yb$^+$ is plotted in Fig. 7.2(a).
Figure 7.2.: Isotope shift measurement with trapped Yb\textsuperscript{+}. (a) Data from a single scan over the \( ^2S_{1/2} \rightarrow ^2P_{3/2} \) transition in \( ^{174}\text{Yb}\textsuperscript{+} \). Error bars denote the quantum projection noise. (b) Plot of a single resonance scan in \( ^{171}\text{Yb}\textsuperscript{+} \). Here, we do not project to bright or dark states but measure PMT counts during the detection bin \( t_{\text{det}} = 2.5 \text{ ms} \). The error bars denote the uncertainties from photon counting statistics. (c) Cavity drift obtained by repeated measurements of the transitions from \( \vert 2S_{1/2}, F = 1 \rangle \) to \( \vert ^2P_{3/2}, F = 1 \rangle \) (circles) or \( \vert ^2P_{3/2}, F = 2 \rangle \) (disks). Offsets of \( \nu_1 = 1811.0 \text{ MHz} \) (\( F = 1 \), circles) and \( \nu_2 = -60.0 \text{ MHz} \) (\( F = 2 \), disks) are added to the measured resonance frequencies. We choose \( \nu_1 \) and \( \nu_2 \) so that the standard deviation for a combined linear fit (black line) is minimized. From its slope, we determine a linear drift of 92 kHz/min. The hyperfine splitting of the \( ^2P_{3/2} \) state is given by the difference \( \nu_1 - \nu_2 = 1751.0 \text{ MHz} \). The result given in Tab. 7.2 is based on the average of two measurement series on different days. (d) Isotope shifts in the \( ^2S_{1/2} \rightarrow ^2P_{3/2} \) transition (circles) and the \( ^2F_{7/2} \rightarrow ^1D_{5/2} \) transition (squares). Error bars are too small to be visible on this scale.

We repeat the experiment for the isotopes \( ^{168}\text{Yb}\textsuperscript{+} \), \( ^{170}\text{Yb}\textsuperscript{+} \), \( ^{172}\text{Yb}\textsuperscript{+} \), \( ^{174}\text{Yb}\textsuperscript{+} \) and \( ^{176}\text{Yb}\textsuperscript{+} \). For each measurement, we frequency-stabilize the laser to the same cavity mode, but with different offset frequencies \( \nu_{\text{eom}} \) given by the modulation frequency of the fiber EOM. The relative frequency of the spectroscopy light compared to the fixed cavity resonance is determined by \( \nu_{\text{rel}} = 2\nu_{\text{eom}} - 2\nu_{\text{aom}} \). We estimate the drift of the cavity by measuring the same resonance at different times as shown in Fig. 7.2(c).

We determine the resonance frequencies by fitting a Lorentzian line shape to the measured data. The uncertainties in the energy shifts are dominated by the standard error of the least-squares fit (0.5–1 MHz) and the uncertainty in the cavity drift during
the measurement time of a few hours. In principle the error should not depend on the abundance of the isotope. However, the measurements with the rare isotopes $^{168}$Yb$^+$ (0.13% abundance) and $^{170}$Yb$^+$ (3.05% abundance, can only be loaded in combination with $^{171}$Yb$^+$) \[149\] take significantly longer due to low ion loading rates. This leads to larger uncertainties for the cavity drift of about 3 MHz, compared to 1 MHz for the more abundant isotopes $^{172}$Yb$^+$, $^{174}$Yb$^+$ and $^{176}$Yb$^+$. We use $\pi$-polarized light and a small magnetic field of $B = 0.05 \text{ mT}$ to avoid errors due to Zeeman shifts of the D2 transition. The results shown in Fig. 7.2(d) and Tab. 7.1 are based on the average of two measurement series on different days. The difference between these datasets is in agreement with the quoted uncertainties.

<table>
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<th>(A^{(3/2)})</th>
<th>$^{121}$Th</th>
<th>$^{163}$Th</th>
<th>$^{164}$Th</th>
<th>$^{164}$Th</th>
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<td>$A^{(1D[5/2])}$</td>
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Table 7.2.: Hyperfine structure constants \(A\) in $^{171}$Yb$^+$ in MHz. The number in brackets denotes the error in the last digit. The magnetic-dipole hyperfine structure constant \(A^{(3/2)}\) measured by our group is consistent with previous measurements (Exp.) but deviates significantly from theory (Th.) predictions. In Ref. \[164\] results are given for a single-electron approach (a) and a many-electron approach (b). The many-electron results give the best agreement with our experimental results by far.

In case of $^{171}$Yb$^+$ we make use of the hyperfine structure (see Fig. 7.1(b)) in order to detect the excitation to the $^2P_{3/2}$ state. We prepare the ion in the \(|F = 0\rangle\) ground state before transferring it to the \(|F = 1, m_F = 0\rangle\) state via rapid adiabatic passage (RAP) using microwave radiation. We apply a laser pulse with a width of 200 ns to excite the $|^2P_{3/2}, F = 1\rangle$ or $|^2P_{3/2}, F = 2\rangle$ states, followed by a second RAP pulse on the \(|F = 0\rangle \rightarrow |F = 1, m_F = 0\rangle\) transition. At the end of this sequence, we perform state-selective fluorescence detection, based on Doppler cooling without microwave coupling of the \(|F = 1\rangle\) and \(|F = 0\rangle\) ground states. During the detection, an ion in the \(|F = 0\rangle\) state appears dark while an ion in the \(|F = 1\rangle\) state scatters light, which allows for detection of the induced population transfer out of the initial \(|F = 1, m_F = 0\rangle\) state.

Experiments with $^{171}$Yb$^+$ are conducted in a magnetic field of 0.18–0.23 mT in order to allow for efficient Doppler cooling on the \(|^2S_{1/2}, F = 1\rangle \rightarrow |^2P_{1/2}, F = 0\rangle\) transition \[79\]. We use linearly polarized light \((\sigma^+ + \sigma^-)\) at 329 nm wavelength to avoid the dipole forbidden \(|^2S_{1/2}, F = 1, m_F = 0\rangle \rightarrow |^2P_{3/2}, F = 1, m_F = 0\rangle\) transition. Due to the symmetric excitation of the transition (see Fig. 7.1(b)) the magnetic field should not lead to a frequency shift of the transition. Measurements at different fields corroborate this assumption.
We repeat the experiment for both hyperfine states and determine the hyperfine energy splitting given in Tab. 7.2. We compare the transition frequencies to the resonance frequency for the isotope $^{172}\text{Yb}^+$. Together with the well-known energy splitting of the ground state of 12642.812 MHz [157] we calculate the isotope shift of the $^2P_{3/2}$ state given in Tab. 7.1. The uncertainty of 2.5 MHz for the isotope shift is again dominated by the error of the least-squares fit of the resonances (1 MHz) and the uncertainty of the cavity drift during the measurement time. For the uncertainty of the hyperfine constant, the cavity drift is less significant as we do not switch between isotopes during the experiment and thus are able to quickly switch between the measurement of the two hyperfine states.

During the spectroscopy of the $^2S_{1/2} \rightarrow ^2P_{3/2}$ transition, the $^2F_{7/2}$ state with a lifetime of $\tau > 10 \text{ yr}$ [114] is populated via decay of the $^2D_{5/2}$ state. After the state-detection, we pump population out of the $^2F_{7/2}$ state by excitation of the $^2F_{7/2} \rightarrow ^1D_{5/2,5/2}$ transition. We stabilize the laser to a wavelength-meter which yields a laser linewidth of better than 10 MHz. Efficient pumping out of the $^2F_{7/2}$ state is achieved in a frequency range of about $\pm 5 \text{ MHz}$ around the chosen lock point. The estimated uncertainty of 20 MHz consists predominantly of the laser linewidth and the uncertainty of the lock point. We only rely on the relative accuracy of the wavelength meter in a very small frequency range of a few GHz. We are confident that this relative accuracy is much better than the absolute accuracy of the wavelength meter which is specified to be 30 MHz. Comparison of the $5s^2^1S_0 \rightarrow 5s5p^3P_1$ transition in $^{88}\text{Sr}$ at 434.829121 THz [169] which we use for calibration$^2$ to the nearby D2 line in $^6\text{Li}$ at 446.799574 THz [170] corroborates this assumption.

