Ion beams from laser-cooled gases

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Ion Beams
from
Laser-cooled Gases

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- Chapter 2:

- Chapter 4:

- Chapter 5:
High-brightness ion sources are crucial for a variety of applications [1], in particular focused ion beam (FIB) systems, in which an ion beam is focused on a sample to a spot that can be as small as a few nanometers. This small spot size makes FIB systems a popular tool for manipulation or examination on the nano-scale. To reach even higher resolution, the quality of the available ion source must be improved. In this thesis a novel beam source is presented that should be able to bring about such improvements. The new source is based on extracting ions from a laser-cooled atomic gas. This source will be described in detail in the next chapters. In this introduction we will give a short overview of existing high-brightness ion sources, their properties and applications.

1.1 Applications of Focused Ion Beams

A scanning electron microscope (SEM) is nowadays an important tool to visualize the microscopic world. This well known electron microscope uses a focused electron beam that is scanned in a raster over the surface of a sample. These incoming electrons interact with the atoms on the sample so secondary electrons are emitted, which contain information about the sample. By detecting these electrons at every raster position of the focused electron beam, an image of the surface can be obtained.

A focused ion beam (FIB) system works very similar as a SEM, but has one clear difference: instead of a focused electron beam it uses a focused ion beam. In both techniques information about the sample can be obtained by detecting particles that leave the sample due to the interactions with the incoming particle beam. In the case of a thin sample, also transmitted particles can be detected. High spatial resolution can only be obtained if both the probe, as well as the effective interaction area inside the sample, are small.
Electrons, at typical operation conditions, do not remove atoms from a sample. For ions, this is strongly dependent on their mass. Heavy ions, which carry a lot of momentum, will sputter atoms much more efficiently than light ions. These light ion species (e.g. He and Li) are therefore very suitable for imaging purposes without directly damaging the sample [2]. In addition, these ions have a small interaction surface area, so high resolution is obtainable. Heavy ion species on the other hand, can, besides imaging, also be used for manipulation of a sample by sputtering away material at a small scale. By detecting and analyzing the removed atoms, even more information about the composition of the sample can be obtained.

In the remainder of this section three relevant techniques will be briefly discussed. First a description of the most common FIB with relatively heavy ions, mainly used for sample manipulation such as micro-machining, will be presented. Secondly, the technique Secondary Ion Mass Spectroscopy (SIMS) that is used to analyze the sample composition is discussed. Finally, a recently developed FIB that uses light He-ions, which can be used as a high resolution microscope, is briefly described.

### 1.1.1 Micro-machining and deposition

The most common focused ion beam systems are based on a gallium Liquid Metal Ion Source (LMIS), which will be discussed in more detail in section 1.2.2. Over the last two decades FIB systems with this source have become an important tool in a wide array of material science and technological applications because they offer both high-resolution imaging as well as micro-machining capabilities [3, 4]. In these systems a Ga-ion beam with energies between 10 and 50 kV is used, with currents ranging from 1 pA to 10 nA [5], that at low current can be focused to a spot size of about 10 nm. When the ions hit the surface, material will be sputtered away, enabling precise machining. Also indirect manipulation of the sample becomes possible if a gas-injection system is added, enabling ion-beam activated deposition and enhanced etching. By combining all these functions a FIB becomes a versatile instrument to perform manipulation at the nano scale.

A schematic overview of a FIB system is depicted in Fig. 1.1. The ions are produced by the ion source on top of the column. The beam is collimated with a condenser lens and is then partially clipped by an adjustable aperture to select the operating current. This beam is then focused onto the sample by the objective lens. Close to the sample a secondary electron detector and gas injection system are present. The beam can be scanned over the sample surface by using the deflector.

Nowadays most systems are dual beam machines that are equipped with a FIB column together with a SEM column. The electrons can be used for the highest resolution imaging without damage, while the ions can be used for sample preparation. For instance, a small cross section can be cut out of the sample with use of the ions that can be subsequently imaged with the electrons. By repetition of such a procedure and combining many images, a 3D model of the sample can be obtained [6].

In the semiconductor industry FIB systems are mainly used for failure analysis [7], mask
Introduction

1.1 LMIS Extractor

1.1.1 Ion beam Condensor lens

1.1.2 Objective

1.1.3 Sample Detector

1.1.4 Gas injector lens

1.1.5 Aperture

1.1.6 Deflector

1.1.7 Objective lens

1.1.8 Gas injector

1.1.9 Sample

**Figure 1.1:** Overview of focused ion beam (FIB) system based on a Ga-liquid metal ion source (LMIS).

repair [3], and circuit editing [5]. For example, with a FIB a wire in an integrated circuit can be cut, while new conductive connections can be created with gas-assisted deposition. This enables faster testing and localization of problems in new chip designs.

At this moment the minimal spot size of these gallium FIB systems is limited by the chromatic aberrations in the lens column due to the energy spread in the ion beam [4]. Furthermore the Ga ions contaminate the surface and can change the electrical and magnetic properties [8] and can also induce strain in the material [9]. A new ion source with lower energy spread and with a different heavy ion species is thus desirable.

### 1.1.2 Secondary Ion Mass Spectroscopy

Chemical information about the top layer of a sample, including elemental composition and chemical structure, can be obtained by analyzing the secondary ions that are removed from the sample by a primary FIB. This is done in the technique (static) Secondary Ion Mass Spectroscopy (SIMS) where the mass spectrum of these ions is acquired. There are three basic mass analyzer types: sector field based, quadrupole based and time-of-flight based [10]. This last technique has the highest sensitivity and will now be discussed in some more detail.

This type of SIMS requires a pulsed focused ion beam on the sample. A schematic
overview of a ToF-SIMS is given in Fig. 1.2. The incoming pulsed ion beam removes and
ionizes material on the surface of the sample. The secondary ions are then accelerated in a
flight tube towards a detector. Particles with the lowest mass will reach the detector before
particles with a higher mass. By recording the distribution in time, the different elements
can be distinguished and a mass spectrum is obtained.

To get a high spatial resolution, it is important that the incoming ion beam can be
focused to a small spot with enough ions per pulse to have enough signal. To get a high mass
resolution, the pulse length of the incoming primary ion beam has to be short [11]. There
is always a compromise between spatial and mass resolution, due to fundamental as well as
practical reasons. Fundamental reasons, such as dose limitations, limit the obtainable signal
from a small spot. Practical reasons, such as increased energy spread for shorter bunches, lead
to larger focal spots. Additionally, heavy incoming ion species are preferred so sputtering
becomes more efficient. An ion source of a heavy ion species that can generate short ion
bunches, which can also be focused to a small spot on a sample is thus desirable.

1.1.3 Ion-Microscopy

When, instead of a heavy ion species, a light ion species is used in a FIB, it becomes a very
interesting alternative for an electron microscope. Due to the development of a commercial
high brightness helium source, which will be discussed in more detail in section 1.2.3, a helium
microscope has been recently developed [12]. It has some significant advantages compared to
a scanning electron microscope (SEM).

The obtainable resolution is always a compromise between different mechanisms that limit
the resolution, such as between diffraction and chromatic or spherical aberrations. This is
illustrated in Fig. 1.3 for a SEM, where the three contributions are schematically represented
in a log-log plot. The spot size contributions of these effects are plotted as function of the
opening angle $\alpha$ of a focusing lens. The influence of both chromatic and spherical aberrations

---

Figure 1.2: Schematic of time-of-flight Secondary Ion Mass Spectroscopy (ToF-SIMS).
Secondary ions, produced by the pulsed primary ion beam, are accelerated to the detector.
Different masses result in different time-of-flight to the detector.
Figure 1.3: Illustration of the compromise between different mechanisms limiting the resolution. The spot size is plotted as function of the opening angle $\alpha$. Diffraction (solid lines) scales with $\alpha^{-1}$, chromatic aberrations (dashed line) with $\alpha$ and the spherical aberrations (dotted line) with $\alpha^3$. For more details see text. Figure adapted from Ref. [13].

are increased for larger openings angles. Diffraction behaves the opposite, the effect on the resolution decreases for larger angles. The optimal resolution is in this case given by the compromise between diffraction and chromatic aberrations, at the crossover position indicated by the black arrow.

For ions the Broglie wavelength is over two orders of magnitude smaller [13], resulting in a shifted diffraction curve in Fig. 1.3, indicated by the red line. The position for optimal resolution now shifts, indicated by the red arrow. A smaller spot is now possible at smaller opening angles. In practice the opening angle is typically 5 times smaller than used in SEMs, which additionally results in a 5 times larger depth of field. Furthermore the excitation volume in the sample due to incoming ions is also smaller under usual operation conditions. The ions have much more momentum and penetrate deeper into the sample, so they do not spread out near the sample surface [12, 14]. Therefore they only emit secondary electrons from a small area around the incoming ions, so high resolution imaging is possible, much better than obtainable with a SEM.

Finally, the secondary electron yield, the number of emitted secondary electrons per incoming particle is much higher for incoming ions than incoming electrons. A better signal to noise ratio can therefore be obtained at the same beam current. The secondary electron yield is also strongly material dependent, so good material contrast is automatically obtained. When, additionally, backscattered helium ions are detected, even better material contrast can be achieved [12]. An ion microscope with a different low-mass ion species would be interesting, because that probably introduces new contrast mechanisms, based on specific
ion-target interactions [15].

1.2 Existing ion sources used in FIB systems

In this section an overview is given of two existing high-brightness ion sources used in the applications discussed in section 1.1. We start with a short introduction of beam quality and the definition of brightness.

1.2.1 Beam quality

The focusability of an ion beam, i.e., how well it can be focused to a small spot size, is determined by the quality of the beam. In most situations the longitudinal and the transverse directions can be described independently, so the quality can be characterized by two parameters: the (transverse) reduced brightness $B_r$ and the longitudinal energy spread $\sigma_U$.

The energy spread $\sigma_U$ is simply defined as the root-mean-square (rms) spread in the beam energy $U$. Due to chromatic aberrations in a focusing column, this can limit the smallest achievable spot size. A low energy spread is thus important to get optimal resolution.

![Figure 1.4: Illustration of the brightness of an ion source. Ions are extracted from area $A$ with a solid angle $\Omega$.](image)

In the transverse direction, the reduced brightness is usually defined as

$$B_r = \frac{1}{U} \frac{\partial^2 I}{\partial A \partial \Omega},$$

with $I$ the beam current, $A$ the (effective) source area, $\Omega$ the subtended solid angle. The different parameters are illustrated in Fig. 1.4. This can be rewritten in terms of the emission temperature $T$ for a source with a uniform current density as

$$B_r = \frac{Je}{\pi kT},$$

(1.2)
where $J = I/A$ is the current density, $k$ Boltzmann’s constant and $e$ the elementary charge.

The usual way to improve the brightness is to extract the same current from a smaller source area $A$. The sources described in the following sections are examples of this principle. In this manner the sources better approximate a theoretical point source, which in principle can be focused to a single point. The current density $J$ close to the source, however, will rise if the source area is reduced. This unfortunately increases coulombic interactions, that may degrade the beam quality.

### 1.2.2 Liquid Metal Ion Source

The current industry standard high brightness ion source for FIB applications is the Liquid Metal Ion Source. There are several types, but the most common one, the needle-type is illustrated in Fig. 1.5. It consists of a rather blunt tip, usually made from tungsten with a reservoir of liquid metal attached. When the reservoir is heated to a suitable temperature, the metal flows and wets the tip [16]. Different metals can be used in principle, but Gallium has the best combination of properties, such as high surface tension and low vapor pressure, which result in the highest brightness.

![Schematic of a gallium liquid metal ion source.](image)

The tip is placed close to an extraction aperture, so a strong electric field can be applied between them. The molten metal is then displaced by the electrostatic stress and this results, in combination with the surface tension forces, in a sharp cone, the so-called Taylor-Gilbert cone [1]. At the end of the sharp cone, where the electric field is strongly enhanced, the field causes field evaporation and subsequent field ionization of the metal atoms. An ion beam is produced from a source area of only several square nanometers, which makes it possible to achieve the high brightness. High brightness can only be realized if a small fraction of the extracted current is used. Typically a current of 1 $\mu$A is extracted for a useable beam current of 10 pA with a reduced brightness of 1 $10^6$ A/(m$^2$srV) [17]. The current density close to the tip is very high ($J \approx 10^{10}$ A/m$^2$ [3]), which results in strong coulombic interactions. These interactions increase the effective source size to about 50 nm [17]. Additionally they
increase the energy distribution, resulting in a relatively large FWHM longitudinal energy spread of about 5 eV [3, 18]. Chromatic aberrations associated with this energy spread limit the smallest focal spot size that can be achieved.

1.2.3 Helium Field Emission Source

A recently developed Helium field emission source enabled the development of a helium microscope as discussed in section 1.1.3. It is an improved version of the source used in a field ion microscope (FIM) [19] developed over 50 years ago.

It consists of a cryogenically cooled, sharp metal needle with a radius on the order of 100 nm [13] in an ultra high vacuum environment (< $10^{-10}$ mbar residual background). By placing the needle close to an extraction electrode and applying a relatively modest high voltage, a strong field near the tip can be produced of about 3 V/Å. When helium gas is added to the system nearby the tip, the gas atoms become polarized in the field and start to accelerate towards the needle. If they are sufficiently close to the needle, the atoms will be ionized by the process of quantum mechanical electron tunneling to the tip [12]. The created ion is immediately accelerated away from the tip, so it does not hit the surface.

![Schematic overview of a He-Field Emission source with a) a bare tip b) a tip with super-structure. Adapted from Ref. [13].](image)

The source is illustrated in Fig. 1.6a. The ionization process takes place at a large number of atoms protruding from the surface of the needle, increasing the source area and thus lowering the brightness. To overcome this, a (proprietary) process has been developed [13] to build a stable and precisely defined three sided pyramid on the apex of the needle, see
Fig. 1.6b. The top of the pyramid has a configuration with three atoms, a so-called trimer. Field enhancements close to this even sharper peak are responsible for the fact that now all ionization takes only place close to these three atoms, see Fig. 1.6b.

By changing the helium pressure, the ion current can be controlled. Typically a current of 10 pA is used, but the current can be varied from 1 fA to 100 pA. It is claimed, with an (conservative) estimate of the (effective) source size of 0.1 nm$^2$, that this results in a reduced brightness of $B_r \approx 5 \times 10^8$ A/(m$^2$srV) [13], approximately 500 times as bright as the LMIS. Also the energy spread is improved compared to the LMIS: it has a measured rms energy spread less than 1 eV.

So this source is well suited for use in a microscope because of the high brightness and low energy spread. Previous attempts to build field emission sources with a small superstructure on top of the tip, produced unreliable results with lifetimes that can not compete with that of the LMIS [16]. These problems may have been solved now by the proprietary process described in [13]. However, it has not yet been demonstrated that this source can also be used to produce different (i.e. heavier) ions than helium with high brightness and good reliability. Helium is ideal because it can easily be purified and has the highest ionization energy of all elements [20]. This helps to prevent unwanted collisions of background gas with the sensitive superstructure, because all other atomic elements that can be present are ionized before they have the chance to collide with the structure. This property enhances the stability of the source. For other elements this might be a problem.

1.3 New concept: Ions from a laser-cooled gas

As discussed in section 1.1, a new high brightness source for FIB applications, that has a low energy spread to overcome the limitations set by the chromatic aberrations, would be a welcome addition. Furthermore it would be interesting if several different ion species, heavy as well as light, can be used, depending on the application. And additionally, if the source is able to operate in a pulsed mode, besides continuous operation, it can also be used for secondary ion mass spectroscopy.

In this thesis a source with these properties is studied. It is a new kind of ion source, that uses a completely different approach to reach high brightness. Instead of trying to reduce the source area $A$ in Eq. (1.2) the source temperature $T$ is reduced. This ultra cold ion source (UCIS), is based on just-above threshold photo-ionization of laser-cooled atoms trapped in a magneto-optical trap (MOT). The current density at the source is much lower than for the sources discussed in previous sections. This reduces the effects of space charge, so low energy spread ion beams become possible. Furthermore, many different atomic species can be laser-cooled (e.g. all alkali metals) making it a versatile source.

Detailed calculations to estimate the performance of the UCIS will be discussed in the next chapter. To give already an idea of its properties, the most important numbers are summarized in table 1.1, together with the properties of the two other discussed sources.
The typical temperature of the ions extracted from this source, which depends on the atomic species, is about 150 µK. Currents from 1 pA to 100 pA can be extracted from a source area with a radius from 5 to 50 µm. Even with these larger source sizes, it can produce a brightness comparable to the LMIS for many different ion species. Only for Helium ions it cannot compete with the high brightness of the Helium field emission source as discussed in the previous section. A next generation UCIS source, briefly discussed in chapter 7, may be able to produce comparable brightness to this field emission source after all.