To the best of our knowledge, this is the most complete (in terms of measured isotopes) and precise measurement of the isotope shifts of the $^2F_{7/2} \rightarrow ^1D_{5/2,5/2}$ transition. In $^{171}\text{Yb}^+$ we drive the transitions $|F = 4\rangle \rightarrow |F = 3\rangle$ and $|F = 3\rangle \rightarrow |F = 2\rangle$ (see Fig. 7.1(b)). We use sidebands at 3940 MHz to excite both transitions efficiently. We find that efficient pumping is achieved in a frequency range of 3930–3950 MHz.

With a hyperfine splitting of the $^2F_{7/2}$ state of 3620(2) MHz [116], we determine an energy splitting of the upper $^1D_{5/2,5/2}$ state of 320(20) MHz and a hyperfine constant $A(^1D_{5/2,5/2}) = -107(6) \text{ MHz}$. There seems to be no previous experimental data available for the $^1D_{5/2,5/2}$ hyperfine splitting, only a theoretical estimation of $A = 199 \text{ MHz}$ [171], which deviates significantly from the value we find in the experiment.

$^2$ Kindly made available by the group of Prof. Florian Schreck
7.3. Results

Figure 7.3.: Branching ratio measurement of the $^2P_{3/2}$ state. Plot of PMT counts during a 100 $\mu$s detection bin versus pulse width of a laser pulse ($t_{329}$), resonant with the D2 transition (blue) and background counts measured without an ion in the trap during the same 100 $\mu$s detection bin (yellow). From the decay time constant $\tau_{\text{dark}}$, we determine the combined decay probability to the $^2D$ states. From the ratio of fluorescence levels $n(D_{5/2})/n(D_{3/2})$, we determine the relative strength of the decays to the $^2D$ manifold. The inset shows a scan over the $^2S_{1/2} \rightarrow ^2P_{3/2}$ resonance at a saturation parameter of $s = 11$ (blue). For comparison the calculated non-saturated line is shown (yellow).

7.3.2. Branching fractions

To measure the branching fractions for decay out of the $^2P_{3/2}$ state, we excite the D2 transition with a short pulse of resonant light, followed by fluorescence detection of 100 $\mu$s duration. From the excited $^2P_{3/2}$ state, the ion decays either back to the ground state from where it may be excited to the $^2P_{3/2}$ state again, or to one of the metastable $^2D$ states.

During the subsequent fluorescence detection, an ion initially in the $^2S_{1/2}$ or $^2D_{3/2}$ state scatters light, while an ion in the $^2D_{5/2}$ state appears dark. By applying a pulse of light resonant with the D2 transition we transfer the population from the initial (bright) $^2S_{1/2}$ to a mixed state of $^2D_{3/2}$ (bright) and $^2D_{5/2}$ (dark). As a result, the photon scattering rate for $t_{329} = \infty$, $\nu_{\text{Ph}}^{(\infty)}$ is only a fraction of the initial rate $\nu_{\text{Ph}}^{(0)}$,

\[ \nu_{\text{Ph}}^{(\infty)} = \nu_{\text{Ph}}^{(0)} \times \frac{f(D_{3/2})}{f(D_{3/2}) + f(D_{5/2})}, \]

where $f(D_{3/2})$ and $f(D_{5/2})$ are the branching fractions into the $^2D_{3/2}$ state and $^2D_{5/2}$ state respectively.
Scanning the width of the resonant excitation pulse, we obtain the PMT counts versus pulse width plotted in Fig. 7.3. A least-squares fit of an exponential decay to the data yields a time constant $\tau_{\text{dark}} = 1.04(4) \mu s$ for the transfer from the initial bright $^2S_{1/2}$ state, to the mixed $^2D$ state with reduced fluorescence.

From the time constant $\tau_{\text{dark}}$ obtained by the fit, the lifetime of the $^2P_{3/2}$ state of $\tau_{p32} = 6.15(9) \text{ ns}$ [108] and the probability to be in the excited state during the laser pulse $p_{P_{3/2}} = 0.48(1)$, we determine the combined branching ratio to both $^2D$ states as follows:

$$p(^2D) = \frac{\tau_{P_{3/2}}}{p_{P_{3/2}} \times \tau_{\text{dark}}}$$

(7.2)

Additionally, we obtain the ratio of the fluorescence at $t_{329} = \infty$ to the initial fluorescence at $t_{329} = 0$ from the measured data as $\nu^{(\infty)}_{\text{Ph}} = 0.104(5)$ to $\nu^{(0)}_{\text{Ph}} = 0.74(2)$. According to Eq. 7.1, this corresponds to $f(D_{3/2})/f(D_{5/2}) = 0.16(1)$. Combining this with the result from Eq. 7.2, we determine branching fractions to the $^2D_{5/2}$ state and $^2D_{3/2}$ state of $1.08(5)\%$ and $0.17(1)\%$ respectively which is in agreement with theoretical predictions from Ref. [111]. The errors include the statistical uncertainties in $\tau_{\text{dark}}$, $\nu^{(0)}_{\text{Ph}}$, $\nu^{(\infty)}_{\text{Ph}}$ as well as uncertainties in the excited state population and the lifetime of the $^2P_{3/2}$ state.

The result is based on two independent measurements on different days. Fitting the individual results of these two measurement yields branching fractions to the $^2D_{5/2}$ state of $1.05(7)\%$ and $1.10(7)\%$ as well as branching fractions to the $^2D_{3/2}$ state of $0.17(1)\%$ for both measurements, which is well within the given uncertainties. As an additional consistency check we perform fits of subsets of the data, using only the even (uneven) time bins. The results are in agreement with the quoted uncertainties.

The saturation parameter $s$ and thus the excited state population probability $p_{p_{32}}$ in Eq. 7.2 is determined by a frequency scan over the resonance. We normalize the power in the $329 \text{ nm}$ beam during the scan by appropriate power settings of the AOM as described above. We choose a short pulse width of $t_{329} = 500 \text{ ns}$ to avoid saturation of
the decay to the \( ^2D_{5/2} \) state. We measure a saturation parameter of \( s = 11 \), the data is shown in the inset of Fig. 7.3. For the branching ratio experiment we tune the laser to resonance and operate the AOM at the frequency of maximum diffraction efficiency which allows us to increase the power in the laser pulse by a factor of 2.2 compared to the scan. Accordingly, we calculate a saturation parameter of \( s = 24(13) \) for the branching ratio experiment, corresponding to a probability of being in the excited state of \( p_{32} = 0.48(1) \). This scan is repeated frequently during the measurement to monitor intensity and frequency drifts.

The cumulative duration of the excitation pulse \( (t_{329} < 12 \mu s) \) and the detection bin \( (t_{det} = 100 \mu s) \) is small compared to the lifetimes of the \( ^2D_{3/2} (\tau > 50 \text{ ms} [113, 160]) \) and \( ^2D_{5/2} (\tau = 7.2 \text{ ms} [81]) \) states. The probability for a decay back to the ground state during that time is less than 0.3% and thus negligible compared to other experimental errors.

### 7.4. Conclusions

We reported on spectroscopic results on the \( ^2S_{1/2} \rightarrow ^2P_{3/2} \) transition in single trapped Yb\(^+\) ions. We find the branching fractions for decay of the \( ^2P_{3/2} \) state to the \( ^2D_{5/2} \) state and \( ^2D_{3/2} \) states to be 1.08(5)% and 0.17(1)%, respectively, in rough agreement with theoretical predictions from single electron methods.

The isotope shifts in the \( ^2S_{1/2} \rightarrow ^2P_{3/2} \) transition in Yb\(^+\) and hyperfine splitting (in \(^{171}\)Yb\(^+\)) of the \( ^2P_{3/2} \) state have been determined. Our results on both agree with previous results from Ref. [162] but are more precise by a factor of 5–9. Our results contradict theoretical predictions obtained from single valence electron approaches for the hyperfine splitting by a factor 2–3.

Calculations of the properties of electronic states in Yb\(^+\) are complicated because energetically low lying states with electrons excited from the \( f \)-shell can strongly interact with states with filled \( f \)-shell. In order to include states with unfilled \( f \)-shell in the calculations a many-electron approach is needed [164]. However, the methods for many-electron calculations are generally less precise compared to single valence electron calculations. In particular, the \( ^2P_{3/2} \) state has a completely filled \( f \)-shell, but mixes strongly with the energetically close \( ^3\left[3/2\right]_{3/2}^{o} \) state of the \( 4f^{135}d6s \) configuration. This mixing could explain the relatively large discrepancy between experiment and theory based on single electron methods [164].
Indeed, the hyperfine constant calculated by a many-electron approach [164] agrees much better with our experimental result. However, the theoretical prediction obtained with the many-electron method still deviates from our experimental result by many standard deviations. Precise knowledge of properties of states with strong mixing to states with holes in the $f$-shell such as the $^2P_{3/2}$ state measured in this work may thus serve as a testbed for many-electron methods in Yb$^+$. 
A.1. Reality checks of the simulation

In this section, we check the accuracy of the simulation algorithm used in chapter 2 in detail using realistic trapping fields that can be achieved in our experiment. A summary of the parameters used in the simulations unless noted otherwise can be found in table 2.1.

The functionality of the random number generation was checked by analysis of the distributions of initial atom coordinates for 10000 events sampled at $T_a = 2 \mu K$ on a sphere of $r_0 = 0.6 \mu m$. By definition, the spatial coordinates automatically lie on the sphere. It is therefore sufficient to check that each coordinate is uniformly distributed in the interval $[-r_0, r_0]$. For the velocities, the distributions of Eq. 2.21 must be obtained. As an example, distributions for $r_{a,1}$, $v_{a,r}$ and $v_{a,\phi}$ are shown in Fig. A.1.

Having a method for the energy determination at hand, it is of importance to check the negligible influence of the start and escape sphere sizes for the atoms. If the sphere radii are picked at the same order as the range of the atom-ion interaction, the immediate change in potential energy after the insertion and extraction of an atom leads to unrealistic kicks in the force on the ion. To check the influence of the sphere
radii on the ion temperature, the inner sphere radius $r_0$ was scanned between 0.2 and 1.8 $\mu$m. The thermalization of a single trapped ion initially at rest with a thermal cloud of atoms at $2 \mu$K was simulated. The outer sphere radius $r_1$ was chosen to be 0.5% bigger than $r_0$. An example for a thermalization curve (blue points) is shown in Fig. A.2 (left). The curve was obtained by averaging over 656 individual runs and fitted with an exponential (see Eq. 2.25) (black line) leading to an equilibrium temperature of $T_{\text{kin}} = 11.4(1) \mu$K on the characteristic time scale of $N_{\text{col}} = 607(2)$ collisions, using $T_0 = 0$ as the initial ion’s temperature. The ion’s energy distribution after thermalization is shown in Fig. A.2 (right). The blue points were obtained from all ion energies of the 656 runs between collision 5000 and 10000 and fitted with a thermal distribution (red, dashed) leading to a temperature of $9.4(2) \mu$K and a thermal distribution with fixed temperature (purple) obtained from the exponential fit (left). The ion’s energies deviate quite a bit from the thermal distributions, showing a longer tail towards high energies, which is a well known behavior [42, 43, 53, 68], caused by the additional kinetic energy due to the micromotion of the ion.

The final temperatures and characteristic number of collisions $N_{\text{col}}$ required for equilibration for the different starting radii are shown in Fig. A.3 and were obtained using the exponential fit model given by Eq. 2.25. For each point, at least 300 runs were averaged. The equilibrium temperature $T_{\text{kin}}$ of the ion shows no dependence on the starting sphere size $r_0$, whereas $N_{\text{col}}$ shows a quadratic behavior over the scanned range. This behavior can be qualitatively explained by the nature of Langevin collisions. For a given collision energy $E_{\text{col}}$, every atom with an impact parameter smaller than $b_c = (2C_4/E_{\text{col}})^{1/4}$ undergoes a Langevin collision and can therefore cause a large energy and momentum transfer that contributes to the thermalization process. The
Figure A.2.: Average kinetic energy of an ion colliding with atoms at 2 $\mu$K averaged over 656 runs to obtain the ion’s temperature (left) from an exponential fit (black) and distribution of the ion’s energies in units of $T_{\text{kin}}$ as defined in Eq. 2.22 after thermalization (right) along with a fitted thermal distribution (red, dashed) and a distribution where the temperature was fixed to the value obtained from the exponential fit (purple).

A fraction of atoms that undergo a Langevin collision $P_L$ and therefore fly into the solid angle element defined by $b_c$ is then given by $P_L = (1 - \cos \left( b_c / r_0 \right)) \approx 1 / 2 \left( b_c / r_0 \right)^2$. For an increasing $r_0$ this automatically demands for a quadratic increase in the required number of total collisions to equilibrate. Unless noted otherwise, $r_0 = 0.6 \mu$m is used in all further simulations as a trade-off between simulation time and realistic atomic densities (see e.g. [172]). Demanding only one atom at a time inside the sphere around one of the ions results in a density of $\rho_a = \frac{1}{16/3\pi r_0^3 \cdot N_{\text{ions}}} < 1.1 \cdot 10^{18} \text{ m}^{-3}$.

To realistically model the atom-ion interaction, one needs to check as well that the temperature of the ion does not strongly depend on the choice of the hard-core radius parameter $C_6$ as introduced in Eq. 2.18. In reality, a repulsive barrier is expected to be at a distance, where the electronic wavefunctions of the atom and ion begin to significantly overlap, typically in the range of hundreds of picometers to a few nanometers. The parameter $C_6$ was therefore scanned in a range between $5 \cdot 10^{-14} \text{ m}^2$ to $5 \cdot 10^{-21} \text{ m}^2$, effectively varying the position of the classical turning point $r_{\text{hc}} = \sqrt{2C_6}$ between 0.1 nm and 316 nm. The results for both final ion temperature $T_{\text{kin}}$ and collisions required for equilibration $N_{\text{col}}$ are shown in Fig. A.4. The points were obtained by averaging the ion’s average kinetic energy over at least 300 runs and fitting it according to Eq. 2.25. For a broad range of barrier radii the final temperature of the ion remains at the same level. For values bigger than $r_{\text{hc}} = 10 \text{ nm}$ the potential is more and more dominated by the repulsive term proportional to $C_6$, preventing Langevin collisions and therefore the ion from micromotion-induced heating as we describe it in our work Ref. [70], where a repulsive barrier is utilized to prevent exactly this heating.
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**Figure A.3.** Equilibrium temperature $T_{\text{kin}}$ as defined in Eq. 2.22 (left) and characteristic number of collisions $N_{\text{col}}$ (right) for an ion colliding with atoms at $2 \mu K$ versus the starting distance $r_0$ between atom and ion. While the equilibrium temperature does not depend on $r_0$ in the scanned regime, the characteristic number of collisions increases quadratically. The lines show a constant (left) and quadratic fit (right).