1.4 This thesis

The outline of this thesis is as follows: in chapter 2 we present a basic model and detailed simulations of the performance of this new source in the regime where it is useful for a focused ion beam (FIB) system. In chapter 3 the details of the experimental setup that has been developed in this project are given. In chapter 4 longitudinal energy spread measurements are presented that show low energy spread is indeed possible. In chapter 5 we demonstrate that this source enables the use of time-dependent acceleration fields that opens new possibilities. Experimental results and models are presented. In chapter 6 more details will be discussed of these time-dependent experiments and additional measurements are presented. In chapter 7 a short outlook is given of future prospects. Finally in chapter 8 the conclusions are discussed and put in a somewhat broader context.
Table 1.1: *Table with the most important properties of the discussed sources.*

<table>
<thead>
<tr>
<th>Properties</th>
<th>UCIS Ultra Cold Ion Source</th>
<th>LMIS Liquid Metal Ion Source</th>
<th>FES Field Emission Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>Current $I$</td>
<td>$0 - 100 \text{ pA}$</td>
<td>$0 - 10 \text{ nA}$</td>
<td>$0 - 100 \text{ pA}$</td>
</tr>
<tr>
<td>Ion species</td>
<td>Alkali metals (e.g. Li, Cs), Alkaline earth metals, Cr, Yb, Nobel gases, ...</td>
<td>Ga</td>
<td>He</td>
</tr>
<tr>
<td>Beam quality (1 pA)</td>
<td>Brightness $B_r$</td>
<td>$3 \times 10^5$</td>
<td>$1 \times 10^6$</td>
</tr>
<tr>
<td></td>
<td>A/(m$^2$ sr V)</td>
<td>A/(m$^2$ sr V)</td>
<td>A/(m$^2$ sr V)</td>
</tr>
<tr>
<td>Energy spread $\Delta U$</td>
<td>0.2 eV</td>
<td>4.5 eV [18]</td>
<td>&lt; 1.0 eV [13]</td>
</tr>
<tr>
<td>Source radius $R$</td>
<td>4.5 $\mu$m</td>
<td>25 nm [17]</td>
<td>$\sim$ 0.3 nm [13]</td>
</tr>
<tr>
<td>(effective)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Temperature $T$</td>
<td>150 $\mu$K</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Chapter 1.

Bibliography


Simulated performance of an ultra-cold ion source

Abstract. At present, the smallest spot size which can be achieved with state-of-the-art Focused Ion Beam (FIB) technology is mainly limited by the chromatic aberrations associated with the 4.5 eV energy spread of the Liquid-Metal Ion source. Here we numerically investigate the performance of an Ultra-Cold Ion source which has the potential for generating ion beams which combine high brightness with small energy spread. The source is based on creating very cold ion beams by near-threshold photo-ionization of a laser-cooled and trapped atomic gas. We present ab initio numerical calculations of the generation of ultra-cold beams in a realistic acceleration field and including all Coulomb interactions, i.e. both space charge effects and statistical Coulomb effects. These simulations demonstrate that with existing technology reduced brightness values exceeding $10^5 \text{A m}^{-2}\text{sr}^{-1}\text{V}^{-1}$ are feasible at an energy spread as low as 0.1 eV. The estimated spot size of the Ultra-Cold Ion source in a FIB instrument ranges from 10 nm at a current of 100 pA to 0.8 nm at 1 pA.

2.1 Introduction

The nanometer milling capability of Focused Ion Beam (FIB) technology has led to its widespread use in nanoscience in general, and the semiconductor industry in particular [1–4]. The minimum focal spot size, and thus the minimum feature size which can be addressed, is ultimately limited by the quality of the ion source at a certain current. At present, the preferred source in a FIB is the Liquid-Metal Ion Source (LMIS) [1, 5] by virtue of its unrivalled beam brightness. For a gallium-based LMIS the reduced brightness can be as high as $10^6 \text{A m}^{-2} \text{sr}^{-1} \text{V}^{-1}$ for a useable beam current of 10 pA and an energy spread of 4.5 eV [1, 5–7]. A FIB equipped with a Ga-LMIS enables a focal spot size of approximately 10 nm diameter, making it an indispensable tool for inspecting the smallest structures in present-day large-scale integrated circuits. However, if the advances in semiconductor technology keep up with Moore’s law, 1–nm ion beam milling capability will be required within a few years time. The 10 nm spot size that can be achieved at present is mainly limited by chromatic aberrations associated with the 4.5 eV energy spread of the Ga-LMIS [8, 9].

Recently, the Ultra-Cold Ion Source (UCIS) was proposed as an alternative for the LMIS [10–12]. The UCIS has the potential of producing ion beams with a reduced brightness and useable current comparable to the LMIS, but with a much smaller energy spread, and may therefore provide us with a route towards 1–nm ion beam milling. The UCIS is based on creating very cold ion beams by near-threshold photo-ionization of a laser-cooled and trapped atomic gas [13]. So far several closely related schemes have been proposed. The original idea was to extract ions from a two-dimensionally laser-cooled atomic beam [10]. Subsequently, it was proposed to use a Magneto-Optical atom Trap (MOT) as cold particle source, allowing both DC and pulsed operation [11]. Very recently it was proposed to use a miniaturized MOT [12]. In [12] estimates were presented for the brightness, energy spread and spot size that can be achieved, but without considering the effect of Coulomb interactions. In particular statistical Coulomb effects can severely degrade the quality of a charged particle beam. It is therefore worthwhile to assess the importance of such effects. Statistical Coulomb effects have been the subject of a great deal of theoretical study; see for example Ref. [14] for a recent review. Unfortunately these theories are generally not suitable to predict source performance, since they can not be applied to the critical initial acceleration stages.

Here we present a detailed particle tracking analysis of the UCIS. The simulations start from conditions which can be realized routinely in a rubidium-based MOT [13]. Furthermore, realistic acceleration fields are used and all Coulomb effects are included, i.e. each and every individual ion is tracked from ionization to a field-free observation plane, while interacting with all other ions. This means that both long-range space-charge effects and statistical Coulomb effects, such as trajectory displacement and the Boersch effect [14], are automatically accounted for in a fully exact manner. The results of the simulations are subsequently used to predict the performance of a Rb-based UCIS in which ions are accelerated to 1 keV in a 100 kV/m extraction field, for beam currents ranging from 1 pA to 100 pA.
We find that for a useable beam current of 1 pA an energy spread as low as 0.1 eV is feasible, at reduced brightness values exceeding $10^5 \text{A m}^{-2} \text{sr}^{-1} \text{V}^{-1}$, which is close to the fundamental thermal limit of a MOT-based ion source, as discussed in Ref. [12]. Note that in Ref. [12] a definition for reduced (or normalized) brightness is used which differs by a factor $4\pi^2$ from the usual definition (see, e.g., Ref. [15], p. 976). For a proper comparison with our results their values of the reduced brightness should therefore be divided by a factor $4\pi^2$.

Our simulations also show that higher currents can be obtained at the cost of an increase in energy spread and a decrease in brightness. We find that the dependence of energy spread on current is very weak, in agreement with a simple model. The brightness decrease with current, however, is unexpected and dramatic: for a useable current of 100 pA the reduced brightness is more than an order of magnitude smaller than at 1 pA, in contradiction with a simple model [12], in which the reduced brightness only depends on the initial atomic density and temperature in the MOT and not on current. We find that the decrease of the reduced brightness is due to disorder-induced heating of the transverse degrees of freedom [16], which is the result of the initial random distribution of the ions.

2.2 Setup

In a MOT the radiation pressure exerted by 3 orthogonal pairs of laser beams of pairwise opposite circular polarizations, in combination with a quadrupole magnetic field, cool the atoms to temperatures below 1 mK and cause the atoms to collect near the point in space where the magnetic field vanishes [13]. The resulting cloud of laser-cooled and trapped neutral atoms, suspended at the center of an accelerating structure, is schematically indicated by the concentric circles in Fig. 2.1.

The laser-cooled and trapped atoms are ionized in a two-step process [17], as is shown in Fig. 2.1. In the first stage, the atoms are excited to an intermediate level by a laser beam that propagates along the symmetry axis of the accelerating structure. In the second step, atoms in the intermediate level are ionized by a second laser beam which is focused in one direction to a thin sheet beam, propagating at right angles with the first. The two-step ionization method allows control over both the shape and the dimensions of the initial ionization volume by carefully tuning the overlap of the excitation and ionization laser beams.

In the simulations in this paper the initial transverse density distribution of the ions is taken to be uniform with radius $R$. This can be accomplished by a uniform excitation laser profile with radius $R$, which is much smaller than the root-mean-squared (rms) size of the atom cloud. Atoms continuously enter the ionization volume from the sides due to thermal motion. Here we assume that the intensity of the ionization laser is adjusted such that the ionization time is comparable to the time it takes to cross the ionization volume. This results in a large fraction of the excited atoms getting ionized while the laser intensity is sufficiently low that the longitudinal density distribution can be assumed near-gaussian with rms width $\sigma_L$ as determined by the rms thickness of the ionizing sheet beam.
As is explained in section 2.3, it is advantageous to minimize the size of the ionization volume. For a current between 1 and 100 pA the typical size of the ionization volume ranges from a few to about hundred micrometer across, much smaller than the typical dimensions of an atom cloud in a MOT. Ions can be extracted continuously from this small volume as long as the number of atoms extracted per unit time is less than the loading rate of the MOT in steady state. Even for currents as high as 1 nA this is not a limiting factor.

Immediately after creation, the ions are accelerated in an electrostatic field, created by a potential difference $V$ across two metal electrodes surrounding the MOT, separated by a distance $d$, as is shown in Fig. 2.1. The laser-cooled ion-beam exits the source through a circular hole with radius $a$ in the negative electrode.

### 2.3 Fundamental performance limits

A commonly used figure of merit for the transverse quality of non-relativistic charged particle beams is the reduced brightness, $B_r$, defined in the conventional way as

$$B_r = \frac{1}{U} \frac{\partial^2 I}{\partial A \partial \Omega},$$

(2.1)

where $A$ is the cross sectional area of the beam, $\Omega$ the corresponding subtended solid angle, and $U$ the average kinetic energy. For an extended source emitting a uniform current density
Simulated performance of an ultra-cold ion source

$J$ at temperature $T$, the resulting brightness is given by [15]

$$B_r = \frac{Je}{\pi kT},$$  \hspace{1cm} (2.2)

where $e$ is the elementary charge and $k$ is Boltzmann’s constant. This equation shows that the maximum achievable beam brightness is fundamentally limited by the temperature and the available flux $\Phi = J/e$ of neutral atoms into the ionization volume.

In the case of a MOT, the neutral atom flux is given by

$$\Phi_{\text{MOT}} = 2 \frac{n v_{\text{th}}}{4},$$  \hspace{1cm} (2.3)

where $n$ is the density of the trapped atoms, and $v_{\text{th}} = (8kT/\pi m)^{1/2}$ is the thermal velocity, with $m$ the atomic mass. The factor 2 in Eq. (2.3) originates from the fact that the influx can be from either side into the ionization volume. We thus find that for a MOT there is an upper bound to the brightness of the extracted beam that is independent of the radius and that scales inversely proportional to the square root of the temperature:

$$B_r,_{\text{MOT}} = 2 \frac{\pi e^2 n}{\sqrt{2\pi mkT}}.$$  \hspace{1cm} (2.4)

The initial rms energy spread $\sigma_U$ is due to the combination of creating particles over a potential difference associated with the rms width $\sigma_L$ of the ionizing sheet beam, and the initial thermal motion of the ions with (atomic) temperature $T$. Let us first consider the case of zero initial temperature: If the initial ionization volume is located at the center of a diode with $a \ll d$, then the $T = 0$ energy spread is given by

$$\sigma_{U_0} = e E_0 \sigma_L,$$  \hspace{1cm} (2.5)

where $E_0 \equiv V/d$. The corresponding $T = 0$ rms longitudinal momentum spread is

$$\sigma_{p_0} = \frac{\sigma_{U_0}}{v_0} = \sqrt{\frac{m e E_0 \sigma_L^2}{d}},$$  \hspace{1cm} (2.6)

where $v_0 = \sqrt{eE_0d/m}$ is the average velocity after acceleration. At finite initial temperature $T$, the thermal rms momentum spread $\sqrt{mkT}$ has to be added in quadrature to obtain the full rms longitudinal momentum spread,

$$\sigma_p^2 = \sigma_{p_0}^2 + mkT.$$

However, for all cases of practical interest $mkT/\sigma_{p_0}^2 = d kT/e E_0 \sigma_L^2 \ll 1$, so the thermal contribution can be neglected and the rms energy spread can be approximated by

$$\sigma_U \approx \sigma_{U_0} \equiv e E_0 \sigma_L.$$  \hspace{1cm} (2.8)
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The width $\sigma_L$ can not be chosen arbitrarily small. The lowest energy spread occurs when the ionization sheet laser beam is focused such that its Rayleigh length is identical to the radius $R$ of the excitation laser, leading to

$$\sigma_L \geq \sqrt{\lambda R / \pi}, \quad (2.9)$$

with $\lambda$ the wavelength of the ionization laser.

The maximum current that can be extracted from a uniformly emitting surface with radius $R$ and flux $\Phi$ is given by $I = \Phi e \pi R^2$. According to Eq. (2.8) and (2.9) the minimum energy spread for a given $n$ and $T$ increases with current, scaling with $I^{1/4}$ according to

$$\sigma_U \geq E_0 \sqrt{\lambda R / \pi} = E_0 \left( \frac{\lambda^2 I}{\pi^3 \Phi e} \right)^{1/4}. \quad (2.10)$$

2.3.1 Rubidium MOT as an ultra-cold ion source

In this paper we use initial conditions which are typical for a rubidium MOT, the workhorse of laser-cooling and trapping [13]. The excitation laser is tuned to the $5^2P_{3/2}$ state of Rb, which implies that the ionization laser operates at $\lambda = 480$ nm. The limiting density in an atom trap is in the order of $10^{18}$ m$^{-3}$ [18] and a temperature $T = 200 \mu$K is routinely achieved in our lab. These values translate into a flux $\Phi = 10^{17}$ atoms m$^{-2}$ s$^{-1}$ and hence a brightness as high as $3 \cdot 10^5$ A m$^{-2}$ sr$^{-1}$ V$^{-1}$, see Eqs. (2.3) and (2.4). Combined with an electric field $E_0 = 100$ kV/m this results in an initial energy spread as low as $0.25$ eV at currents as large as $100$ pA, see Eq. (2.10).

Although these estimates of the initial low energy spread and high brightness of the UCIS are very encouraging, it is not a priori clear that the above numbers can be realized in a realistic setup. Realistic acceleration fields and statistical Coulomb effects may decrease the brightness significantly.

2.4 Numerical approach

The setup under investigation has been simulated with the GPT [19] code. This code solves the 3D equations of motion of each and every ion, in terms of velocity $v_i$ and position $r_i$ of each particle $i = 1, 2, \cdots, N$, including all pairwise Coulomb interactions:

$$m \ddot{r}_i = \sum_{j=1 \atop j \neq i}^{N} \frac{e^2}{4 \pi \epsilon_0} \frac{r_j - r_i}{|r_j - r_i|^3} + eE_E(r_i), \quad (2.11)$$

with $E_E$ the externally applied acceleration field. In this approach all Coulomb effects are calculated from first principles. It therefore automatically covers the Boersch effect, trajectory displacement, and space-charge effects [14].
Simulated performance of an ultra-cold ion source

For the external field we start from an analytical expression for the potential due to an infinite perfectly conducting plate at \( z = 0 \) with a circular hole with radius \( a \), which separates a uniform electric field \( E_0 \hat{z} \) at \( z = -\infty \) from a zero electric field at \( z = +\infty \) \([20]\),

\[
V_E(r) = \frac{E_0 a}{\pi} \left[ \sqrt{\frac{\rho - \mu}{2}} - \frac{|z|}{a} \arctan \sqrt{\frac{2}{\mu + \rho}} \right],
\]

(2.12)

where \( \mu = \left( x^2 + y^2 + z^2 \right)/a^2 - 1 \) and \( \rho = \sqrt{\mu^2 + 4z^2/a^2} \). The origin of the coordinate system is at the center of the circular hole, and the \( z \)-axis is perpendicular to the conducting plate. If a voltage \( V = E_0 d \) is applied across two such plates, separated by a distance \( d \gg a \), then the electric field is given by \( E_E = E_E^+ - E_E^- \), where

\[
E_E^\pm(r) = -\nabla V_E \left( x, y, \frac{d}{2} \pm z \right) + E_0 \hat{z} H \left( z \pm \frac{d}{2} \right),
\]

(2.13)

with \( H \) the Heaviside step function. Equations (2.12) and (2.13) provide us with a convenient way to accurately describe the non-uniform acceleration field of a diode as shown in Fig. 2.1, which contains all the features of a real field, and which can be varied with only two parameters: The aperture radius \( a \) and spacing \( d \).

All initial particle coordinates are chosen randomly in an uncorrelated way to correctly model the stochastic nature of the ionization process. The initial transverse position distribution is uniform within radius \( R \). The initial longitudinal distribution is gaussian with rms width \( \sigma_L \). The initial velocity distribution is thermal with temperature \( T \) (and hence \( \sigma_v_x = \sigma_v_y = \sigma_v_z = \sqrt{kT/m} \)). The appearance of new particles in time is modeled by a Poisson process with rate \( I/e \) reflecting the random arrival times of the atoms in the ionization volume.

2.5 Results

The setup shown in Fig. 2.1 has been simulated with the GPT code for a large number of currents ranging from 1 to 100 pA. The starting point is a rubidium MOT with a temperature \( T = 200\mu\text{K} \), corresponding to velocities \( v_{th} = 0.22\text{m/s} \), and a density \( n = 10^{18}/\text{m}^3 \). A voltage \( V = 2\text{kV} \) is applied across a \( d = 20 \text{mm} \) gap, resulting in an electrostatic field \( E_0 = 100\text{kV/m} \) and an initial energy spread in the sub-eV range, see Eq. (2.10). The radius \( a \) of the aperture is 1 mm, which turns out to be sufficiently large to prevent that non-linear fields affect the quality of the extracted beam. The particle distribution is analyzed 20 mm from the MOT center, i.e. 10 mm downstream from the aperture.

In Fig. 2.2 the resulting rms energy spread (top) and peak reduced brightness (bottom) are plotted as function of current. Figure 2.2 also shows the fundamental limits for the energy spread and brightness according to Eqs. (2.10) and (2.4). Figure 2.3 shows the transverse phase-space distribution (top row), the energy distribution (middle row), and the uncorrelated
Figure 2.2: Crosses: simulated rms energy spread (top) and reduced brightness (bottom) as function of current; open circles: reduced brightness calculated using transverse beam temperatures; dash-dotted lines: fundamental limits calculated using Eqs. (2.4) (bottom) and (2.10) (top).
angular distribution (bottom row) for beam currents $I = 1, 10, \text{and} \ 100 \ \text{pA}$. In the following we will first treat the energy spread, followed by a discussion of the transverse phase-space distribution, disorder-induced heating and the reduced brightness. We end with a prediction of attainable spot size in a FIB instrument.

2.5.1 Energy spread

The energy distributions shown in Fig. 2.3 clearly reflect the gaussian intensity profile of the ionization laser beam. The solid lines are gaussian fits from which the rms widths $\sigma_U$ are determined. The centers of the gaussian energy distributions are shifted by about 0.1 eV from the 1 keV final energy due the fact that the particles have not reached their final energy yet at the observation plane, see Eq. (2.12). In Fig. 2.2 the values of $\sigma_U$ resulting from the simulations are plotted as a function of current. Also plotted is the dependence of $\sigma_U$ on current according to Eq. (2.10), indicated by a dash-dotted line, which gives a fundamental lower limit for the energy spread.

It is clear that the simple geometrical model for the energy spread, discussed in Sec. 2.3, provides an accurate description: for small currents, which require a small initial beam radius $R$, the rms thickness $\sigma_L$ of the ionizing sheet beam can also be chosen small, so the ions can be extracted from an increasingly narrow cross section. This leads to an increasingly lower energy spread that ranges from below 0.3 eV at high current (100 pA) to below 0.1 eV at low current (1 pA).

2.5.2 Phase-space distribution

The slant in the transverse position ($x$) – angle ($x'$) phase-space distributions in Fig. 2.3 shows that diverging beams are created, which is mainly due to the negative lens effect or ‘exit kick’ of the aperture. For a particle beam starting from zero velocity at the center of a diode with $a \ll d$ it can be shown that the focal length is given by $F = -2d$, i.e. $F = -40 \ \text{mm}$ in our case. The negative lens gives rise to a linear correlation between transverse position $x$ and angle $x'$ with a slope $dx'/dx = F^{-1} = 25 \ \text{m}^{-1}$. This is in good agreement with the results of the simulations for all three currents, implying that the effect of space charge on the beam divergence is small.

Apparently, the overall behavior of the ion beams is very similar for all three currents. A closer inspection, however, of the transverse phase-space distributions in Fig. 2.3 reveals some subtle and interesting differences: the 1 pA beam has a well-defined narrow core and a halo consisting of particles which are scattered out of the core; for 10 pA the relative size of the halo is much smaller, while at 100 pA there are hardly any outliers. To further investigate the differences we show the uncorrelated angular distributions in the bottom row of Fig. 2.3. These distributions have been extracted from the top-row full phase-space distributions by first removing the linear correlation, i.e., by collimating the beam with an ideal positive lens, thus minimizing the angular widths, and subsequently making histograms of the angular
Figure 2.3: Transverse phase-space distribution (top row), energy distribution (middle row), and uncorrelated angular distribution (bottom row) for $I = 1, 10$ and $100$ pA. Note the changing scales. The solid lines are gaussian fits.
Simulated performance of an ultra-cold ion source

distributions of the particles. These angular distributions are fitted with a gaussian profile, as is shown in Fig. 2.3. The gaussian angular distribution corresponds to a thermal transverse velocity distribution, from which the transverse temperature $T_t$ can be extracted. We find at $I = 1$ pA a transverse beam temperature $T_t = 190 \mu$K which is virtually the same as the original ion temperature $T = 200 \mu$K. At higher currents there is significant heating of the transverse degrees of freedom: $T_t = 740 \mu$K at $I = 10$ pA, and $T_t = 2800 \mu$K at $I = 100$ pA.

2.5.3 Disorder-induced transverse beam heating

The rise of the transverse beam temperature, and the concomitant decrease in brightness, can be attributed to disorder-induced heating [16]: immediately after ionization the ions move with the very small velocities of the cold atomic gas, which means their kinetic energy is much smaller than the excess potential energy arising from their random spatial distribution. Subsequently the excess potential energy is converted into random motion of the ions and therefore into thermal energy.

Disorder-induced heating in a stationary ultra-cold plasma will lead to a final temperature $T_f$ of the order of the Coulomb interaction energy between neighboring ions [16],

$$ kT_f \approx \frac{e^2}{4\pi\varepsilon_0 a}, $$

where $a = (4\pi n/3)^{-1/3}$ is the Wigner-Seitz radius and $n$ the ion density. This final temperature is reached on a timescale of the order of the inverse plasma frequency $\omega_p^{-1} = \sqrt{m \varepsilon_0 / n e^2}$. In our system the initial ion density $n_0$ at the onset of the acceleration process is approximately given by

$$ n_0 \approx \Phi \sqrt{\frac{m}{e E_0 \sigma_L}} \approx 10^{14} \text{ m}^{-3}, $$

implying that a temperature $T_f \approx 1$ K is reached within $\omega_p^{-1} \approx 1 \mu$s, which is approximately the time it takes for the ions to reach the observation plane. However, this final temperature is never reached, because the density decreases as the particles are accelerated, both lowering the final temperature and slowing down the heating process. Nevertheless, only a small amount of disorder-induced heating is sufficient to explain the observed temperature rise.

In principle disorder-induced heating only depends on the current density, and should therefore not increase with current. However, this only holds if the system size is much larger than the average interparticle spacing. In our case the average interparticle spacing at initiation is approximately $n_0^{-1/3} \approx 20 \mu$m, which is larger than the transverse beam size $2R = 9 \mu$m at 1 pA, but smaller than the transverse beam size $2R = 90 \mu$m at 100 pA. Obviously, no disorder-induced transverse beam heating will occur if there are no neighbors in the transverse direction. In this so-called ‘pencil beam’ regime the asymptotic behavior towards zero current, and thus to zero transverse size, is that there is no transverse heating and hence no reduction in brightness. On the opposite side of the current range, at 100 pA, we are nearing the ‘Holtsmark’ regime. Here, the transverse size is so large compared to
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the interparticle spacing that heating becomes independent of current. Disorder-induced heating of the transverse degrees of freedom is therefore suppressed at $I = 1 \text{ pA}$, becomes increasingly important at higher currents, and starts to level off at 100 pA, in agreement with the simulation results shown in Fig. 2.2.

To check whether there are any other heating effects contributing, we did simulations in which the ions are started from an ordered ‘Hammersley’ lattice [22] instead of a random distribution, but which are in all other aspects identical to the simulations presented in the earlier sections. In these simulations we find that no significant heating occurs, implying that other heating mechanisms are less important, at least in the first stages of acceleration. As a separate check we did simulations in which the initial energy spread was artificially decoupled from the extracted current. This did not affect the transverse heating at all, implying that the transverse temperature does not depend on energy spread. This shows that there is no significant transverse heating due to equilibration between the relatively ‘hot’ longitudinal degrees of freedom and the relatively ‘cold’ transverse degrees of freedom: the transverse heating cannot be attributed to a reverse version of the Boersch-effect.

2.5.4 Reduced brightness

By substituting the current density at the observation plane, $J = 1.6 \times 10^{-2} \text{ A/cm}^2$, and the transverse temperature $T_t$ obtained from the gaussian fits in Fig. 2.3 into Eq. (2.2), we find for the reduced brightness at the observation plane $B_r = 3 \times 10^5 \text{ A m}^{-2} \text{ sr}^{-1} \text{ V}^{-1}$ at $I = 1 \text{ pA}$, $B_r = 8 \times 10^4 \text{ A m}^{-2} \text{ sr}^{-1} \text{ V}^{-1}$ at $I = 10 \text{ pA}$, and $B_r = 2 \times 10^4 \text{ A m}^{-2} \text{ sr}^{-1} \text{ V}^{-1}$ at $I = 100 \text{ pA}$. These estimates are indicated by open circles in Fig. 2.2. The observed decrease of the reduced brightness with beam current is due to transverse beam heating, and can therefore be attributed entirely to statistical Coulomb effects.

Equation (2.2) allows us to make an estimate of the reduced brightness, but it is not immediately clear whether the value of $B_r$ thus obtained represents the entire beam (the average brightness), or only a very small part (peak brightness), or something in between. For this reason a robust calculation of the reduced brightness, that is not sensitive for statistical outliers in the distribution of the simulated beams has been done, based on the definition given in Eq. (2.1), using a numerical approach [21] outlined in the Appendix. This method allows us to unambiguously calculate the average reduced brightness of any fraction of the beam, including the peak brightness. Figure 2.2 shows the peak brightness calculated in this way (crosses), as a function of the total beam current.

The calculated curve agrees very well with the estimates based on Fig. 2.3. We find that at 1 pA the peak brightness is close to the fundamental limit of a few times $10^5 \text{ A m}^{-2} \text{ sr}^{-1} \text{ V}^{-1}$, indicated by a dash-dotted line. For higher currents the peak brightness gradually decreases due to statistical Coulomb effects to about $10^4 \text{ A m}^{-2} \text{ sr}^{-1} \text{ V}^{-1}$ at 100 pA.

Fig. 2.4 shows the average brightness as function of beam fraction, for $I = 1$, 10 and 100 pA, obtained by numerically skimming off the beam by removing outliers according to the recipe in the Appendix. The overall behavior for all currents is identical: only a small
fraction, on the order of 10-20%, needs to be skimmed to obtain very good average brightness. This is most pronounced for the 1 pA case, where reducing the current by 10% results in an average brightness which is larger than half the peak brightness.

2.5.5 Attainable FIB spot size

The high brightness and low energy spread of the UCIS makes it an ideal source for a FIB instrument. In order to estimate attainable spot size as function of current we assume downstream electrostatic acceleration to a typical value of $V_p = 30$ kV. The accompanying decrease in ion density allows us to assume that downstream heating effects are negligible compared to the heating already accounted for at the source. The spot size $d_p$ is given by

$$d_p = \left( \frac{IC_c^2 \sigma_U^2}{B_r V_p^3} \right)^{1/4},$$

where $C_c$ is the chromatic aberration coefficient of the focusing system. If we assume a realistic $C_c = 20$ mm, the expected spot sizes are 9.6 nm at 100 pA, 2.4 nm at 10 pA and 0.8 nm at 1 pA.

2.6 Conclusion

On the basis of particle tracking simulations of an Ultra-Cold Ion source, using realistic acceleration fields and including all Coulomb interactions, we conclude that reduced brightness values in the order of a few times $10^5$ A m$^{-2}$ sr$^{-1}$ V$^{-1}$ are attainable at an rms energy spread below 0.1 eV. In comparison, the best quoted value for the LMIS is a reduced brightness of $10^6$ A m$^{-2}$ sr$^{-1}$ V$^{-1}$ at an energy spread of 4.5 eV [1, 6, 7]. The combination of high brightness
and low energy spread of the Ultra-Cold Ion source allows 100 pA to be focused on a 10 nm spot, whereas a sub-nm spot size is feasible if the current is reduced to 1 pA.

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Appendix 2.A Robust Brightness Estimation

Inspired by Ref. [21] the following procedure was used to calculate the reduced brightness for any fraction of the beam, and to obtain a robust estimate for the peak brightness. The input of the algorithm is the discrete set of transverse phase space particle coordinates $x_i = (x_i, y_i, x'_i, y'_i)$, where $i = 1, 2, \ldots, N$ with $N$ the total number of particles in the beam.

We start from the definition of the average brightness of the entire beam $B_r$, which naturally follows from integrating Eq. (2.1) over transverse positions and angles,

$$\bar{B}_r = \frac{I}{U \cdot \epsilon}, \quad (2.17)$$

with $\epsilon$ the 4D hypervolume in $(x, y, x', y')$ space, occupied by all the particles in the beam as they pass the observation plane. Because of the discrete nature of the particle distribution, the 4D volume $\epsilon$ can in principle be calculated in may ways.

We define $\epsilon$ as the volume of a 4D hyperellipsoid, whose shape and orientation are extracted from the $4 \times 4$ beam sigma matrix,

$$\Sigma = \begin{pmatrix}
\langle x \cdot x \rangle & \langle x \cdot x' \rangle & \langle x \cdot y \rangle & \langle x \cdot y' \rangle \\
\langle x' \cdot x \rangle & \langle x' \cdot x' \rangle & \langle x' \cdot y \rangle & \langle x' \cdot y' \rangle \\
\langle y \cdot x \rangle & \langle y \cdot x' \rangle & \langle y \cdot y \rangle & \langle y \cdot y' \rangle \\
\langle y' \cdot x \rangle & \langle y' \cdot x' \rangle & \langle y' \cdot y \rangle & \langle y' \cdot y' \rangle 
\end{pmatrix}, \quad (2.18)$$

where $\langle \cdots \rangle$ indicates averaging over the entire distribution. The directions of the principal axes of the ellipsoid are given by the eigenvectors of the sigma matrix and the lengths of the principal axes follow from the corresponding eigenvalues.

The hyperellipsoid as defined by Eq. (2.18) can be scaled simultaneously in all four dimensions, such that both the orientation and aspect ratios remain constant. Once a point lies on the surface of such a scaled hyperellipsoid, it will remain on this surface for any downstream linear transport system. Although the shape and orientation of the ellipsoid will vary according to the beamline optics, its volume will remain constant. The volume $\epsilon_i$ of a scaled hyperellipsoid which just touches the 4D phase-space position $x_i$ is given by

$$\epsilon_i = \frac{\pi^2}{2} \sqrt{\det(\Sigma)} \left( x_i^T \cdot \Sigma^{-1} \cdot x_i \right)^2. \quad (2.19)$$
Using Eqs. (2.18) and (2.19) the set \( \{ \epsilon_i | i = 1, 2, \cdots, N \} \) can be generated. By sorting the list of \( \epsilon_i \) values and renumbering them in such a way that \( \epsilon_1 < \epsilon_2 < \cdots < \epsilon_N \), we may now define a unique curve of average brightness as function of beam fraction \( f_i = i/N \):

\[
\bar{B}_r(f_i) = \frac{1}{U} \frac{f_i \cdot I}{\epsilon_i}.
\]

(2.20)

Clearly, for calculation of the average brightness of the entire beam the volume \( \epsilon = \epsilon_N \) should be used. The peak brightness \( B_{r,\text{peak}} \) is obtained by linear extrapolation of the \( \bar{B}_r(f) \) curve to zero beam fraction \( f = 0 \). This is a robust implementation of the definition given in Eq. (2.1), avoiding inaccuracies arising from the fact that when going to zero beam fraction, the number of data points, over which one should average, also goes to zero.

As a refinement to the procedure, already suggested in [21], we use the above method iteratively and base the sigma matrix from Eq. (2.18) on the 50\% particles with the smallest \( \epsilon \) in order to prevent that outliers affect the overall shape of the ellipsoids.