**Figure A.4.** Equilibrium temperature $T_{\text{kin}}$ as defined in Eq. 2.22 (left) and characteristic number of collisions $N_{\text{col}}$ (right) for an ion colliding with atoms at $2 \mu K$ versus the repulsive barrier radius $r_{hc}$. The red points were obtained using a higher numerical precision as explained in the text.

mechanism. For the smallest value of $r_{hc} = 0.1 \text{ nm}$, the ion temperature seems to be a factor of 1.5 higher than in the regime between 0.3 to 10 nm, which can be explained by numerical errors due to the increasing steepness of the hard core barrier for low values of $r_{hc}$ leading to large changes in acceleration in a hard core collision. Therefore, this point was simulated again with a five times smaller tolerance in the adaptive step-size Runge-Kutta propagator, leading to the red points, in agreement with the values for larger $r_{hc}$. The number of collisions required for thermalization $N_{\text{col}}$ seems to first slightly decrease for higher values of $r_{hc}$ but shows a dramatic increase by around a factor of two at $r_{hc} = 77 \text{ nm}$. Note that at this point the potential energy minimum caused by the attractive $C_4$-term of the potential becomes comparable to the collision
energy, dominated by the atom temperature of $2\,\mu\text{K}$. Therefore, the intermediately released kinetic energy during a Langevin collision becomes negligible. For even higher values of $r_{hc}$ the thermalization process speeds up again due to the quadratically increasing geometric cross section for repulsive collisions. For all further simulations, $r_{hc} = 1\,\text{nm}$ is used, which is around three times larger than the classical turning point of the Li-Yb$^{+}$ system [62, 80] but still produces similar results with less numerical effort due to the weaker forces involved.

During propagation, the Runge-Kutta propagator adjusts the size of the time steps in order to stay below a given relative accuracy parameter $p_{\text{tol}}$. It therefore propagates the system once by a full time step and once by two half time steps and compares the relative difference in propagated coordinates between both methods. If the maximum relative difference between one of the coordinates (including velocity) is bigger than the desired tolerance, the propagation step is repeated using an adjusted time step. To ensure a sufficiently small tolerance $p_{\text{tol}}$, further tests were performed. Firstly, the allowed tolerance was scanned from $p_{\text{tol}} = 10^{-5}$ to $10^{-15}$ as a parameter for the propagation of a single ion starting at a randomly chosen kinetic energy sampled from a thermal Distribution at $T_{\text{kin}} = 13\,\mu\text{K}$, leading to $E_{\text{kin}}/k_{B} = 20.5\,\mu\text{K}$ in the presented case. The trajectories including the velocities for the individual runs were stored to compute the relative deviation in kinetic energy for each tolerance with the one from the smallest value\(^1\), $p_{\text{tol}} = 10^{-15}$,

$$
\delta E_{\text{kin}}(p_{\text{tol}}) = \left| \frac{E_{\text{kin}}(p_{\text{tol}}) - E_{\text{kin}}(10^{-15})}{E_{\text{kin}}(10^{-15})} \right|.
$$

(A.1)

Because collisions with atoms can cause a dramatically different change in trajectory for each tolerance, no atoms were introduced in this test. The ions were propagated for 120 ms, a timescale that typically corresponds to 10000 collisions in the simulation. Due to the large amount of data, the trajectories were stored only during the last millisecond of propagation. The resulting relative deviations $\delta E_{\text{kin}}(p_{\text{tol}})$ are shown in Fig. A.5 (left). Due to the adaptive step-size algorithm, it is not possible to have the trajectories for each tolerance stored at the exact same time steps each, therefore the kinetic energy $\delta E_{\text{kin}}(10^{-15})$ was interpolated using cubic polynomials to match the time grid of the other tolerances, possibly leading to a small amount of interpolation noise. For clarity, only the values for $p_{\text{tol}} = 10^{-6}$ (green), $10^{-10}$ (blue) and $10^{-14}$ (red) are shown along with their time averages (straight lines). In Fig. A.5 (right) the time

\(^1\) Note that values of $p_{\text{tol}} < 10^{-15}$ can cause numerical instabilities due to the close by machine precision limit $\epsilon$ for which the numerical addition/subtraction $1.0 \pm \epsilon = 1.0$. On a 64-bit computer, $\epsilon \approx 2.22 \cdot 10^{-16}$ for double precision floating point numbers, according to the IEEE-754 standard.
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Figure A.5.: Relative deviations in kinetic energy for a single trapped ion for different values of the adaptive step-size algorithm tolerance $p_{\text{tol}}$ versus propagation time (left). For clarity only the values for $p_{\text{tol}} = 10^{-6}$ (green), $10^{-10}$ (blue) and $10^{-14}$ are shown in the left plot, along with the time averages (lines). The time averages for the other scanned tolerances are shown on the right, along with an exponential fit. Averaged deviations for the other values of $p_{\text{tol}}$ are shown, approximately following an exponential behavior (solid line) with exponent $n \approx 0.78$. While for a tolerance of $p_{\text{tol}} = 10^{-6}$ the time averaged relative deviation is $< 11\%$, $p_{\text{tol}} = 10^{-8}$ delivers acceptable values of $\langle \delta E_{\text{kin}}(p_{\text{tol}}) \rangle \leq 0.2\%$ already.

Similar to the tests for $C_6$ and $r_0$, also the influence of the tolerance parameter $p_{\text{tol}}$ on the final ion temperature $T_{\text{kin}}$ and required collisions $N_{\text{col}}$ to equilibrate was investigated. The results are shown in Fig. A.6. Each point was obtained from taking the average of $\bar{E}_{\text{kin}}$ over at least 300 individual runs and fitting the curves according to Eq. 2.25. Both observables do not change significantly from $p_{\text{tol}} = 10^{-12}$ to $10^{-6}$,

Figure A.6.: Final ion temperature $T_{\text{kin}}$ (left) and characteristic number of collisions required to equilibrate $N_{\text{col}}$ (right) for an ion colliding with atoms at $2\,\mu K$ versus tolerance parameter $p_{\text{tol}}$ used in the adaptive step-size propagator. The inset shows a magnified version of the plot from $p_{\text{tol}} = 10^{-12}$ to $10^{-6}$.
only the point at $p_{\text{tol}} = 10^{-5}$ shows a dramatic increase in both $T_{\text{kin}}$ and $N_{\text{col}}$ due to increasing numerical errors. For all further simulations $p_{\text{tol}} = 10^{-10}$ is used (unless noted otherwise) as a trade-off between precision and computational effort.

A final check for both energy conservation of the propagator during collisions as well as physical behavior of the system is to investigate the secular case, where the time-dependent trapping potential of the Paul trap is replaced by a 3D harmonic oscillator potential with the secular trap frequencies of the Paul trap. From a thermodynamic point of view, the ion should then thermalize to the same temperature as the atomic bath and the total energy during each collision should be conserved since no micromotion energy can be transferred to the secular oscillation. The resulting thermalization curve, averaged over 608 individual runs along with a histogram of the energy distribution is shown in Fig. A.7. The histogram was taken from all points between collision

![Figure A.7: Thermalization curve of a single ion trapped in harmonic oscillator potential colliding with atoms at 2 $\mu$K, using the secular trap frequencies of the employed Paul trap potential (left). The distribution of average kinetic energies according to Eq. 2.22 in units of $T_{\text{kin}}$ (right) shows a perfect thermal behavior. The exponential fit (left) as well as the fitted thermal distribution lead to a final temperature of $T_{\text{ion}} = 2 \mu$K.

3000 and 5000 and is in perfect agreement with a thermal distribution (solid line) at 2 $\mu$K, the same temperature as the atomic bath. Also the exponential fit of the thermalization curve (left) leads to the same value, thus indicating a correct physical behavior of the numerical model.

To finally investigate the energy conservation of the collisions, the energy transfer between atom and ion in each collision was investigated by comparing the atom and ion energies before and after a collision, at the points in time $t_0$ when an atom is introduced on the sphere with radius $r_0$ with the point in time $t_1$ when that atom escapes the sphere defined by $r_1$. The energy transfer on an ion trapped in the harmonic oscillator potential is shown in Fig. A.8 (right), taken from one of the 608 individual runs
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Figure A.8.: Change in energy of a harmonically trapped ion within each collision with atoms at 2 $\mu$K (left) and total change in energy of the atom-ion system for each collision (right). The solid line shows the averaged energy gain of the system per collision.

from the simulation used for Fig. A.7 (left). The plot shows the ion’s energy transfer $\Delta E_{\text{ion}} = E_{\text{ion}}(t_1) - E_{\text{ion}}(t_0)$ for each collision and ranges on scales limited by the atom energies. For the atom, a corresponding curve can be obtained. In Fig. A.8 (right) the level of energy conservation $|\Delta E_{\text{ion}} + \Delta E_{\text{atom}}|$ is shown. The averaged error in total energy in each step is less than 0.12 nK (dark blue line) and therefore negligible on the typical energy scales of the simulations. Note that this error is mainly caused by the sudden but tiny jump in potential energy when the atom is introduced and extracted. With reasonable effort this could be corrected in the energy determination and atom injection scheme, but is only of interest for much higher densities and lower temperatures that may anyways require a quantum mechanical treatment. We therefore conclude that the employed propagator produces physical results with reasonable precision.

A.2. Reality checks of the Fourier method

In this section, we check the accuracy of the presented Fourier method for determining the average kinetic energy of an ion crystal. Unless stated otherwise, we use a linear chain of four ions at around 100 $\mu$K and let them thermalize by collisions with a cloud of atoms at 2 $\mu$K.

To test the Fourier analysis method for obtaining the temperature of an ion crystal, we compare the temperature $T_{\text{fft}}$ of Eq. 2.37 with the temperature obtained from the average kinetic energy $T_{\text{kin}}$ (Eq. 2.22) as shown in Fig. A.9. For a step-size of $\Delta t_{\text{fft}} = 50$ ns, sufficient to resolve frequency components of up to $f_{\text{max}} = 20$ MHz,
there is no significant improvement when increasing the number of steps from 16384 (red) to 32768 (black), the relative deviation from $T_{\text{fft}}$ to $T_{\text{kin}}$ is at around 2.5% on average over a broad range of temperatures. This leads to the conclusion that a frequency resolution of $\Delta f_{\text{fft}} = 1/(N_{\text{fft}} \Delta t_{\text{fft}}) \approx 1.2 \text{ kHz}$ is a good choice.

To find a sufficient number of grid points while leaving the frequency resolution constant, we vary $\Delta t_{\text{fft}}$ inversely with $N_{\text{fft}}$, as shown in Fig. A.10. For all combinations with $\Delta t_{\text{fft}} \leq 200 \text{ ns}$, the relative deviation from $T_{\text{kin}}$ is approximately the same. At $\Delta t_{\text{fft}} = 400 \text{ ns}$ (gray) the maximum resolvable frequency is $f_{\text{max}} = 2.5 \text{ MHz}$, being too close to the micromotion sidebands at around $f_{\text{rf}} = 2 \text{ MHz}$ and therefore leading to a much lower energy, dominated by only the low frequency parts. To be on the safe side, we chose the combination $\Delta t_{\text{fft}} = 50 \text{ ns}$ and $N_{\text{fft}} = 16384$ for our system.

While during the collision processes very fast dynamics demanding for an adaptive step size algorithm may occur, the fastest timescale during the temperature determination is set by the micromotion oscillation at $f_{\text{rf}} = 2 \text{ MHz}$ in the case for $q_z^2 \ll 1$. Therefore, a fixed step-size propagator with $\Delta t_{\text{kin}} \ll 1/f_{\text{rf}}$ is sufficient. In order to save computation time, we use the same fixed step-size propagator for the Fourier transformation energy determination as for obtaining the average kinetic energy. We therefore choose the time grid to be integer subdivisions of the Fourier grid, $\Delta t_{\text{kin}} = \Delta t_{\text{fft}}/n, n \in \mathbb{N}$. To find a sufficiently small $\Delta t_{\text{kin}}$ to resolve the micromotion oscillations at $f_{\text{rf}} = 2 \text{ MHz}$, we compare the kinetic temperature as defined in Eq. 2.22 for different propagation
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Figure A.10.: Average kinetic energy of a four-ion crystal colliding with atoms at 2 µK (left) obtained by the Fourier method for several combinations of Fourier grid sizes \(N_{\text{fft}}\) and grid spacings \(\Delta t_{\text{fft}}\), resembling a variation of the maximally resolvable frequency \(f_{\text{max}}\). All curves besides for \(N_{\text{fft}} = 2048\) (gray) lie on top of each other, deviating from the average kinetic energy \(T_{\text{kin}}\) by less than 5% (right).

time steps \(\Delta t_{\text{kin}}\) with the temperature obtained using the smallest time step 2.5 ns as a reference. For time steps up to 40 ns we obtain relative deviations of less than 0.05% from the kinetic energy derived using time steps of 2.5 ns when averaged over 8 ms propagation time over the whole temperature range. To be on the safe side, we chose \(\Delta t_{\text{kin}} = \Delta t_{\text{fft}}/10 = 5\) ns.

A.3. Excess micromotion in a linear four-ion crystal

The obtained results for average kinetic energy and secular energy are shown in Fig. A.12. Each point was fit by averaging over at least 30 individual runs. The resulting average kinetic energies expressed as \(T_{\text{kin}}\) (left) follow approximately the same quadratic behavior as in the case of a single ion, indicating that the main part of the kinetic energy is stored in the micromotion. The quadratic fits (solid blue lines) lead to the increase parameters \(\theta_{E_{\text{rad}}} = 7.45(3) \mu K \cdot (V/m)^{-2}\), \(\theta_{E_{\text{ax}}} = 2705(15) \mu K \cdot (V/m)^{-2}\) and \(\theta_{\delta\phi_{rt}} = 4005(16) \mu K \cdot \text{mrad}^{-2}\), in almost perfect agreement with the single ion case. For all three cases the theoretical approximate energies due to the micromotion is shown as dashed blue lines. To verify the validity of these curves, the average kinetic energy for a crystal without atoms, initialized at zero secular temperature was simulated as well (red points). Only for the case of radial excess micromotion the theoretical prediction (dashed blue) deviates significantly from the red points, indicating the approximate nature of the prediction at high radial micromotion amplitudes.
### A.3. Excess micromotion in a linear four-ion crystal

#### Figure A.11.

Visualization of the normal mode movement for a trapped linear four-ion crystal in descending order with respect to the eigenmode frequency. The arrows indicate the direction and amplitude of the respective mode. The modes are shown along with their respective eigenfrequencies \( f_{th} \) obtained from the diagonalization of the secular approximation and the values \( f_{fft} \) obtained numerically from Fourier analysis of the mode spectra. Typical names of the modes are shown on the right column. The center-of-mass (c.o.m.) modes represent the upper and lower limit of the frequencies.