**Bibliography**


Experimental setup

In this chapter the ultracold ion source setup with its different parts will be discussed. More details and background information will be given here that is not present in the coming chapters where the measurements and simulations are presented. An overview of the setup is shown in Fig. 3.1. Inside a vacuum chamber an accelerator structure is placed in which rubidium atoms are cooled and trapped with laser radiation. A two-step photo ionization process is used to ionize a small volume of the atoms in the cold atomic cloud, to create a ultracold ion bunch. The ions are accelerated by the field in the accelerator, created by either a DC voltage or a voltage pulse. Finally, the ions are detected on a multi channel plate (MCP) detector assembly with phosphor screen.

3.1 Vacuum enclosure and accelerator structure

The accelerator structure used in the experiments is placed inside a vacuum chamber. The chamber has a height of 44 cm and a length and width of respectively 46 cm and 35 cm. It has many ports (12 CF40, a CF100, a CF160 and 4 CF200), mainly for optical access and mounting the accelerator, see Fig. 3.1 and Fig. 3.2. The chamber can be pumped down by a turbo molecular pump (250 l/s) and finally pumped to a pressure of $P < 3 \times 10^{-9}$ mbar by only using an ion getter pump (150 l/s) to prevent mechanical vibrations. One of the ports is used to let rubidium inside the chamber. It is connected to a rubidium ampul that can be closed by a CF16 valve. It is heated to about 30°C to get the needed partial rubidium vapor pressure ($\approx 5 \times 10^{-9}$ mbar) in the chamber. Furthermore, a short beam line is connected to one of the flanges of the vacuum chamber.

The accelerator structure used in the experiments, depicted in Fig. 3.3, is placed inside the vacuum chamber. The accelerator is a rotationally symmetric coaxial structure designed
Figure 3.1: Partially cut open side view of the experimental setup. The accelerator structure is located in the chamber. The divergent horizontal MOT beam is shown that uses the internal mirror of the accelerator and a mirror and lens mounted on the end of the chamber.

Figure 3.2: Frontview of the experimental setup. The main chamber is pumped by a ion getter pump and a turbo molecular pump. An optical platform is mounted on top of the chamber.
for voltages up to 30 kV and risetimes down to 300 ps [1]. The outer conductor is grounded while a high voltage can be applied to the inner conductor. An internal mirror and holes in the outer conductor are present to accommodate the laser beams needed for laser cooling, ionization and diagnostics. The accelerator has an exit-hole for the ions with a diameter of 20 mm that is located at 20 mm from the inner conductor. For the experiments, only the shape of the field in the region where the ions are accelerated is important. The potential at the center of the structure, where the ions are created, has a value of 0.49 ± 0.01 [1] times the applied potential on the inner conductor. The electric field inside the accelerator was calculated with the SUPERFISH poisson solver [2], the resulting field is shown in Fig. 3.4 and Fig. 3.5. More details can be found in [1].

Figure 3.3: A cross-section of the accelerator structure [1]. A high voltage can be applied to the inner conductor while the outer conductor is grounded. Holes in the outer conductor and the internal mirror are available to accommodate for the laser beams for the MOT at the position indicated with the arrow.
Figure 3.4: Illustration of the calculated electric field in the cylindrically symmetric accelerator structure. The iso-potential lines in the field are plotted as black solid lines. The arrows show the direction and the strength of the field at a specific position.

Figure 3.5: Calculated electric field on axis of the accelerator structure with $V_a = 1000$ V. a) the potential b) the z-component of the electric field.
3.2 Laser Setup

The optical transitions of $^{85}$Rubidium used for cooling and trapping are illustrated in Fig. 3.6. A rubidium magneto-optical trap (MOT) [3] needs two lasers to operate, a main trapping laser and a repump laser to re-excite atoms that unwantedly ended up in the wrong ground state ($5S_{1/2}F = 2$). The most important properties of $^{85}$Rb are shown in table 3.1. The linewidth of the used atomic transition is $\approx 6$ MHz, so to create a stable MOT setup, the lasers have to be frequency stable well below this linewidth. An overview of the whole laser system with the optics used to stabilize and manipulate the frequency is given in Fig. 3.7. In this section the different sub-systems are explained in more detail.

![Level diagram of $^{85}$Rb of the hyperfine levels used for laser cooling and trapping.](image)

The trapping laser (780 nm) is a commercial tapered amplifier diode laser system (Toptica DLX) with an output power of about 900 mW. It is locked to the $5S_{1/2}F = 3 \rightarrow 5P_{3/2}F = 4$ transition frequency of $^{85}$Rb using modulation transfer spectroscopy [4], explained in more detail below. After a fraction of the output is split off for the locking system, the rest is divided over two output beams: One for the MOT and one for independent excitation of the trapped atoms. Three acousto-optical modulators (AOMs) (IntraAction ATM-801A2) with a center frequency of 80 MHz are used in double-pass configuration, see Fig. 3.7. They are placed in the output beams as well as in the lock system, so the detuning of the output beams can be independently controlled from $\approx -30$ to 30 MHz. Additionally they can be used to switch the output beams on and off in several microseconds.
Figure 3.7: A schematic overview of the laser systems with optics to stabilize and manipulate the frequency of the lasers. The different functional areas are shown with the dashed boxes. The complete system is mounted in a closed box (black lines) for laser safety and temperature stability.
Experimental setup

Table 3.1: Table with properties of $^{85}\text{Rb}$ relevant for laser cooling on the $5S_{1/2}F=3 \rightarrow 5P_{3/2}F=4$ transition.

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Atomic mass</td>
<td>$m$</td>
<td>$85$ a.m.u.$=1.41 \times 10^{-25}$ kg</td>
</tr>
<tr>
<td>Wavelength</td>
<td>$\lambda$</td>
<td>$780.24$ nm ($\text{in vacuum}$)</td>
</tr>
<tr>
<td>Natural linewidth</td>
<td>$\Gamma$</td>
<td>$5.98$ MHz</td>
</tr>
<tr>
<td>Lifetime of $5P_{3/2}(F=4)$</td>
<td>$\tau$</td>
<td>$1/(2\pi\Gamma)$ = $26.63$ ns</td>
</tr>
<tr>
<td>Saturation intensity</td>
<td>$I_0$</td>
<td>$1.64$ mW cm$^{-2}$</td>
</tr>
<tr>
<td>Doppler temperature limit</td>
<td>$T_D$</td>
<td>$\hbar\Gamma/2k_B = 142.41$ $\mu$K</td>
</tr>
</tbody>
</table>

The repump light is produced by another commercial diode laser system (Toptica DL 100) with a output power of $\approx 100$ mW. The repump transition $5S_{1/2}F=2 \rightarrow 5P_{3/2}F=3$ is $2915.1$ MHz shifted with respect to the trapping transition. A frequency offset lock has been built to lock this laser frequency with respect to the trapping laser, more details are described below. A saturated absorption spectroscopy [$5$] system, see Fig. 3.7 is still available to make the search for the right atomic transition easier.

3.2.1 Modulation Transfer Spectroscopy

The saturation polarization spectroscopy setup that was used before [$5$] to lock the trapping laser has been replaced by modulation transfer spectroscopy [$4$]. This technique is chosen because it is much less sensitive for temperature and intensity fluctuations, and therefore enhances the long term stability. Both methods are based on the detection of Doppler free absorption in a glass cell with Rubidium ($p \approx 2 \times 10^{-7}$ mbar) by using two counter propagating beams, a probe and a pump beam. The absorption of the probe beam is measured with a photo detector.

The modulation transfer spectroscopy is strongly related to the better known frequency modulation spectroscopy [$6$], where a probe beam is frequency modulated so the derivative of some spectroscopic feature can be measured with use of phase sensitive detection. In modulation transfer spectroscopy, not the probe, but a counter propagating pump beam is modulated instead. Only close to an atomic transition, modulation can be transferred from the pump beam to the probe beam by a nonlinear, four wave mixing effect [$4$]. By again performing phase sensitive detection on the probe beam, a signal is acquired that is zero except close to a resonance, see Fig. 3.9. There it has a distinct feature with a zero-crossing exactly at the resonance. The position of this zero-crossing is in first order independent of laser intensities, laser alignment or cell temperature, which makes it ideal for locking.

Our system is a copy of the system described in [$4$] with some minor adjustments to use it with our equipment. The optical configuration is shown in the left bottom corner of Fig. 3.7. An electro-optical modulator (EOM) (Thorlabs EO-PM-NR-C1) operating at $8.2$ MHz is used to modulate the pump beam. A function generator (HP 33120A) creates
the modulation signal, but cannot produce the required voltage for the EOM so a resonant LRC circuit is used to amplify, see Fig. 3.8. The modulation on the probe beam is detected by a photo diode (Thorlabs DET10A) and amplified to the required level, so it can finally be mixed with the modulation signal for phase sensitive detection. The mixing phase can be adjusted by changing the cable length to the mixer, as well as with a small change in frequency due to the LRC resonance of the EOM. As last step, the mixer output is filtered by a high order 30 kHz lowpass filter and amplified.

In Fig. 3.9 the measured signal of the modulation transfer spectroscopy is plotted as function of the laser frequency. To illustrate the improvement, also the (old) signal is plotted measured with saturated polarization spectroscopy. The new signal has a much sharper peak without an offset so the zero-crossing is well defined. By looking at the signal to noise ratio, the frequency fluctuations due to the electronics in the lock system are estimated below 150 kHz.

The spectroscopy signal is used as an error signal for a control loop that locks the laser. The laser frequency can be adjusted by slightly changing the external cavity length by a piezo in the laser and by changing the current through the laser diode. A PID controller (Toptica Laselock) is used that modifies the piezo voltage as well as the current of the laser to get optimal results. The stability of the locked laser is estimated with use of the remaining error signal and gives a \( \text{rms} \) frequency fluctuation \( \approx 1 \) MHz, well below the natural linewidth of \( ^{85}\text{Rb} \).
Experimental setup

3.2.2 Frequency offset lock

The modulation transfer spectroscopy described in previous section does not create a clear signal at the $5S_{1/2}F = 2 \rightarrow 5P_{3/2}F = 3$ transition needed for the repumper. So another solution is needed. This atomic transition frequency is 2915.1 MHz higher than the trapping transition. By using a frequency offset lock system, as described in this section, the repump laser can be locked with a fixed frequency offset with respect to the stabilized trapping laser.

The basic idea of the system is simple. By heterodyning both lasers on a photo detector a beat note is generated with a frequency that is equal to the difference between the lasers. If this beat frequency is exactly the frequency difference between the atomic transitions, the laser is tuned to the right wavelength. A signal proportional to the difference between the beat and the required frequency is needed to stabilize the laser with a feedback loop. This signal can be created by using a phase-locked loop.

Both laser beams (1 mW) are mixed into a single mode fibre, shown in the bottom right corner of Fig. 3.7. A half wave plate is added so the polarization direction of both lasers can be made identical. The beat signal ($\approx 3$ GHz) is measured with a fast fibre-coupled photo-diode (Thorlabs FDS02). A schematic overview of the electronics is given in Fig. 3.10. The beat signal is first amplified to the required level. Processing the signal at these high frequencies is difficult, so the frequency is first reduced by a factor eight with a divider.
Figure 3.10: Block schematic of the frequency offset lock electronics. The beat signal (≈ 3 GHz) is measured by a fast fibre coupled photo diode and then frequency divided by 8 so the processing occurs around 375 MHz. After the signal amplitude is stabilized, the signal enters a phase-locked loop where the voltage controlled oscillator (VCO) is locked to the input frequency by a control loop with phase-sensitive detection. The output of the controller is a measure for the frequency difference in respect to the setpoint. A switch in the output is added so no output signal is created when no beat signal is present.

To make the system independent of input power fluctuations, the signal is amplitude stabilized by a limiter and a band pass filter. The range of this filter (354 – 370 MHz) is chosen to correspond to the required working regime of 2832 to 2960 MHz.

The signal is then fed into a phase-locked loop where it is mixed with the signal from a local oscillator. This is created by a temperature stabilized voltage controlled oscillator (VCO) with a long term stability better than 50 kHz. In the phase-locked loop, the frequency of the VCO is adjusted by the PI controller (180 kHz bandwidth) to make the output of the mixer zero. When that happens, the loop is locked and the VCO has the same frequency as the incoming beat signal. The output of the PI controller is thus a measure for the beat frequency.

The required beat frequency, the frequency set point, can be specified by the set point voltage. This voltage is added to the VCO input, illustrated in Fig. 3.10. The required frequency is generated by the VCO if this voltage is directly applied. So, if the loop is locked,
the output of the controller is proportional to the difference between the beat and the set point frequency, exactly what is needed as error signal.

When there is no input signal, or when it is outside the required frequency window, the phase-locked loop cannot lock. An auto reset feature is added to the PI controller so it keeps searching for a usable signal. Scanning the VCO frequency is needed because the controller can only lock if at some moment the VCO frequency gets close to the input frequency. To prevent output while no suitable beat signal is present, an switch in the output is added. Only when a radio frequent (RF) signal is detected after the band filter, a digital TTL output is generated and the switch is closed; in other cases the output is just zero.

To stabilize the laser frequency, the offset lock system is connected to the PID module (Toptica PID110) of the laser controller. The output of the offset lock system is used as the error signal. To be able to auto relock, additionally the TTL output is connected to the search logic of the PID module. If there is no suitable beat signal, the laser controller now enters into a search mode and scans the laser frequency until the offset lock system detects a input signal in range. From there the PID electronics take over and stabilize the laser.

![Graph](image)

**Figure 3.11:** Measurement to check the absolute accuracy of the frequency offset lock system. The number of trapped atoms in the MOT as function of the offset frequency of the repump lock are shown (squares). The dotted line is a fit. The two vertical lines show the (expected) position of the two transitions.

The remaining error signal is used to estimate the stability of the laser lock, which gives a $\text{rms}$ fluctuation 900 kHz, probably limited by the linewidth of the trapping laser. To have an indication of the absolute accuracy of this lock system in combination with the modulation transfer spectroscopy of the trapping laser, a simple experiment is performed. The number of trapped atoms in the magneto-optical trap (MOT) is measured as function of
the frequency setpoint of the repump laser, shown in Fig. 3.11. The two repump transitions $5S_{1/2}F = 2 \rightarrow 5P_{3/2}F = 2$ and $5S_{1/2}F = 2 \rightarrow 5P_{3/2}F = 3$ separated by 63 MHz can be clearly observed and show that stable and reproducible locking over the whole range is possible. A small shift of the observed peak positions (0.6 MHz and 2.2 MHz) can probably be ascribed to details in the dynamics of the MOT and the interaction of the atoms with the magnetic fields.

3.3 Magneto optical trap

Our UCIS setup uses a standard $^{85}$Rb magneto-optical trap (MOT) configuration [3]. The MOT consists of three orthogonal pairs of counter propagating circularly polarized 780 nm laser beams together with a quadrupole magnetic field.

![Figure 3.12: Schematic illustration of a vapor-cell MOT. In the capture volume, defined by the volume where the laser beams intersect, the atoms can be cooled and trapped. Only particles with a velocity below the capture velocity are trapped (trajectories A and B). Atoms entering the volume with higher velocities will not be trapped (trajectories C and D) and are only deflected.](image)

3.3.1 MOT geometry

There exist different ways of loading the MOT with atoms. The simplest method is used here, namely loading directly from a room temperature rubidium background gas, a so called
vapor-cell MOT. Atoms with a velocity below the capture velocity $v_c$ that enter the capture volume (the area of the intersection of the laser beams) will be cooled and trapped, illustrated in Fig. 3.12. For a Rubidium MOT with typical parameters, $v_c \approx 30 \text{ m/s}$ [7] is relatively high, so sufficient atoms are present in the low velocity tail of the Boltzman distribution to create a substantial atom cloud.

The trapping and cooling beams have a large diameter of roughly 15 mm to enhance the loading of atoms. Typically a red detuning of 16 MHz is used with beam intensities of about 10 mW/cm$^2$. Two of the laser beam pairs are positioned diagonally through the accelerator and vacuum chamber as illustrated in Fig. 3.2. These beams are mixed with light from the repump laser. To make the alignment easier, the beams are retro-reflected to create the counter propagating beams. The downside of this is that at high atomic density a shadow will be cast in these counter propagating beams and cause an imbalance. This limits the maximum density and can create instabilities, for more details see [8]. In future experiments, where higher atomic density is required, they can easily be replaced by two separate beams.

The horizontal beam pair, in the direction of the ion beam, is not retro-reflected and uses two separate laser beams. Because it is impossible to place a laser mirror on the z-axis without interfering with the ions, one laser beam is placed at a small angle of 5 degrees, see Fig. 3.1. The other laser beam is sent in through the bottom of the chamber using the internal mirror in the accelerator. The counter propagating beam enters the chamber through a 16CF window and is focused by a lens ($f = 30 \text{ mm}$) so a divergent beam is created. In this case it can be reflected with a small mirror ($5 \times 5 \text{ mm}^2$) mounted 20 mm from the optical axis, see Fig. 3.1, and still have the right beam diameter at the MOT position. The beam angle and divergence have only a minor effect on the performance of the laser cooling.

The required magnetic field is created by two magnetic coils in anti-Helmholtz configuration that produce a quadrupole field with a gradient of $10 - 20 \text{ G/cm}$ inside the vacuum chamber. The coils are made out of a hollow copper tube, with 4 turns with a diameter of about 100 mm for each coil. The distance between the two coils is about 100 mm. They are water cooled so they can be used with a typical current of 180 A. Three pairs of compensation coils are present around the vacuum chamber to be able to slightly adjust the magnetic zero of the quadrupole, so that the position of the atomic cloud in the MOT can be changed.

### 3.3.2 MOT diagnostics

The fluorescence light of the atomic cloud is imaged on two CCD cameras (uEye 2230-M) positioned at the top and the side of the vacuum chamber, see Fig. 3.2. The side camera uses a window mounted on the ion-getter pump. The top window is also needed for the ionization laser, see next section, so a dichroic mirror is used to separate the two beams, illustrated in Fig. 3.13. A bandpass filter is added to remove the unwanted remaining ionization laser light. The fluorescence light is imaged on the CCD camera as well as a photodiode to measure the dynamics of the MOT such as the loading rate.

The absolute position of the MOT can be calibrated by imaging the holes in the outer
conductor of the accelerator. This is needed to obtain the exact position in the accelerator where the ions will be created. Software has been written to automatically analyze the fluorescence images. The images are fitted with a two dimensional Gaussian distribution. From that the absolute center position and \textit{rms} widths of the trapped rubidium cloud are calculated with a precision of about 0.5 mm. The detected fluorescence power $P_{\text{det}}$ is, after calibration, a measure for the number of trapped atoms $N$ namely:

$$N = \frac{P_{\text{det}}}{\hbar \omega \Gamma f \mu},$$

with $\hbar \omega$ the energy of the emitted photon ($\approx 1.6$ eV), $\Gamma (\approx 6$ MHz) the decay rate from the excited state, $f$ the fraction of atoms in the excited state ($\approx 0.5$) and $\mu$ the detection efficiency ($\approx 5 \times 10^{-5}$). Typically $10^7 - 10^8$ rubidium atoms are trapped in cloud with a Gaussian density distribution with an \textit{rms} radius of 1 mm, which has a central density of $10^9 - 10^{10}$ atoms/cm$^3$.

### 3.4 Ionization

A two-step photo-ionization process [9] is used to ionize the atoms, so only atoms in the cross-section of the two laser beams are ionized. It starts by turning off the trapping laser for several tens of microseconds. Next, a separate, horizontal, focused 780 nm excitation beam is
turned on, which excites a part of the atoms to the $5P_{3/2}F = 4$ state. This excitation beam is mixed with the horizontal trapping beam that enters from the bottom and is reflected by the internal mirror in the accelerator, see Fig. 3.1.

![Figure 3.14: Illustration of the optics on the plateau mounted on top of the vacuum chamber. The light of both ionization lasers, the pulsed dye laser and the fibre coupled diode laser are mixed together and focused into the cold rubidium cloud. The laser spot size is monitored with a CCD camera.](image)

A second laser beam (479 nm) is focused vertically through the atomic cloud, intersecting with the excitation laser beam. It is tuned just above the ionization threshold, so the atoms are ionized while almost no extra energy is added to the system. Two different lasers were used to produce the ionization light. The first laser is a tunable pulsed dye laser system (Quanta-Ray PDL3, rms pulse length 2.5 ns, 100 µJ energy per pulse), pumped by the third harmonic of a Nd:YAG laser. Its repetition rate is limited to 10 Hz by the pump laser. A fraction of the pulse is split off to a wavemeter (Lambdameter LM-007) to precisely monitor its wavelength. The pulse is transported to the plateau on top of the vacuum chamber, see Fig. 3.14, where it is focused into the atomic cloud.

For CW experiments and experiments that need a higher repetition rate, a second laser system is used instead, a commercial frequency-doubled diode laser system (Toptica TA-SHG 110) operating at 479 nm with a power of 250 mW. An acoustic optical deflector (Intraaction ADm-70) is used as shutter, which can produce pulses down to 150 ns FWHM.
with a repetition rate up to 100 kHz. The chopped laser beam is then fibre coupled in a single mode fibre and also transported to the optics platform, where it is directed over the same path as the other laser beam and focused into the cloud.

A small fraction of the light is measured by a photo-detector (Thorlabs DET110) to monitor the timing and intensity. After passing through the final focusing lens, the light gets reflected downwards towards the atomic cloud by the dichroic mirror in Fig. 3.13. A small part of the light leaks through the mirror and is used to measure the laser profile at exactly the MOT position with use of a CCD camera (Sanyo), see Fig. 3.14. The same is done with another camera for the excitation laser beam. The images of both cameras are automatically fitted with a 2D Gaussian distribution function to extract the sizes and positions of the laser spots and thus the ionization volume.

The size of the ionization volume can be controlled by changing or moving the lens so the spot size at the cloud position is changed. The \( \text{rms} \) spot sizes used in the experiments varied from about 25 to 250 \( \mu \text{m} \).

### 3.5 Acceleration voltages

Depending on the experiment a simple DC or a time-dependent voltage is applied to the accelerator structure. The DC voltages are generated by a computer-controlled high-voltage supply (Ultravolt HVRack) that can output voltages from \(-6\) to \(6\) kV.

![Figure 3.15: Schematic overview of the bipolar high-voltage pulser. The output (out) of the pulser can be switched between three states, a positive high-voltage level \(V_p\), zero and a negative high-voltage level \(V_n\) by changing the state with the TTL input signals. A voltage divided output (mon) is available to monitor the output.](image)

Two different systems are used to create the time-dependent voltages. The first system is a homemade bipolar high voltage pulser \((-2500\) to \(2500\) V) based on two Behlke switches, see Fig. 3.15. The output of the pulser can be quickly switched between three states: a positive
high voltage $V_p$, zero and a negative high voltage level $V_n$ created by the DC high-voltage power supply. By combining different states with specific durations, different time-dependent output pulses can be generated. The minimum length of a state is about 100 ns. A repetition rate up to 30 kHz can be used, depending on the voltages, limited by the maximum current of 3.3 mA of the high-voltage power supply. The risetime ($< 50$ ns) is short compared to the time ions stay in the accelerating field. An example output pulse, measured with a high voltage probe while connected to the accelerator is shown in Fig. 3.16.

As second system, a high-speed (5 MHz bandwidth) high-voltage amplifier (Falco WMA-300) is available that can generate output voltages from $-150$ to $150$ V with a risetime of about 100 ns. The input signal of the amplifier is supplied by a computer controlled arbitrary waveform generator (Agilent 33220A). The output is monitored with a high-voltage probe. This system is not limited to simple pulse patterns, but all kinds of waveforms are possible. It can operate reliably at low voltages in contrast to the other system.

### 3.6 Ion beam diagnostics

To measure the properties of the ion beam, a multi-channel plate (MCP) with phosphor screen (Burle) is used, see Fig. 3.17. It has a diameter of 40 mm and is mounted at a distance between 30 cm and 100 cm from the center of the accelerator, depending on the experiment. This device consists of an array of millions of very thin glass capillaries with a diameter of 10 $\mu$m coated with a resistive material. A voltage difference is applied between the front and the back side of the plate, which makes each channel function as an independent
secondary-electron multiplier tube: an incoming ion (or electron) generates some secondary electrons when it hits the wall of a channel, that are again accelerated in the applied field and in turn generate more electrons when they hit the wall, so an avalanche is started. The electrons leaving the MCP are then finally accelerated towards a P20 phosphor screen. A grounded grid in front of the detector (spacing of 5 µm, 50% open area) is used to shield the electric field in the vacuum chamber, in case the front of the MCP is not at ground potential.

![Diagram of the MCP detector assembly with phosphor screen](image)

**Figure 3.17:** Illustration of the MCP detector assembly with phosphor screen. A grounded grid shields the electric field in the vacuum chamber. The spatial distribution is measured with a CCD camera, the time-dependent current is extracted from the phosphor screen and converted to a voltage signal by a transimpedance amplifier.

A CCD camera (Apogee Alta U9000) is used to image the phosphor screen to get the spatial information of the ion beam. It has 3056 × 3056 pixels with a size of 12 × 12 µm. The phosphor screen is imaged on the ccd chip with a single lens (150 mm diameter) with a magnification of 1/1.8. These images are, after background substraction, fitted with a 2D gaussian distribution function, to extract the horizontal and vertical widths of the ion distribution.

In the case of a pulsed ion beam, the temporal distribution of the ion bunch is recorded simultaneously with the images. With use of a transimpedance amplifier (time constant < 10 ns, output 1 V/mA) connected to the phosphor screen illustrated in Fig. 3.17, the time-dependent current is measured on an oscilloscope (Agilent 6000 series, 500 MHz BW). The moment in time the ion bunch starts to be accelerated is defined by the ionization laser beam or the electric field pulse, depending on the experiment. Both are also recorded by the scope, the ionization laser beam by a photodiode and the voltage pulse by a high voltage probe. From these signals the total charge of the bunch (Q), the time-of-flight (T) and the spread in time-of-flight (σT) are extracted.

To measure the absolute charge, the gain of the MCP operating at specific settings needs to be calibrated. Typically a front MCP voltage of −300 V is used and a voltage difference
between the front and the back plate of 1000 V. For the calibration, measurements are performed with a separate Faraday cup, as well as using the MCP itself as charge collector. The absolute charge is then measured with a calibrated charge amplifier (Canberra 2004) and compared with the integrated signal of the transimpedance amplifier. A total average gain of $550 \pm 100$ has been found for the MCP, including the detection efficiency.

3.7 Timing generator

Depending on the exact experiment, a different sequence of steps have to be performed in time for a single measurement. Precise control and stability of the timing sequence is crucial. To make this possible a programmable pulse generator (PPG) has been built together with EAG\textsuperscript{1} based on a field-programmable gate array (FPGA). It has 16 TTL outputs and runs at a clock of 100 MHz, so the smallest timestep is 10 ns. A sequence up to 6144 output states can be defined all with their own durations, enabling the creation of any needed pattern directly by this hardware. Software has been written to be able to easily program the sequence and make it possible to define variables for different elements in the sequence, such as a delay or some pulse length.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{Fig3.18.png}
\caption{Illustrative timing diagram of the experiment. The trapping lasers are turned off before the excitation and ionization laser pulses are switched on. Depending on the experiment, a DC electric field is used, or a pulsed field that is switched on after ionization. After some delay the ion bunch is measured on the MCP.}
\end{figure}

An illustration of a typical timing sequence is shown in Fig. 3.18. After the atoms are laser-cooled and trapped in the MOT, the trapping lasers are turned off with use of the AOM to make it possible to only ionize a small subvolume of the atomic cloud. Next the separate

\textsuperscript{1}the Experiment Automation Group (EAG) at the Eindhoven University of Technology
excitation and ionization beams are turned on, creating the ion bunch. Depending on the experiment, a DC electric field is present or a field is switched on after ionization. Finally the ion bunch is detected when it hits the MCP detector.

### 3.8 Computer control

Due to the complexity of the setup, many different parameters of different (sub)systems have to be controlled and monitored to be able to perform reliable experiments. Furthermore, it is often needed for our measurements to repeat the experiment while other parameters are varied or to scan several parameters simultaneously. To make this possible in an acceptable amount of time, the setup has been automated so it can perform parameter scans and automatically collect the required data. To keep up with the amount of data that can now be relatively easily acquired, also the data analysis of the raw data is automated. In this section more details of the computer control will be discussed.

![Figure 3.19: Schematic overview of structure of the computer control. The main scan controller program controls the hardware in the setup through the connected client programs. Two types of clients exist, hardware clients (HW) and acquisition clients (AQ). See text for more details.](image)

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A flexible modular design is chosen so it is easy to accommodate for changes or additional (sub)systems. A schematic overview of the system, written in c (LabWindows), is given in Fig. 3.19. The central program, the so-called scan controller, arranges all the system parameters and the data acquisition. It does not communicate directly to hardware, but uses specialized client programs to do that instead. The communication between the scan controller and these clients programs takes place over the network so the clients can be located at several different computers.

If a client program connects to the scan controller, it can define one or more scannable parameters, for example the voltage and current setpoint of a power supply. Additional information about the parameter, such as the maximum range and the unit used is also handed out. The information is collected and stored in a internal variable table and displayed on the graphical user interface (GUI). If a parameter is adjusted by a user, the new value is sent to the client which then updates the specific hardware. To perform an automatic scan, a simple script can be loaded in the scan controller that defines the required combinations of parameters and values that need to be scanned.

Figure 3.20: *Simplified flowchart of scan series performed by the scan controller program.*

The clients are divided in two types, the hardware clients and the acquisition clients. The hardware clients are used for devices that have to be set to some specific value before the real measurement takes place, for example the DC acceleration voltage and the ionization pulse length. The acquisition clients represent hardware that collects the data, for example an oscilloscope or a CCD camera.

When a scan starts, it will loop over all the possible combinations of parameters. Every scan step starts with updating all the changed parameters of the clients, as illustrated in
Fig. 3.20. An event system is implemented, so clients can signal the controller when the hardware is updated to the new value and is stable again. The controller waits until all the clients are ready. Subsequently the acquisition clients are signalled that they can start acquiring the data. The destination and filename for the data is distributed by the controller, so the data is stored in an organized way. The controller also saves the specific parameter values at every step. Finally it waits until all the clients are ready, before proceeding with the next scan step until it is finished.

3.9 Conclusion

A reliable experimental setup has been built to perform the ultracold ion beam experiments. A MOT is created inside an accelerator structure and its properties can be observed by looking at the fluorescence light. Enhancements of the frequency lock systems increased the reproducibility and the long term stability of the system. The spatial as well as the temporal distribution of the ion beams can be measured with the MCP detector. And finally, the setup has been automated so it is easier and faster to collect the required data.

Bibliography


Abstract. We present time-of-flight measurements of the longitudinal energy spread of pulsed ultracold ion beams, produced by near-threshold ionization of rubidium atoms captured in a magneto-optical atom trap. Well-defined pulsed beams have been produced with energies of only 1 eV and a root-mean-square energy spread as low as 0.02 eV, two orders of magnitude lower than the state-of-the-art gallium liquid-metal ion source. The low energy spread is important for focused ion beam technology by enabling milling and ion-beam-induced deposition at sub-nm length scales with many ionic species, both light and heavy. In addition, we show that the slowly moving, low energy-spread ion bunches are ideal for studying intricate space charge effects in pulsed beams. As an example we present a detailed study of the transition from space charge dominated dynamics to ballistic motion. A new effect has been observed, space charge-induced energy spread reduction, which is due to a cancellation of acceleration forces by space charge forces.
4.1 Introduction

The importance of Focused Ion Beam (FIB) applications for nanotechnology can hardly be overstated. FIBs are used for structuring at the nanometer scale both by accurate removal of material by sputtering and by high precision ion-beam-induced deposition. For this reason FIBs have become indispensable tools for circuit editing in the semiconductor industry [1]. In addition FIBs enable determination of the elemental, isotopic, and molecular composition of surfaces using Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS), making ToF-SIMS one of the most sensitive surface analysis techniques [2].

FIB performance is presently limited by the properties of the commonly preferred Liquid Metal Ion Source (LMIS). The gallium-based LMIS FIB offers the highest spatial resolution. The smallest focal spot size of $\sim 10 \text{ nm}$, is limited by the energy spread of the Ga$^+$ source [1]. However, to keep up with Moore’s law, the semiconductor industry will soon require milling and deposition at the 1 nm scale. In addition, for ToF-SIMS heavier elements, like cesium, are preferred for their higher sputter yield. In particular the use of ToF-SIMS in the life sciences requires projectiles heavier than Ga [3]. Unfortunately this goes at the expense of spatial resolution, which can only be reached at present with the Ga-based LMIS FIB.

Recently a new ion source was proposed, the Ultra Cold Ion Source (UCIS), which is based on extraction of ions from a laser-cooled atomic gas [4–6]. The UCIS promises a much smaller energy spread than the LMIS at comparable brightness, enabling $\leq 1 \text{ nm}$ focal spot sizes. In addition the UCIS is suited for many elements, in particular the alkalis: Cs for ToF-SIMS with high spatial resolution and high sputter yield; Li as an alternative for He in the recently developed ion microscope [7].