<table>
<thead>
<tr>
<th>movement</th>
<th>( f_{th}^{th} ) [kHz]</th>
<th>( f_{fft}^{fft} ) [kHz]</th>
<th>mode name</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>154.0</td>
<td>153.8(6)</td>
<td>x c.o.m.</td>
</tr>
<tr>
<td></td>
<td>152.8</td>
<td>152.6(6)</td>
<td>y c.o.m.</td>
</tr>
<tr>
<td></td>
<td>148.0</td>
<td>147.7(6)</td>
<td>x tilt</td>
</tr>
<tr>
<td></td>
<td>146.8</td>
<td>146.5(6)</td>
<td>y tilt</td>
</tr>
<tr>
<td></td>
<td>139.2</td>
<td>139.2(6)</td>
<td>x drum</td>
</tr>
<tr>
<td></td>
<td>137.9</td>
<td>137.9(6)</td>
<td>y drum</td>
</tr>
<tr>
<td></td>
<td>129.4</td>
<td>129.4(6)</td>
<td>z anti-stretch</td>
</tr>
<tr>
<td></td>
<td>127.4</td>
<td>127.0(6)</td>
<td>x zigzag</td>
</tr>
<tr>
<td></td>
<td>126.0</td>
<td>125.7(6)</td>
<td>y zigzag</td>
</tr>
<tr>
<td></td>
<td>102.3</td>
<td>102.5(6)</td>
<td>z egyptian</td>
</tr>
<tr>
<td></td>
<td>73.5</td>
<td>73.2(6)</td>
<td>z stretch</td>
</tr>
<tr>
<td></td>
<td>42.4</td>
<td>42.7(6)</td>
<td>z c.o.m.</td>
</tr>
</tbody>
</table>
Figure A.12.: Average kinetic energy of a linear four-ion crystal colliding with atoms at 2 µK (left, blue) expressed as $T_{\text{kin}}$ and temperature of the secular motion (right) versus micromotion causing parameters. The results for the kinetic energy were fit with quadratic function (solid blue curves). The dashed blue curves show the approximate theoretical amount of energy stored in the excess micromotion according to Eqs. 2.10, 2.13 and 2.17 respectively. The red points correspond to simulated values for the non-interacting case, in approximate agreement with the theoretical behavior. The dashed gray lines indicate the $s$-wave temperature limit. The secular part of the average kinetic energy is shown on the right. The insets show the difference between the solid and dashed blue curves, resembling the micromotion-induced heating. Green points were obtained using a fixed starting/escape sphere, blue with a comoving sphere.
To quantify the micromotion-induced heating effect on the secular motion, the secular temperature was extracted as described in section 2.5. In all three cases the dependence on the scanned parameter seems to be a bit weaker than quadratic. The temperature dependence of the individual modes is discussed in section 2.6.4.

In all three cases, the number of collisions required to equilibrate (not shown in the figures) show a similar behavior as in the single ion case, besides the fact that they are $N_{\text{ions}} = 4$ times higher because of the reduced effective density of atoms.

### A.4. Photodiode comparator box

To avoid damage of the ion trap due to misaligned dipole trapping beams, we monitor the difference in power between the ingoing and outgoing path. If the power between the beams shows a significant difference, the laser shuts down automatically by an interlock signal. We therefore use two infrared sensitive photodiodes\(^2\), one behind the last mirror before the trapping beam enters the vacuum system for the first time (PD1) and one behind the first mirror after the trapping beam exits the vacuum system for the second time (PD2), effectively measuring the transmission of these mirrors, which can be easily on the order of 100 mW. The photodiodes are connected to a homebuilt circuit board. Within the circuit, the photocurrent is measured as the voltage drop across a variable resistor from 100 – 110 kΩ to adjust for small differences of the mirror’s transmission coefficients. The photovoltages $U_{\text{PD1,PD2}}$ are then buffered with a unity gain operational amplifier (OPA551) each and fed into a differential amplifier (INA117P). The differential amplifier also takes an additional offset voltage $U_{\text{of}}$ and produces $U_D = U_{\text{PD2}} - U_{\text{PD1}} + U_{\text{of}}$ as an output voltage. The offset voltage can be set with a potentiometer to be from 0 – 120 mV and ensures that the difference $U_D > 0$ V in normal operation. Finally, a comparator (LM393) is used to compare $U_D$ with 0 V. In normal operation, the comparator produces an output voltage of 24 V. In the case of an obstacle between PD1 and PD2 leading to a drop in $U_{\text{PD2}}$, the difference voltage drops below 0 V and the comparator follows to 0 V within less than a millisecond as an output, leading to a shutdown of the dipole trap laser. By carefully choosing the offset voltage, one can also ensure a shutdown when dust particles accumulate on the optics and viewports between PD1 and PD2. For alignment, the output voltage can be set manually to 24 V, overriding the photodiode signals. Note that the circuit board was

\(^2\) Thorlabs SM1PD1A
A. Appendix

Figure A.13.: Circuit diagram for a photocurrent comparator box. The circuit measures the photocurrent as a voltage drop across variable resistors for up to three photodiodes (PD0-2) and produces 24 V or 0 V as an output voltage, depending on the sign of the voltage differences between PD2 and PD1 as well as PD1 and PD0. Both voltage differences can be shifted by up to +120 mV using the potentiometers $R_{00,01}$. The input voltages for the IC’s are produced by the simple voltage regulator circuit from a bipolar ±24 V source as shown in the inset. All IC’s supply voltage inputs are equipped with a 100 nF bypass capacitor, which is not drawn for simplicity.

designed to accept one more photo diode input (PD0) to monitor power loss also on other parts of the beam path. A schematic can be found in Fig. A.13.
A.5. Calculation of magnetic fields

In order to precisely calculate the magnetic field $\vec{B}$ of a coil, we make use of the Biot-Savart law,

$$\vec{B} = \nabla \times \vec{A} = \frac{\mu_0}{4\pi} \int \mathrm{d}^3 r' \nabla \times \frac{\vec{J}(r')}{|\vec{r} - \vec{r}'|}$$  \hspace{1cm} (A.2)$$

which can be derived from Maxwell’s equations. Here, $\mu_0$ denotes the vacuum permeability and $\vec{J}$ the current density. For a simplified calculation, we assume infinitely thin wired, which is justified because the distance to the atoms in the experiment usually is much larger than the coil wire diameter. Equation A.2 then simplifies after some work to the following expressions for the axial and radial field components $B_z$ and $B_r$ of a single wire loop with diameter $r_0$ and a distance $z_0$ from the origin

$$B_z = \frac{\mu_0 I}{(2\pi)\sqrt{(r_0 + r)^2 + (z - z_0)^2}} \left( K\left(\frac{r_0^2 - r^2 - (z - z_0)^2}{(r_0 + r)^2 + (z - z_0)^2}\right) + \frac{4\pi r_0}{(r_0 + r)^2 + (z - z_0)^2} E\left(\frac{4\pi r_0}{(r_0 + r)^2 + (z - z_0)^2}\right) \right)$$

$$B_r = \begin{cases} \frac{\mu_0 I (z - z_0)}{(2\pi)\sqrt{(r_0 + r)^2 + (z - z_0)^2}} \left( \frac{(z - z_0)^2 + r^2}{(r_0 + r)^2 + (z - z_0)^2} E\left(\frac{4\pi r_0}{(r_0 + r)^2 + (z - z_0)^2}\right) - K\left(\frac{4\pi r_0}{(r_0 + r)^2 + (z - z_0)^2}\right) \right), & r > 0 \\ 0, & r = 0 \end{cases}$$  \hspace{1cm} (A.3)$$

with the elliptic integrals

$$K[m] = \int_{0}^{\frac{\pi}{2}} \frac{d\theta}{\sqrt{1 - m \sin^2 \theta}}, \quad m \in (0, 1)$$

$$E[m] = \int_{0}^{\frac{\pi}{2}} \sqrt{1 - m \sin^2 \theta} \, d\theta, \quad m \in (0, 1)$$  \hspace{1cm} (A.5)$$

which can be evaluated efficiently using for example Wolfram Mathematica’s built in functions EllipticK[m] and EllipticE[m].
A. Appendix

A.6. Circuit diagram of the H-bridge driver

This section contains the circuit diagram of the H-bridge driver used to switch the polarity of the lower MOT coil and the lower Feshbach coil.