After first preliminary experiments [8], the UCIS potential of delivering beams of LMIS brightness was recently demonstrated [9]. In this paper we present detailed ToF energy spread measurements on rubidium ion bunches extracted from a UCIS. We have produced Rb$^+$ ion beams with a root-mean-squared (rms) energy spread of only $0.02 \text{ eV}$, two orders of magnitude smaller than the state-of-the-art Ga-based LMIS. These extremely low energy spreads have been realized by extracting ion bunches at energies as low as 1 eV. Since energy spread can be conserved during further acceleration, chromatic aberration can be virtually eliminated at beam energies typical for FIB operation, i.e. 30 keV. In combination with the recently measured brightness of such beams [9], this implies that sub-nm focal spot sizes are within reach for Li$^+$, Cs$^+$ and many other ionic species.

The extreme degree of control over beam properties afforded by UCISs opens up completely new applications as well. First, ultra-low beam energies with meV energy spread and nm spatial resolution allow direct ion deposition, highly controlled excitation of localized surface states, and precision surface chemistry, all without sputter damage.

Second, the UCIS in pulsed mode opens up new regimes of space charge dominated beams at very low velocities. As we show in this paper, this allows investigation of intricate space charge effects in slow motion (ion velocities of $\sim 10^3 \text{ m/s}$) and therefore in great detail. As an
example, we have studied the transition from space charge dominated dynamics to ballistic motion. Such a model system is of great importance for the study of ill-understood beam phenomena like space charge-induced instabilities, emittance growth and halo formation. These nonlinear space charge effects play a decisive role in the beam formation for the most demanding applications such as heavy ion fusion, high energy colliders, and free electron lasers. The only system at the moment fully dedicated to the study of such space charge effects is UMER [10, 11], which employs a 10 keV electron beam in a ring.

The basis of a UCIS is a laser-cooled and trapped atomic gas inside a magneto optical trap (MOT), which is ionized by near-threshold photoionization. By applying an electric field a cold ion beam is created, as is schematically illustrated in Fig.4.1. The thermal energy of these ions (100 µK ∼ 10^{-8} eV) is very low, giving rise to a very high brightness. An additional longitudinal energy spread is introduced due to the initial longitudinal size of the ionization volume. A more detailed description of the source and its expected performance is given in our previous paper [4].

**Figure 4.1:** A schematic overview of the experimental setup. A cold cloud of rubidium (a) is trapped inside a cylindrically symmetric accelerator structure (b). After pulsed ionization (c), ions are accelerated to the MCP detector (d) where the temporal distribution is measured (e).

### 4.2 Experimental setup and method

In our experiments we use $^{85}$Rb in a standard vapor cell MOT configuration [12], which consists of 3 orthogonal pairs of circularly polarized 780 nm laser beams. A quadrupole magnetic field with a gradient of 10 G/cm is produced by two coils in anti-Helmholtz configuration placed around the accelerator inside the vacuum chamber. Typically $10^7 - 10^8$ Rb atoms are captured in a cloud with a Gaussian density distribution with an rms radius of
1 mm and a central density of $10^9 - 10^{10}$ atoms/cm$^3$. To produce ions a two step photo-ionization scheme is used. First Rb atoms are excited to the 5p level by the trapping laser, from where the atoms are ionized by a 2.5 ns rms, 480 nm pulsed dye laser tuned just above the ionization threshold. The ionization laser beam is focused through the cold atom cloud in a direction perpendicular to the electric field (see Fig.4.1). In this way a cylinder of charged particles is created with an rms radius $\sigma_R = 32 \pm 1 \mu$m.

DC voltages up to $V_A = 5$ kV are applied across the electrodes, which are approximately 20 mm apart. For technical details of the accelerator structure, see Ref. [13]. The quadrupole magnetic field is kept on, but this has a negligible effect on the trajectories. Charged particles are created at the center of the acceleration region, in a local electric field $E_0 = V_A/d_{\text{eff}}$, where $d_{\text{eff}} = 27$ mm. They travel about 10 mm before exiting the accelerator, resulting in an energy of $U = 0.49eV_A$. The size $\sigma_R$ of the ionization volume in the accelerator field $E_0$ gives rise to an initial rms energy spread

$$\sigma_U = e\sigma_R E_0,$$

so that $(\sigma_U/U)_{\text{initial}} = 0.2 \%$ for $\sigma_R = 32 \mu$m.

At a distance of 29 cm from the accelerator center a MCP detector assembly is used to detect the ions. The temporal distribution is measured by recording the time dependent current with a transimpedance amplifier. The rms time resolution $\tau_D$ of the detection system is $9 \pm 1$ ns, which also includes the laser pulse length.

Time-of-flight (ToF) measurements have been performed by pulsed photo-ionization of the cold atoms in the DC acceleration field. The time-dependent current is recorded on an oscilloscope, together with a photodiode signal of the pulsed laser. The charge $Q$ in a bunch is measured with 5% accuracy by integrating the current signal. Both the photodiode signal and the current signal are fitted with a gaussian distribution to determine the average ToF $T$ and the rms bunch length $\sigma_T$. The ion beam consists of isotopical pure $^{85}$Rb so there is no dispersion due to mass differences. The relative spread in arrival time $\sigma_T/T$ is therefore a measure for the longitudinal energy spread $\sigma_U/U$ in the bunch:

$$\frac{\sigma_U}{U} = \frac{2\sigma_T}{T} \frac{1}{(1 - \epsilon)},$$

where $\epsilon \approx 0.13$ is a geometric correction factor.

### 4.3 Results

Measurements of the energy spread as function of the beam energy are shown in Fig. 4.2. Different curves correspond to different amounts of charge in a bunch, ranging from $Q = 0.026$ fC to $Q = 13$ fC. The results shown are averages over 10 bunches. At higher voltages $\sigma_T$ is close to the time constant $\tau_D$ of the detection system, so a deconvolution is performed by quadratically subtracting $\tau_D$. 

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Two different regions can be clearly observed in the plot. At higher acceleration voltages the curves of the different bunch charges coincide, implying that space charge forces only play a minor role. In this region the relative energy spread $\sigma_U/U$ is less than 0.2 %, as expected on the basis of Eq. (4.1). At lower voltages, however, the curves clearly depend on the charge in the bunch, and thus space charge is important in this region. With beam energies as low as 1 eV, this is not unexpected. At these low energies it is possible to produce beams with an rms energy spread $\sigma_U = 0.02$ eV, two orders of magnitude lower than the LMIS.

### 4.4 Simulations

To get a better understanding of the behavior, particle tracking simulations have been performed with the use of the GPT code [14]. The DC electric field inside the accelerator has been calculated with the Superfish poisson solver [15]. All the ions in the bunch are tracked individually with all mutual Coulomb interactions included, using the Barnes Hutt algorithm [16] to reduce the calculation time.

In Fig. 4.2 the simulation results are shown for five different charges. The directly calculated energy spread is indicated by dotted curves. Also the same procedure used in the

![Figure 4.2: Measured energy spread $\sigma_U$ as function of the beam energy $U$ for various bunch charges (scatter plots) together with the results of the GPT simulations (dotted and solid curves). The dotted curves have been calculated directly in the GPT simulations; the solid curves have been calculated by applying the ToF procedure of Eq. (4.2).](image-url)
experiment can be performed, by using Eq. (4.2) (shown as solid lines). Both are in remarkably good agreement with the experimental data, without any fit parameter.

The observed behavior can be fully explained in terms of space charge forces and acceleration fields, the only ingredients in the GPT simulation. This implies that all the data can be scaled to a single curve by dividing both the acceleration voltage and the observed energy spread by the bunch charge, as shown in Fig. 4.3.

### 4.5 Analytical model

The energy spread at higher acceleration voltages is dominated by the initial spread in position in the acceleration field due the size of the ionization volume, as described by Eq. (4.1). In this region the energy spread depends linearly on the acceleration voltage, indicated by the dashed line in Fig. 4.3.

\[
\sigma \sim \sqrt{U}
\]

This can be understood as follows; The space charge expansion takes place on a timescale \( \sim \omega_p^{-1} \) with \( \omega_p = \sqrt{n_{ion} e^2 / (m \epsilon_0)} \) the plasma frequency, \( n_{ion} \) the initial peak ion density, \( m \) the ion mass, and \( \epsilon_0 \) the permittivity of free space. In the region where the square root behavior appears, the bunches move so slowly that most of the internal (space charge) potential energy in the bunch has been converted into kinetic energy before it

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**Figure 4.3:** The five measured energy spread curves from Fig. 4.2 scaled by the bunch charge to a single curve. The simple analytical model given by Eq. (4.3) (dotted and solid lines) and Eq. (4.1) (dashed line) are plotted. The inset shows the data without the scaling.
hits the detector. In that case for each particle the asymptotic velocity \( v_{sp} \) due to the space charge expansion can be added to the velocity \( v_0 \) due to the accelerating fields. The energy spread is then given by:

\[
\sigma_U = \frac{1}{2} m \left( \langle (v_0 + v_{sp})^2 \rangle - \langle v_0 + v_{sp} \rangle^2 \right) = m \sigma_{v_{sp}} \langle v_0 \rangle, \tag{4.3}
\]

where \( \langle \rangle \) denotes averaging over all the particles and \( \sigma_{v_{sp}} \) is the rms space charge expansion velocity. Since \( v_0 \sim \sqrt{U} \) this model gives indeed the observed square root behavior.

The asymptotic space charge velocity \( v_{sp} \) can be easily calculated for a uniform sphere. With a correction factor \( \eta \) for the geometry this can be used to estimate the final space charge velocity for the gaussian, cylindrically shaped bunch:

\[
\sigma_{v_{sp}} = \eta \sqrt{\frac{2}{3}} \sigma_R \omega_p. \tag{4.4}
\]

In Fig. 4.3 the resulting model curve, obtained by combining Eq.(4.3) and Eq.(4.4) and taking \( \eta = 0.4 \), is indicated by a dotted line. It shows good agreement with the measured data. In the inset the separate curves for the different charges, without the scaling, are plotted together with the measured data.

**Figure 4.4:** Measurements (scatter plots) of \( \sigma_U/U \) as function of \( U \) for \( \sigma_R = 32 \) and 180 \( \mu \text{m} \), with respectively, \( Q = 0.42 \text{ fC} \) and \( Q \approx 0.5 \text{ fC} \). Also shown are simulation results for \( \sigma_R = 180 \mu \text{m} \) (solid line), \( \sigma_R = 110 \mu \text{m} \) (dashed line), \( \sigma_R = 32 \mu \text{m} \) (dotted line).

## 4.6 Crossover region

In the crossover region around the intersection of the dashed and the dotted lines, where both space charge forces and the initial size contribute, an interesting effect occurs for large values
of $\sigma_R$. In Fig. 4.4 $\sigma_U/U$ is plotted as a function of $U$ for $\sigma_R = 180 \, \mu\text{m}$ and $\sigma_R = 32 \, \mu\text{m}$ with, respectively, $Q \approx 0.5 \, \text{fC}$ and $Q = 0.42 \, \text{fC}$. At high voltages we find that the relative energy spread goes to a constant value (Eq.(4.1)), which can indeed be controlled by changing the size of the ionization volume. This implies that even much lower relative energy spreads can be achieved than reported in this paper by further reduction of the ionization laser beam waist. At the lowest voltages again space charge dominates, so $\sigma_U/U \propto U^{-1/2}$.

In the crossover region ($10 \, \text{eV} < U < 100 \, \text{eV}$) however, the relative energy spread for $\sigma_R = 180 \, \mu\text{m}$ is significantly lower than the asymptotic high-voltage value. In this region space charge forces apparently give rise to a reduction of the relative energy spread. This counterintuitive effect can be understood as follows: in the high-energy regime, where space charge effects can be neglected, the particles in the back of the bunch acquire a higher velocity than the ones in front, simply because they are accelerated over a longer distance. In the low-energy space charge dominated regime, on the other hand, the particles in the back acquire a lower velocity than the ones in front as they are decelerated by space charge forces. In the crossover regime these two effects cancel, leading to a further reduction of the relative energy spread. Related effects have been predicted in simulations of high-density electron bunch dynamics [17, 18]. GPT calculations also show this behavior for large values of $\sigma_R$ (see Fig. 4.4). The agreement between simulation and experiments for $\sigma_R = 180 \, \mu\text{m}$ is not as good as for $\sigma_R = 32 \, \mu\text{m}$, which we attribute, at least partially, to distortion of the ionization laser beam profile. Further investigation is required to understand the detailed mechanism behind this subtle and possibly useful effect.

### 4.7 Conclusions

In summary, we have presented time-of-flight energy spread measurements on ion-bunches from an ultra cold ion source, which show that very low energy spread ion beams can indeed be produced. This result will certainly hold for continuous operation of the source, because space charge effects will be much less important at demonstrated currents of 1.4 pA [9] and achievable currents of 100 pA [4]. The lowest energy spread observed here, $\sigma_U = 0.02 \, \text{eV}$, constitutes a two orders of magnitude improvement over the state-of-the-art Liquid Metal Ion Source. Well-defined, low-divergence, monochromatic beams with energies of only 1 eV have been produced, creating entirely new possibilities for highly controlled ion-surface interaction, without sputtering damage. In addition, we have shown that the slowly moving ion bunches provide a model system for studying space charge effects in pulsed beams. The transition from space charge dominated dynamics to ballistic flight has been studied in great detail. Furthermore a new effect has been observed, space charge induced energy spread reduction, that could be used to lower the energy spread even further.
Bibliography


Time-dependent manipulation of ultra-cold ion bunches: Part I

Abstract. All applications of high brightness ion beams depend on the possibility to precisely manipulate the trajectories of the ions, or more generally, to control their phase-space distribution. We show that the combination of a laser-cooled ion source and time-dependent acceleration fields gives new possibilities to perform precise phase-space control. We demonstrate reduction of the longitudinal energy spread and realization of a lens with control over its focal length and sign, as well as the sign of the spherical aberrations. This creates new possibilities to correct for the spherical and chromatic aberrations which are presently limiting the spatial resolution.

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2In chapter 6 the results of this chapter are repeated in a more detailed discussion.
Chapter 5.

5.1 Introduction

High brightness ion beams are crucial for a variety of applications such as focused ion beam (FIB) systems [1] and ion microscopes [2]. Recently, a new kind of ion source was proposed, the ultra cold ion source (UCIS) [3, 4], based on laser-cooled atoms. The UCIS is characterized by a low effective source temperature [5] and an extended source size [3]. Compared to liquid metal ion sources (LMIS) [7] and ionic liquid ion sources [8] it offers the advantage of a much reduced energy spread [6] and thus reduced chromatic aberration in FIB columns at comparable (predicted) brightness. In comparison with the He-gas field emission source [2], the brightness is lower, but stable operation is possible with isotopically pure and strictly singly ionized beams of several ionic species, both light (e.g. Li\(^+\)) as well as heavy (e.g. Rb\(^+\), Cs\(^+\)). This makes it an attractive source for ion microscopy as well for sputtering applications. In this Letter we show that, additionally, the UCIS enables manipulation of the ions by time-dependent electric fields to control both the longitudinal and the transverse phase-space distribution. Not only linear, but also higher order beam manipulations are possible, which opens exciting new possibilities to correct for spherical and chromatic aberrations which are presently limiting the spatial resolution [1].

The idea of time-dependent manipulation has been discussed before. In secondary ion mass spectroscopy [9, 10] for example, it is used to improve the mass resolution. Aberration correction with time-dependent electric [11, 12] and magnetic fields [13] has been the subject of several theoretical studies, but has not yet been demonstrated experimentally [11]. The use of time-dependent fields to manipulate ion bunches is therefore not limited to the UCIS source; however, the properties of the UCIS make practical implementation easier. The low initial thermal velocities and the extended source area of the UCIS allow the creation of well-defined beams at very low energies [6]. The small velocities of the ions then allow temporal manipulation at experimentally feasible timescales. In this Letter, we demonstrate how this may be used for reduction of the longitudinal energy spread caused by the initial size of the source, the limiting factor up to now [6]. We also show that it is possible to create a versatile, fully adjustable lens with control over the sign of the focal length and the spherical aberration coefficient. Importantly, we circumvent Scherzer’s theorem [11, 14], a major restriction in conventional static cylindrical systems, which states that spherical aberration coefficients are always positive, so cancellation of the aberration is not possible. With time-dependent fields there is no such restriction. We show that by switching the lens voltage, the sign of the coefficient can be reversed. This may lead to the development of aberration-corrected focusing columns.

5.2 Theory time-dependent manipulation

In our UCIS experiments, a laser-cooled atomic cloud is trapped inside a cylindrically symmetric accelerator structure. Part of the cloud is pulsed ionized to create ion bunches, which
Figure 5.1: A schematic overview of the experimental setup. A laser-cooled cloud of rubidium (a) is trapped inside a cylindrically symmetric accelerator structure (b). After pulsed ionization (c), ions are accelerated to the MCP detector (d) where both the transverse spatial distribution (e) and the temporal distribution are measured (f).

are subsequently accelerated in the z-direction, see Fig. 5.1. The symmetry of the system makes it possible to write the complete field as an expansion in the z-component of a (static) on axis electric field $E_z(z)$ [15]. The time-dependent electric field is modeled as $E_z(z, t) = e_z(z)\alpha V_a(t)$, with $V_a(t)$ the time-dependent anode voltage and $e_z(z) = E_z(z)/\int_0^\infty E_z(z)dz$ the normalized electric field distribution on axis, with $\alpha$ the ratio of the potential on the position of the ions and the potential at the cathode. If the bunch size does not change much during acceleration, then the characteristic transverse momentum spread $\Delta p_r$ and the characteristic longitudinal momentum spread $\Delta p_z$ outside the accelerator field are given by

$$\Delta p_r = q\alpha \int_0^\infty V_a(t) \left(-\frac{1}{2} e'_z(z)\sigma_{r_0} + \frac{1}{16} e''_z(z)\sigma^3_{r_0} + \ldots\right) dt,$$

$$\Delta p_z = q\alpha \int_0^\infty V_a(t) \left(\frac{1}{2} e'_z(z)\sigma_{z_0} + \frac{1}{2} e''_z(z)\sigma^2_{z_0} + \ldots\right) dt,$$

where $q$ is the ion charge, $\sigma_{r_0}$ the initial root mean square (rms) transverse size, $\sigma_{z_0}$ the initial rms longitudinal size, and a prime denotes the derivative with respect to $z$.

The anode voltage function $V_a(t)$ enables independent control of both the linear and higher order terms in the expansion. This is illustrated in Fig. 5.2a where the first term of these expansions is shown as a function of $z$. By switching with a unipolar (Fig. 5.2b) or a bipolar pulse (Fig. 5.2c), the contributions of the different field terms in Eq. (5.1) can be changed.

### 5.3 Experimental Setup

Our UCIS consists of a rubidium-85 vapor-cell magneto-optical trap (MOT). Typically $10^8$ Rb atoms are trapped in a cloud with a $\text{rms}$ radius of 1 mm. A two-step photo-ionization process
is used to selectively ionize a small volume inside the trapped atomic cloud, see Fig. 5.1: a focused 780 nm laser beam propagating along the z-direction, excites atoms to the 5p level. A 479 nm laser beam perpendicular to the excitation beam, ionizes a fraction of the excited atoms, creating an ion bunch with initial sizes $\sigma_z = 200 \pm 20 \mu m$ and $\sigma_r = 250 \pm 30 \mu m$. For details of the accelerator structure, see [16]. The anode voltage $V_a$ can be switched between three states: zero, a positive high voltage level ($V_p$), and a negative high voltage level ($V_n$) with a switch time of 50 ns.

At a distance $L = 0.64$ m from the center of the accelerator, a 40 mm diameter multi channel plate detector (MCP) with phosphor screen is mounted. A CCD camera is used to capture images of the phosphor screen that contain the spatial information of the ion bunches. Simultaneously the temporal distribution of the ion bunch is recorded on an oscilloscope by using a transimpedance amplifier connected to the phosphor screen. From the oscilloscope signal the total charge $Q$ of the bunch, the time-of-flight $T$ to the detector and its rms spread $\sigma_T$ are extracted. The beam energy $U$ is calculated from $T$ with $U = (1/2)m(L/T)^2$, and the relative energy spread $\sigma_U/U$ is given by the relation $\sigma_U/U = 2\sigma_T/T$.

### 5.4 Results longitudinal manipulation

In Fig. 5.3a we present results of the longitudinal phase-space manipulation. By time-of-flight measurements, the beam energy $U$ and the relative energy spread $\sigma_U/U$ were determined. The relative energy spread $\sigma_U/U$ due to the acceleration can be approximated by $\sigma_U/U = 2\Delta p_z/p_z$, with $p_z$ the average ion momentum, and $\Delta p_z$ given by Eq. (5.1b). First we look
Figure 5.3: Results of measurement with a unipolar voltage pulse. The beam energy \( U \) is varied by changing the pulse duration \( \tau \) from 100 ns up to 2 \( \mu \)s while keeping \( V_p \) constant. Three curves (black, red and blue squares) with respectively \( V_p = 1000, 500 \) and 250 V are shown. In a) the longitudinal relative energy spread \( \sigma_U/U \) versus \( U \) is plotted and in b) the transverse size on the detector \( \sigma_x \) in the x-direction versus \( U \). Additionally a DC- measurement (purple circles) is presented where \( V_p \) is varied. Particle tracking simulations are depicted as solid curves (unipolar pulses) and a dashed curve (DC).

at the DC-measurements, indicated by the purple circles in Fig. 5.3a. For the DC case \( (V_a(t) = \text{constant}) \) Eq. (5.1)b results to the lowest order in \( \sigma_{z_0} \) in \( \sigma_U/U = \sigma_{z_0}|e_z(0)| \), with \( e_z(0) \) the normalized electric field at the initial position of the bunch \( (z = 0) \). Because \( U \) and \( \sigma_U \) are both proportional to the acceleration voltage, the relative energy spread \( \sigma_U/U \) is independent of beam energy, as is clearly illustrated by the data in Fig. 5.3a. In DC fields, a small relative energy spread can therefore be realized only by choosing a small initial \( \sigma_{z_0} \).

By using time-dependent fields \( \sigma_U/U \) can be reduced without changing \( \sigma_{z_0} \); with a unipolar switch function of duration \( \tau \), the accelerating field can be turned off while the ion bunch is still being accelerated. The time spent in the field is then the same for all ions, independent of their initial position. From Eq. (5.1b) then follows (in lowest order)

\[
\frac{\sigma_U}{U} = \sigma_{z_0}|e_z(z_s) - e_z(0)|, \tag{5.2}
\]

with \( z_s \) the position of the center of the bunch when the field is turned off \( (t = \tau) \). If the field is switched off after the ions have left the accelerator field, Eq. (5.2) reduces to the expression derived for the DC-case. In the idealized case of a perfectly homogeneous electric field inside
the accelerator, i.e. $e_z(z_s) = e_z(0)$, the first term exactly cancels the second term in Eq. (5.2). If the field is not homogeneous, the first term still partially reduces the energy spread.

In Fig. 5.3a measurements are shown performed with such a unipolar pulse, indicated by black, red and blue squares. The relative energy spread $\sigma_U/U$ is measured as a function of $U$ by varying $\tau$ from 100 ns up to 2 $\mu$s. The measurements have been done for three different $V_p = 2000$ V, 1000 V and 500 V at a bunch charge of $\approx 0.5$ fC. The encircled points correspond to pulse durations for which the ions have already left the accelerator at $t = \tau$, and are therefore not influenced by the field switching. In that case the relative energy spread coincides with the DC measurements. For shorter $\tau$, both $U$ and $\sigma_U$ are reduced, but $\sigma_U$ reduces more than $U$, because the influence of the field derivatives in Eq. (5.1b) is smaller. For even shorter $\tau$, $T$ becomes so long that space charge effects start to increase $\sigma_U$. This is the same effect as observed in [6]. In the region where space-charge effects are not important, the curves for different $V_p$ have the same shape and can in fact be made to overlap by scaling the $U$ axis proportional to $V_p$.

To quantitatively understand the measurements, particle tracking simulations were performed with the GPT [17] code. The electric field inside the accelerator was calculated with the SUPERFISH Poisson solver [18]. All the ions in the bunch are tracked individually with all mutual Coulomb interactions included. The initial conditions are the same for all simulations, and are chosen with values within measurement uncertainty. The simulation results are depicted as dashed (DC) and solid (unipolar switch) curves in Fig. 5.3. Good agreement with the data is obtained. Small deviations from the simulations occur in the low-energy region, where space-charge effects become significant. A reduction of a factor of three of the relative energy spread is obtained. To improve the reduction even further, optimization of the field shape is required.

5.5 Results transverse manipulation

Now we discuss manipulation of the transverse phase-space. Simultaneously with the time-of-flight signals, the spatial ion bunch distribution on the detector was captured by the CCD camera. This is shown in Fig. 5.3b where the transverse spot size $\sigma_x$ on the detector is plotted as a function of $U$. The behavior in longitudinal ($z$) and transverse ($x$) direction is very similar, as expected in view of the strong similarities between Eqs. (5.1a) and (5.1b).

The divergent field at the exit hole of the accelerator structure acts as a lens with a focal strength given by $1/f = -\Delta p_r/(\sigma_{r_0} p_z)$. The lens effect is described by the first term in the expansion in Eq. (5.1a). When the bunch velocity is assumed constant while passing through the divergent part of the field, a simple expression can be derived. In the DC-case this results in $1/f = -1/4e_z(0)$, corresponding to a negative focal length $f = -33$ mm for our accelerator structure. This lens effect can be observed in the DC measurements (purple circles) in Fig. 5.3b. At high energy the bunch size is increased due to the lens by a constant factor of 16 compared to the initial size, at lower energies ($U < 200$ eV), the spot blows up.
even further due to space charge.

The results of the unipolar experiments are indicated by the black, red and blue symbols in Fig. 5.3b. For this unipolar case, the focal strength can be written as

\[
\frac{1}{f} = \frac{1}{4} \left( e_z(z_s) - e_z(0) \right).
\]  

(5.3)

The encircled points of the curves correspond to measurements where \( \tau \) is again so long that the ions experience the full divergent field. When \( \tau \) is reduced, the field is switched off while the ions are still in a divergent part of the field, so the radial momentum spread \( \Delta p_r \) is reduced (see field diagram in Fig. 5.3b). As is clear from Eq. (5.3), the negative lens strength is then also reduced, resulting in a smaller spot on the screen. At even shorter \( \tau \), and thus lower \( U \), space-charge starts to increase the spot size again.

Instead of simply turning the field off with a unipolar pulse, it is also possible to change the sign of the radial electric field with a bipolar pulse (see Fig. 5.4). By choosing a suitable bipolar pulse, the radial momentum an ion receives can be inverted, so the diverging accelerator field can now be used as a positive lens. For this pulse the focal strength can be approximated with

\[
\frac{1}{f} = \frac{1}{4} \left( \frac{V_p}{V_n} e_z(z_s) - e_z(0) \right).
\]  

(5.4)

Clearly, the focal strength can be controlled by changing the duration and amplitudes of the pulse. As a side effect, also the field in the \( z \)-direction is reversed, so the ions start to decelerate.

In Fig. 5.4 measurements are shown of the spot size on the detector when a bipolar pulse with \( V_p = 1000 \) V and \( \tau = 633 \) ns is applied. The negative voltage \( V_n \) has a duration longer than the time the bunch spends in the accelerator. The figure clearly shows that when \( V_n \) is increased, the bunch first focuses on the detector and then starts to over-focus. Phosphor screen images are added to illustrate the effect. The bunch is focused on the detector when \( V_n = 540 \) V; in that case it is accelerated to \( U = 280 \) eV with the positive pulse and decelerated to \( U = 180 \) eV by the negative pulse. Again, measurements agree well with particle tracking simulations, indicated by the solid curve.

So far, we have shown that we can control the linear term in Eqs. (5.1a) and (5.1b) with the time-dependent fields, but clearly control of higher orders is also possible. As a demonstration we change the spherical aberration due to the exit fields of the accelerator. To determine the amount of spherical aberrations the transverse position \( x \) on the detector is measured as a function of the initial position \( x_0 \). The position \( x_0 \) is changed by moving the ionization laser focus. When the exit lens is aberration free, the relation between \( x_0 \) and \( x \) is simply linear \((x = Ax_0)\); when spherical aberrations are present, a third order term appears \((x = Ax_0 - Cx_0^3)\) which is the result of the \( e_z''' \) term in Eq. (5.1a). By changing \( V_a(t) \) the integral of this term can be controlled (see diagrams Fig. 5.5). From the linear coefficient \( A \) the focal length is obtained by \( f = -L/(A - 1) \) and the third-order coefficient \( C \) is related to the \( C_s \) coefficient by \( C_s = f^3C \), if the bunch is focused on the detector. The spotsize
$\delta_s$ due to spherical aberrations in a focusing system is given by $\delta_s = C_s \alpha^3$, with $\alpha$ the lens acceptance angle [11].

A bipolar and a tripolar switch function were used in the experiment in Fig. 5.5. For each, three measurements are shown with $f \simeq L$. A horizontal line ($A = 0$) would correspond to a focus precisely on the detector, a positive linear slope to a focus behind the detector and a negative slope to a focus in front of the detector. In Fig. 5.5a the deviation from linear behavior is clear, and fits well with a third order term (solid curves). The bipolar pulse results in $C_s = -1.1 \pm 0.1 \times 10^4$ m. By changing only to a tripolar pulse Fig. 5.5b, the sign of the aberration coefficient is reversed to $C_s = 4.0 \pm 0.2 \times 10^4$ m. This shows that manipulation with time-dependent fields can be used to achieve aberration corrected systems.

5.6 Conclusion

In conclusion, we have shown that phase-space manipulation of ultra cold ion beams with time-dependent acceleration fields is experimentally feasible. We have shown that a unipolar pulse can be used to reduce the relative energy spread, a bipolar pulse can be used to change the sign of a lens, and finally, a tripolar pulse can be used to change the sign of the spherical aberration coefficient. Even more complex pulses will enable further possibilities.
Figure 5.5: Demonstration of the sign reversal of the spherical aberration coefficients. The position $x$ of the ion bunch on the detector is recorded as function of the initial ionization volume position $x_0$ (scatter plots). In all measurements $V_p = 1000$ V. The curves are fitted with the relation $x = Ax_0 - Cx_0^3$ (solid curves). Results are shown of measurements using (a) a bipolar pulse ($C < 0$) and (b) a tripolar pulse ($C > 0$).

Bibliography


Abstract. Recently a new kind of high-brightness ion source has been introduced, the ultra cold ion source (UCIS) based on photo-ionization of laser-cooled atoms. In this paper we show that the combination of such a source and time-dependent acceleration fields opens new possibilities. Precise manipulation of the bunch distribution in both longitudinal and transverse phase-space is made possible. We demonstrate reduction of the longitudinal relative energy spread by switching the field. In transverse direction we present the realization of a lens with control over its focal length and sign, as well as the sign and strength of the spherical aberrations by only changing the time-dependent fields. The experimental results of both effects is investigated on the basis of a simple analytical model and precise particle tracking simulations.
6.1 Introduction

A new kind of ion source [1, 2] has recently been introduced that is interesting for high-brightness applications. High brightness is achieved by going to very low temperatures, instead of reducing the emission area of the source. This source, the ultra cold ion source (UCIS), is based on the photo-ionization of laser-cooled atoms trapped in a magneto-optical trap (MOT). It can have a brightness that is comparable [3] to the current industry standard Ga-liquid metal ion source (LMIS) [4], but with much lower energy spread, as we showed recently [5]. In addition, many different elements can be used, in particular the alkali-metals. Light species, such as Li, are interesting for ion microscopy applications [6], while heavier elements, as for example Cs, are useful for sputtering applications.

The low energy spread enables the creation of well-defined beams at energies as low as a few eV [5]. The combination of low beam energies and pulsed operation of the UCIS make it possible to change the acceleration field while the ions are being accelerated. The utilization of time-dependent acceleration fields enables the control of both the longitudinal and the transverse phase-space distribution of the ion bunch. Not only linear, but also higher order beam manipulations are possible, which opens new possibilities to correct for spherical and chromatic aberrations which are presently limiting the spatial resolution [7].

The idea of time-dependent manipulation has been discussed before. In (time-of-flight) Secondary Ion Mass Spectroscopy (SIMS) [8] for example, which can be used to obtain the chemical composition of a surface, it can be used to improve the mass resolution. By using time-dependent fields, short primary ion bunches can be created [9], as well as time-focusing of the secondary ions [10, 11]. Also aberration correction with time-dependent fields has been the subject of several theoretical studies [12], but has not yet been demonstrated experimentally. In Ref. [13] a scheme is proposed to perform spherical and chromatic aberration compensation in an electron microscope with switched electric fields. In Ref. [14] the aberrations of a time-dependent magnetic lens has been studied theoretically.