Figure A.14.: Circuit diagram for empowering the Intersil HIP4081a H-bridge driver IC as it is used to switch the polarity of the lower Feshbach and lower MOT coil in our experiment. The polarity and disable TTL inputs are isolated with TIL111 optocouplers. For the MOT coil, the disable input (pin 3 of the IC) is connected to ground, as no fast switch off is required. The polarity switch needs to be provided as original and inverted signal at pin 5 and 6. Pin 8 and 9 can be used to set a delay between the gate output voltages. The outputs to the high side MOSFET gates (pin 11 and pin 20) are equipped with fast bootstrap diodes and large capacitors to ensure a quick pump of charge to the gates, according to the application notes [173]. Pin 12 and 19 are connected to the source pins of the high side MOSFETs. For the low side MOSFET gates (pin 13 and 14, 17 and 18), no charge pump circuit is required, as the power supply ground of the coils is shared with the H-bridge driver, thus pin 14 and 17 are effectively connected to ground.
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Samenvatting

Dit proefschrift beschrijft een experimentele opstelling die gebruikt wordt om ultrakoude $^6$Li atomen te creëren en te overlappen met laser-gekoelde Yb$^+$ ionen. De opstelling is ontworpen om het zogenaamde quantum regime van wisselwerkende atomen en ionen te onderzoeken. Het quantum regime is nog in geen enkel experiment bereikt omdat de elektrische velden die de ionen op hun plaats houden voor opwarming kunnen zorgen. Dit komt omdat ionen in een Paul val een zeer snelle microbeweging ondergaan. Tijdens een botsing met een atoom kan er energie worden overgedragen op de ionen-atomen mix, waardoor het systeem niet koud genoeg is om het quantum regime te bereiken. Recentere berekeningen hebben laten zien dat dit effect kan worden tegen gegaan door hele zware ionen te gebruiken in combinatie met lichte atomen. In ons experiment gebruiken we Yb$^+$ ionen en $^6$Li atomen, met een massa verhouding van 24-29 (afhankelijk van het gebruikte Yb$^+$ isotop). Dit is de grootste massa verhouding die bereikt kan worden met elementen die eenvoudig te laser koelen zijn. Gedurende mijn onderzoek is het quantum regime helaas nog niet bereikt, maar ik kon wel aantonen dat aan de experimentele opstelling slechts enkele kleine verbeteringen moeten worden aangebracht voordat het regime wel bereikt kan worden, zoals beschreven in hoofdstuk 2. Ik heb ook gekeken naar de spin van een enkel ion terwijl het botsingen ondergaat met een wolk van koude, gepolariseerde atomen (hoofdstuk 6). Ik heb gemeten dat de spin van het ion zich al na enkele botsingen uitricht in de richting van dat van de atomen. Deze resultaten hebben we vergeleken met voorspellingen gebaseerd op moleculaire structuur en verstrooiing berekeningen van Dr. Michal Tomza. Ondanks het feit dat de metingen ver buiten het quantum regime zijn verricht geven de resultaten verrassend genoeg toch een indicatie van wat er kan gebeuren als het quantum regime wordt bereikt. De resultaten wijzen op het bestaan van magneto-moleculaire of Feshbach resonanties tussen atomen en ionen in het quantum regime. Deze resonanties spelen een belangrijke rol in de fysica van ultrakoude neutrale atomen, waar ze gebruikt worden om de interactie tussen atomen af te stemmen. De uiteindelijke observatie van Feshbach resonanties tussen atomen en ionen zou een belangrijke stap betekenen in de atoomfysica, omdat het allerlei nieuwe mogelijkheden geeft voor het bestuderen van quantum veel-deeltjes fysica en applicaties in quantum technologie.

Het proefschrift beantwoord specifiek de volgende wetenschappelijke vragen:

- Ik heb berekend dat het quantum (of s-wave) regime binnen bereik moet zijn in ons systeem, rekening houdend met realistische experimentele parameters. Wat betreft de atomen heb ik experimenteel vastgesteld dat het quantum regime kan
worden bereikt, door een ultrakoud Li gas te maken op de locatie van de ionen. Om de ionen koud genoeg te maken moeten er enkele verbeteringen worden aangebracht aan het experiment, zodat zogenaamde excess microbeweging beter gedetecteerd en gecompenseerd kan worden. Ook zal het nodig zijn om onze temperatuur meting van het ion te verbeteren, zodat we kunnen bewijzen dat het quantum regime bereikt is. Hiervoor kan de laser bij 329 nm (de D2 lijn van \( \text{Yb}^+ \)) gebruikt worden. Een studie van de spectroscopie van de D2 lijn is ook onderdeel van dit proefschrift (hoofdstuk 7).

- We hebben gemeten dat de spin van het ion snel uitgewisseld wordt met dat van de atomen tijdens botsingen. We hebben ook gemeten dat sommige botsingen de totale spin niet conserveren (zogenaamde spin relaxatie). We kunnen echter niet erg nauwkeurig vast stellen of dit misschien komt omdat er zich atomen met de verkeerde spin ophouden in de atoom wolk, waardoor het slechts lijkt alsof de spin niet geconserveerd is. We houden daarom de gemeten waarschijnlijkheid aan als bovenste limiet. Nieuwe metingen met atomen gevangen in de dipool val waarmee we betere controle hebben over de atomen (beschreven in hoofdstuk 5) zullen uitwijzen wat de werkelijke relaxatie waarschijnlijkheid per botsing is. Overigens komt de gemeten waarschijnlijkheid wel ruwweg overeen met theoretische voorspellingen.

- Door de metingen te vergelijken met moleculaire structuur en verstrooiing berekeningen hebben we achterhaald dat de snelle uitwisseling het gevolg is van een groot verschil tussen de zogenaamde singlet en triplet verstrooiingslengte in \( \text{Yb}^+/^6\text{Li} \). Dit is een erg belangrijk resultaat omdat dit erop wijst dat er brede Feshbach resonanties zouden moeten bestaan in het quantum regime, en bij experimenteel realiseerbare magneetvelden.
Summary and outlook

This thesis describes an experimental setup for preparing an ultracold cloud of $^6\text{Li}$ atoms, overlapped with trapped, laser-cooled Yb$^+$ ions. The apparatus was designed to explore the so-called quantum regime of interacting atoms and ions. This regime has not been reached in any experiment up until now, because the electric fields used for trapping the ions can cause heating. In particular, the ions undergo rapid driven motion (micromotion) when kept in a Paul trap, from which energy can be transferred to the atom-ion mixture when a collision occurs. Calculations show that this effect may be mitigated by using a heavy ion and a light atom. In our experiment, we use the ion-atom combination with the largest mass ratio that allows for straightforward laser cooling, Yb$^+$/\(^6\text{Li}\), giving a mass ratio of 24-29 (depending on the ionic isotope).

During my research, the quantum regime was not reached yet in our setup, but I could demonstrate that only a few improvements should be made to achieve this goal. Besides this, I studied the spin of a single ion held in a cold cloud of spin-polarized atoms and found that the spin of the ion aligns with that of the atoms after only a few collisions. We compared these measurements to molecular structure and scattering calculations performed by Dr. Michał Tomza. Surprisingly, even though the measurements were performed well outside the quantum regime, the results do give an indication of what could happen when the quantum regime were reached. In particular, the results suggest the existence of broad magneto-molecular (Feshbach) resonances in the ultracold regime. These resonances play a pivotal role in ultracold neutral atomic systems for tuning the interactions between atoms, but have never been seen between atoms and ions. The observation of Feshbach resonances between atoms and ions will have a huge impact on atomic quantum physics as it will open up completely new possibilities in studying quantum many-body physics as well as in quantum technology.

Specifically, this work answers three scientific questions.

- We calculated that our system can reach the quantum (or s-wave) regime of atom-ion collisions, taking into account realistic parameters and levels of micromotion that should be within reach. We have demonstrated experimentally that the requirements for the atoms can be achieved by creating an ultracold atomic cloud within the ion trap. For the ions, minor improvements on the ion trap are needed to compensate so-called excess micromotion. The implementation of improved micromotion detection and temperature determination schemes
Summary and outlook

will be crucial for proofing thermalization below the \( s \)-wave temperature. The \( 329 \text{ nm} \ ^2S_{1/2} \rightarrow ^2P_{3/2} \) transition that was investigated in this work could serve for Raman thermometry to achieve this.

- We found that the ionic spin rapidly exchanges with the atomic spin. Apparent spin-nonconserving relaxation rates may be due to impurity atoms in the wrong spin state. Thus, the measured rates can only be seen as an upper limit. So far, our combination of species shows the highest ratio of spin exchange to spin-relaxation rates of all systems. Further insight on the spin-relaxation and spin-coherence within an atomic bath could be obtained by employing the recently realized optically trapped atomic cloud, that allows for better control.

- By employing \textit{ab initio} quantum scattering calculations, we find that the large spin-exchange rates result from a large difference between triplet and singlet scattering length, surprisingly even for collision energies far above the \( s \)-wave limit. As an encouraging result, this points towards the existence of broad Feshbach resonances close to the \( s \)-wave limits at experimentally feasible magnetic fields.

Detailed summary

In chapter 2 we employed classical Monte-Carlo simulations of the atom-ion scattering process, involving realistic parameters that can be reached in our experiment. We found that for the hypothetical case of optimal micromotion compensation, the collision energy between atoms and ions is on average much lower than the \( s \)-wave energy threshold \( k_B T_s \) of the system. For the micromotion limits measured, we computed collision energies 2-11 times higher than the \( s \)-wave energy, leading to the conclusion that with modest improvements in detection and compensation, the quantum regime of ultracold collisions should be within reach. Further, we analyzed the collision dynamics of a linear ion crystal with ultracold \( ^6 \text{Li} \) atoms and found very similar limits and cooling dynamics. For the case of a two dimensional ion crystal, we presented a method for sympathetic cooling with dramatically reduced micromotion induced heating by only immersing the central ion, sitting in the rf node of the trapping field.

We presented the setup of our experiment in chapter 3. We described in detail the hybrid atom-ion vacuum system and the trap, the magnetic field generation and switching and the complex optical-, laser and microwave setup required to trap and cool both
$^6\text{Li}$ and Yb$^+$. Further, we outlined the hardware and software used to control the experiment.

In chapter 4 we presented the tools and techniques required for trapping, cooling, state preparation and detection of $^{171}\text{Yb}^+$ and $^{174}\text{Yb}^+$. We employed the ions as a tool to calibrate the magnetic fields and to estimate the local vacuum condition within the ion trap. Further, we characterized the ion trap setup, including trap frequency, excess micromotion and heating rate measurements, providing the experimental input for chapter 2.

The preparation of the atomic sample was described in chapter 5. We presented the sequence required to create an atomic cloud of $^6$Li and to transport it magnetically into the ion trap as it was used for the measurements in chapter 6. Further, we implemented an optical dipole trap and presented the first successful evaporative cooling results within the ion trap, reaching atom temperatures far below the $s$-wave limit of atom-ion collisions.

Motivated by the idea of a buffer-gas cooled qubit, we investigated the behavior of the ionic spin in a spin polarized atomic bath within chapter 6. We found large spin-exchange rates of the ion, leading to the polarization of the ion’s spin parallel to the polarization of the atoms. The measured spin-relaxation rates form an upper limit, as apparent spin-nonconserving collisions could in fact be spin-allowed collisions with atoms accidentally prepared in a lower spin state. We modeled the system using ab-initio quantum scattering calculations, from which we conclude that the fast spin exchange rates result from a large difference between singlet and triplet scattering lengths. Thus, the existence of broad Feshbach resonances in atom-ion scattering can be expected for our combination of species.

In chapter 7 we performed spectroscopic measurements on both, the 329 nm $^2S_{1/2} \rightarrow ^2P_{3/2}$ and 638 nm $^2F_{7/2} \rightarrow ^1D[5/2]_{5/2}$ transition, for all stable Yb$^+$ isotopes except $^{173}\text{Yb}^+$. We also measured the branching fractions from the excited $^2P_{3/2}$ state to $^2D_{3/2}$ and $^2D_{5/2}$ and the hyperfine constants of $^2P_{3/2}$ and $^1D[5/2]_{5/2}$ for the isotope $^{171}\text{Yb}^+$. The results improve previously published data by a factor of 5 to 9. This will be beneficial when using the 329 nm laser in Raman configuration and when adding a 411 nm shelving laser, driving the $^2S_{1/2} \rightarrow ^2D_{5/2}$ transition, as here the low lying $^2F_{7/2}$ state is populated.
Future plans and improvements

The loading and cooling efficiency of the atomic $^6$Li sample is sufficient for attaining the quantum regime of atom-ion collisions for now. Thus, adding more complexity to the optical setup is not required for the observation of atom-ion interactions in the $s$-wave regime. For the determination of the shape of atom-ion Feshbach resonances the stability of the magnetic fields should be characterized and potentially optimized via active control loops. For future experiments such as studying the interaction of a molecular BEC with the ion, cancellation of the residual magnetic field curvatures may be required.

The limiting factor for reaching the quantum regime in the current setup is the average kinetic energy of the ions, caused by micromotion induced heating during thermalization of the ion with the atoms as we have seen in chapter 2 and 4. Nevertheless, the prospects of reaching $s$-wave collision energies are good as the desired levels of micromotion lie within values reported in literature [89] and the required improvements rely on the implementation of established compensation and detection techniques [72]. A first major improvement will be the addition of two pairs of compensation electrodes in the horizontal plane of the ion trap to have full control over the radial stray electric fields. In fact, a copy of our ion trap has been manufactured and modified recently to fulfill these requirements. Additionally, to improve the micromotion detection techniques, a 411 nm laser system has now been implemented to perform micromotion sideband-resolved spectroscopy on the 22 Hz wide $^2S_{1/2} \rightarrow ^2D_{5/2}$ clock transition in Yb$^+$ [81]. As we have seen in chapter 2, thermalization requires around 35–38 Langevin collisions when the ion is initially at rest, corresponding to no secular energy. In the current setup, we estimate the energy of the ion to be much larger, on the order of the Doppler temperature $T_D = 0.5 \text{ mK}$. In Sect. 4.10 we indeed found $T_{\text{ion}} \approx 4 \text{ mK}$. To reduce the number of collisions required to thermalize with the atomic bath it is thus beneficial to add an additional cooling stage for the ion, e.g., by employing resolved-sideband Raman cooling [174] by using the 329 nm laser, which is planned.

A completely different approach to tune the interaction strength between atoms and ions is the use of Rydberg-dressed atoms [34, 70], which we recently started to implement [98, 175]. Here the idea is to Rydberg-dress the atomic cloud, thus increasing the polarizability of the atoms. As the atom-ion interaction potential is directly proportional to the polarizability, this gives a handle to tune the interaction over a broad range by just changing the detuning and intensity of the dressing laser.
Submitting this work would not have been possible without the outstanding support of my family and especially my parents during my entire studies. Thank you for being there.

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After finishing my diploma thesis, luckily Dr. René Gerritsma could convince me to start a PhD in his new group, where I could learn many new things and thank you for giving me this opportunity, your support and a great time. During the first two years we had to challenge many things not being directly related to physics, e.g. ordering, soldering, milling, designing, building which was a great variety from my former theory work. Thanks to my amazing colleagues René, Jannis, Norman, Thomas S., Thomas F., Juan and Henrik, we could set up a machine that most of the time worked and when something failed we never ran out of ideas to improve it, such that the machine started to deliver results during the last two years and will hopefully continue to do in the following projects, hopefully also with continued great theory support from Dr. Michał Tomza. Also I need to thank the group of Prof. Selim Jochim for sharing lots of their experience and ideas and their help in the design phase of our experiment. It was a good experience seeing this machine growing and working and being part of the team, inside and outside the university, thank you!

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List of publications

*Trapped ions in an ultracold Rydberg gas.*

*Prospects of reaching the quantum regime in Li-Yb+ mixtures.*

*Dynamics of a single ion spin impurity in a spin-polarized atomic bath.*

*Spectroscopy of the $^2S_{1/2} \rightarrow ^2P_{3/2}$ transition in Yb II: Isotope shifts, hyperfine splitting, and branching ratios.*

*Observation of collisions between cold Li atoms and Yb+ ions.*

*Trapped ions in Rydberg-dressed atomic gases.*

*Controlling the transport of an ion: classical and quantum mechanical solutions*