Recently, we demonstrated manipulation of ultra cold ion bunches with time-dependent fields [15]. In this paper we will present additional measurements and discuss the experimental results in more detail. We start in section 6.2 by deriving a simple general model to get insight into bunch manipulation with time-dependent fields in both the longitudinal and the transverse directions. Next, in section 6.3, we apply the model to describe the linear bunch manipulation for several specific pulse shapes, that are also used in the experiment. The experimental setup is briefly discussed in section 6.4. In section 6.5 we present the experimental results of longitudinal phase-space manipulation. We show that the relative energy spread of the bunch can be reduced by switching the field off while the bunch is still in the accelerator. In section 6.6 we present experimental results of transverse bunch manipulation. We show that by using more complex pulse shapes, the accelerator field can be used as an adjustable lens with control of both the strength and the sign of the lens. And finally, in Sec. 6.7, we demonstrate that also non-linear manipulation is possible. We present
measurements that show that the strength and the sign of the spherical aberration coefficient of the lens can be controlled by only changing the time-dependent acceleration voltage.

6.2 Model of time-dependent bunch manipulation

The concept of time-dependent bunch manipulation is simple; if an ion-bunch is created inside an accelerating electric field, the field can be changed in time by applying a time-dependent voltage to the accelerating structure. The effective field the ions experience while being accelerated can thus, within some limits, be controlled without the need to change the geometry. For time-scales relevant for the ions, induced magnetic fields and propagation of electromagnetic waves in the structure do not play any significant role. The time-dependent electric field is thus simply the static electric field that is rescaled in time.

In this section a simple model is derived to shed light on the principle of bunch manipulation with these time varying fields. This model will also be used in the subsequent sections to explain the experimental results. In our UCIS experiment described in this paper, we create cold ion bunches from a laser-cooled atomic cloud, illustrated in Fig. 6.1. A part of the cold atomic cloud, located in the center of an accelerator structure, is pulse-ionized so an ion bunch is created that is accelerated in the $z$-direction. Both the longitudinal as well as the transverse phase-space of the bunch will be affected by the time-dependent field.

![Figure 6.1: A schematic overview of the experimental setup. A laser-cooled cloud of rubidium (a) is trapped inside a cylindrically symmetric accelerator structure (b). After pulsed ionization (c), ions are accelerated to the MCP detector (d) where both the transverse spatial distribution (e) and the temporal distribution are measured (f).](image-url)

In the experiment a cylindrically symmetric accelerator structure is used. The symmetry of the system makes it possible to write a static acceleration field $\vec{E}(r,z) = E_r \vec{e}_r + E_z \vec{e}_z$ as
an expansion in the z-component of the on-axis electric field $E_{0z}(z)$ [16]:

$$
E_r(r, z) = -\frac{1}{2} E_{0z}'(z)r + \frac{1}{16} E_{0z}''(z)r^3 + \cdots ,
$$

(6.1a)

$$
E_z(r, z) = -E_{0z}(z) - \frac{1}{4} E_{0z}''(z)r^2 + \cdots ,
$$

(6.1b)

where a prime denotes the derivative with respect to $z$ and $r$ is the radial direction.

If a time-dependent anode voltage $V_a(t)$ is applied, the electric field $\vec{E}$ varies in time. Then it is convenient to introduce the static normalized field distribution $e_z(z) = E_{0z}(z)/\phi(z_0)$, with $z_0$ the starting position of the ions and the (static) potential given by $\phi(z) = \int_z^{\infty} E_{0z}(z')dz'$. Due to this definition $e_z(z)$ has the unit of $1/m$. In the experiment the potential at the anode $\phi(z_a)$ is directly controlled, but not the potential $\phi(z_0)$ at the initial position of the ions. By defining $\alpha = \phi(z_0)/\phi(z_a)$ for the static field, the time-dependent field on axis can now be written as $E_z(z, t) = e_z(z)\alpha V_a(t)$.

![Figure 6.2: Schematic drawing of the test particles in the bunch used in the calculation.](image)

The acceleration field is in general not homogeneous, so particles at different positions inside the bunch experience different forces. To describe these effects, we consider the difference in electric field between a test particle and the center particle, as is illustrated in Fig. 6.2. We consider two kinds of test particles: one that is displaced radially (white circle), and one displaced longitudinally in the z-direction (gray circle). The characteristic behavior of the bunch can be obtained by placing the test particles at an initial displacement equal to the rms bunch sizes, respectively $\sigma_{r_0}$ and $\sigma_{z_0}$. By writing the field difference as a series expansion in the displacement, the characteristic relative momenta $\Delta p_r$ and $\Delta p_z$ of the test
particles after acceleration with respect to the central particle can be calculated:

\[ \Delta p_r = q \alpha \int_0^\infty V_a(t) \left( -\frac{1}{2} e'_z(z(t)) \sigma_r(t) + \frac{1}{16} e''_z(z(t)) \sigma_r(t)^3 + \ldots \right) dt, \]  
\[ \Delta p_z = q \alpha \int_0^\infty V_a(t) \left( e'_z(z(t)) \sigma_z(t) + \frac{1}{2} e''_z(z(t)) \sigma_z(t)^2 + \ldots \right) dt, \]

where \( q \) is the ion charge and \( z(t) \) describes the position in the field of the center particle; \( \sigma_r(t) \) and \( \sigma_z(t) \) describe the bunch size as function of time, and thus the relative position of the test particles.

The model can be simplified by assuming that the relative positions of the test particles with respect to the center particle do not change during acceleration, so \( \sigma_r(t) = \sigma_{r0} \) and \( \sigma_z(t) = \sigma_{z0} \). Furthermore, an anode voltage switch function \( \tilde{V}_a(z) \) can be defined as function of the center position of the bunch instead of time. This results in

\[ \Delta p_r = q \alpha \int_{z_0}^{\infty} \frac{\tilde{V}_a(z)}{v_z(z)} \left( -\frac{1}{2} e'_z(z) \sigma_{r0} + \frac{1}{16} e''_z(z) \sigma_{r0}^3 + \ldots \right) dz, \]  
\[ \Delta p_z = q \alpha \int_{z_0}^{\infty} \frac{\tilde{V}_a(z)}{v_z(z)} \left( e'_z(z) \sigma_{z0} + \frac{1}{2} e''_z(z) \sigma_{z0}^2 + \ldots \right) dz, \]

with \( v_z(z) \) the velocity of the center of the bunch as function of its position.

Equations (6.3) clearly show that the anode voltage function \( \tilde{V}_a(z) \) enables independent control of both the linear and higher order terms in the field expansion and thus phase-space manipulation of the bunch. This is illustrated in Fig. 6.3. In Fig. 6.3a the situation is shown...
for a constant anode voltage $V_a$. By switching with a unipolar (Fig. 6.3b) or a tripolar pulse (Fig. 6.3c), the contributions of the different field terms in Eq. (6.3) can be changed.

### 6.3 Theory linear manipulation

In this section the effects of the linear (first order) terms in the general Eqs. (6.3a) and (6.3b) are studied in more detail. Expressions are derived for the focal length, both transversely and longitudinally, for specific cases of the anode voltage function $V_a(t)$.

#### 6.3.1 Transverse - Static field

The linear transverse focusing or defocusing behavior is described by the first order term in $\sigma_{r0}$ in Eq. (6.3a). In the limit of a thin lens, the transverse focal length $f_t$ is defined by

$$\frac{1}{f_t} = -\frac{1}{\sigma_{r0}} \frac{\Delta p_r}{p_z}, \tag{6.4}$$

with $p_z$ the average ion momentum. If we assume that the change in $v_z(z)$ in the fringe fields, i.e. in the region of appreciable radial field components, is negligible then we find for a static acceleration field:

$$\frac{1}{f_t} = -\frac{1}{4} e_z(z_0). \tag{6.5}$$

This shows that the divergent field at the exit of the accelerator works as a negative lens.

#### 6.3.2 Transverse - Switched field

For a time-dependent acceleration field, the focal strength can be calculated by combining Eq. (6.4) and Eq. (6.3a), resulting in

$$\frac{1}{f_t} = \frac{1}{4} \int_{z_0}^{\infty} \frac{\tilde{V}_a(z)}{V_a(z_0)} e'_z(z) dz. \tag{6.6}$$

Here we assumed that the change in final beam energy $U$ is negligible in comparison to the static case: $U \approx U_s$.

From Eq. (6.6) it is clear that the focal length $f_t$ can be modified by time-dependent manipulation by choosing some specific anode voltage function $V_a(t)$, and thus $\tilde{V}_a(z)$. We start with a simple unipolar voltage pulse of duration $\tau$ and amplitude $V_p$, as shown in Fig. 6.3b. The accelerating field can be turned off while the ion bunch is still being accelerated in the field. By introducing $z_{s1}$ as the position of the center of the bunch at the moment the field is turned off ($t = \tau$), the focal strength given by Eq. (6.6) can be written as

$$\frac{1}{f_t} = -\frac{1}{4} \left( e_z(z_0) - e_z(z_{s1}) \right). \tag{6.7}$$
If the field is switched off after the ions have left the accelerator field \((e_z(z_{s1}) = 0)\), Eq. \((6.7)\) reduces to the expression derived for the static case. If the field is switched off earlier, the \(e_z(z_{s1})\) term reduces the focal strength.

Instead of simply turning the field off with a unipolar pulse, it is also possible to change the sign of the radial electric field with a bipolar or multi-polar pulse. By choosing a suitable multi-polar pulse, the radial momentum an ion receives can even be inverted, so the diverging accelerator field can now be used as a positive lens as well.

We now consider the effect of a tripolar pulse, as defined in Fig. 6.3c: the pulse starts with a positive amplitude \(V_p\) and duration \(\tau\), is subsequently switched to the negative voltage \(V_n\) for a duration of \(\tau_n\), and finally switched back again to the positive voltage \(V_p\). The first switch occurs at position \(z_{s1}\), the second switch occurs at position \(z_{s2}\). For this pulse the focal strength can be approximated with Eq. \((6.6)\) as

\[
\frac{1}{f_t} = -\frac{1}{4} \left[ e_z(z_0) - \frac{V_p - V_n}{V_p} \left( e_z(z_{s1}) - e_z(z_{s2}) \right) \right].
\]  

\((6.8)\)

The focal strength can be controlled by either changing the negative voltage \(V_n\) or by changing the pulse durations \(\tau\) and \(\tau_n\), which result in different \(z_{s1}\) and \(z_{s2}\). Note that Eq. \((6.8)\) also describes bipolar pulses \((e(z_{s2}) = 0)\) and unipolar pulses \((V_n = 0\) and \(e(z_{s2}) = 0)\).

### 6.3.3 Longitudinal - Static field

In the longitudinal direction a similar result can be obtained; a longitudinal focal length can be defined as

\[
\frac{1}{f_t} = -\frac{1}{2} \frac{\Delta p_z}{p_z}.
\]  

\((6.9)\)

Under the same assumptions as in the transverse direction, i.e. \(v_z(z)\) changes negligibly in the fringe field region, this results for the static case in

\[
\frac{1}{f_t} = \frac{1}{2} e_z(z_0) = -2 \frac{1}{f_t}.
\]  

\((6.10)\)

and is thus positive. This can be understood as follows: an ion created in the back of the bunch travels a larger distance in the field than an ion created in the front. The particle in the back therefore acquires a higher velocity than a front particle. Because of this correlated velocity difference in the bunch, the front particles are overtaken by the back particles. The bunch is maximally compressed at the focal point.

Equation. \((6.10)\) shows that the longitudinal and transverse focal strength differ by a factor \(-2\), which is due to the zero divergence of the electric field: \(dE_z/dz = -2dE_r/dr\). The longitudinal and transverse focal lengths are thus always coupled and cannot be set independently.

This longitudinal focus determines both the bunch length and the energy spread. The contribution of the initial velocities of the cold ions to the energy spread is generally very
small, and can therefore be neglected in comparison to the spread induced by the acceleration field. This will be discussed in more detail in Sec. 6.3.5. The relative energy spread \( \sigma_U/U \) due to the acceleration can be approximated by \( \sigma_U/U = 2 \Delta p_z/p_z \), with \( \Delta p_z \) given by Eq. (6.3b). In lowest order we thus find that the longitudinal focal length and the energy spread are related by

\[
\frac{\sigma_U}{U} = 2 \frac{\sigma_{z_0}}{|f_l|},
\]

resulting in

\[
\frac{\sigma_U}{U} = \sigma_{z_0} e_z(z_0),
\]

with \( e_z(z_0) \) the normalized electric field at the initial position of the bunch \( z = z_0 \). We thus find that the relative energy spread is also independent of the beam energy. In static fields, a small relative energy spread can therefore only be realized by choosing a small initial \( \sigma_{z_0} \).

### 6.3.4 Longitudinal - Switched field

Similar to the transverse case, the longitudinal focal length for a time-dependent field is given by

\[
\frac{1}{f_l} = -\frac{1}{2} \int_{z_0}^{\infty} \frac{\dot{V}_a(z)}{V_a(z_0)} e'_z(z) dz,
\]

(6.13a)

\[
= -2 \frac{1}{f_l},
\]

(6.13b)

with again the assumption that the change in final beam energy \( U \) is negligible in comparison to the static case: \( U \approx U_s \).

By using time-dependent fields, the focal length \( f_l \) can be adjusted, so \( \sigma_U/U \) can be reduced without changing the initial longitudinal size of the ionization volume \( \sigma_{z_0} \). With a simple unipolar voltage pulse as illustrated in Fig. 6.3b, the accelerating field can be turned off while the ion bunch is still being accelerated. The time spent in the field is then the same for all ions in the bunch, independent of their initial position. Using Eq. (6.13) the focal strength for a unipolar pulse can be approximated by

\[
\frac{1}{f_l} = \frac{1}{2} (e_z(z_0) - e_z(z_{s1})).
\]

(6.14)

According to Eq. (6.11) the relative energy spread is then given by

\[
\frac{\sigma_U}{U} = \sigma_{z_0} |e_z(z_{s1}) - e_z(z_0)|.
\]

(6.15)

If the field is switched off after the ions have left the accelerator field, Eq. (6.15) reduces to the expression derived for the static case. In the idealized case of a perfectly homogeneous electric field inside the accelerator, i.e. \( e_z(z_{s1}) = e_z(z_0) \), the first term exactly cancels the second term in Eq. (6.15), which correspond to a focal length \( f_l = \pm \infty \). If the field is not homogeneous, the first term still partially reduces the energy spread.
6.3.5 Longitudinal - Thermal limitations

So far, we neglected the initial velocities of the cold ions. These thermal velocities correspond to an initial energy spread of only $\approx 20$ neV. In this section we will show they still can play a role in the longitudinal phase-space manipulation. They set a clear limit on the reduction of the energy spread that can be achieved by turning the field off with a unipolar pulse, as discussed in the previous section. We will start by discussing the acceleration process in the longitudinal phase-space ($z$-$p_z$), as depicted in Fig. 6.4.

For clarity a perfectly homogeneous acceleration field with a hard edge is assumed and space charge effects are neglected. In Fig. 6.4a the phase-space evolution of an ion bunch with a relatively large initial length ($\sigma_{z0}$) is shown. Several snapshots of the bunch at different moments in time are sketched. The bunch starts in the left bottom corner with an initial momentum spread $\sigma_{p_z0}$ due to the initial temperature and an initial length $\sigma_{z0}$ due the size of the ionization laser waist. The bunch immediately starts to accelerate in the field. Because the field is homogeneous, all ions experience the same force and thus gain the same momentum. At the same time the shape undergoes a linear transformation in the $z$-direction due to the finite initial momentum spread.

In the static case (green) this continues until the bunch reaches the edge of the accelerator. Not all ions reach the edge at the same moment. Particles in the back of the bunch, that are still inside, keep on being accelerated in contrast to the particles in front, which are already outside the accelerator. This transforms the bunch in a non-linear way, as illustrated in the figure. The momentum spread is now clearly increased compared to the initial spread. This corresponds to the (correlated) energy spread due to the initial bunch length as discussed before, see Eq. (6.12). If the field is turned off before the bunch reaches the edge (red), this transformation does not happen. The momentum spread stays the same and the bunch only drifts further in the $z$-direction. The momentum spread is smaller than in the static case, so by switching off the accelerating field, the energy spread can indeed be reduced.

The final momentum spread $\sigma_{p_z}$ in the static case can be reduced by decreasing the initial size as illustrated in Fig. 6.4b where the time evolution of an initially shorter bunch is shown. This is in contrast to the switched case where the spread is independent of the initial size $\sigma_{z0}$. This may even result in a larger momentum spread than in the static case.

In the switched field case $\sigma_{p_z}$ is conserved, which limits the lowest energy-spread that can be attained. The final energy spread $\sigma_U$ is then given by

$$\sigma_U = \frac{\sigma_{p_z0} p_z}{m} \quad (6.16)$$

with $p_z$ the final average momentum of the bunch. This can also be written in terms of energy and temperature as

$$\sigma_U = \sqrt{2kT U}, \quad (6.17)$$

where $k$ is Boltzmann’s constant and $T$ the initial temperature of the ions.
Figure 6.4: Illustration of the phase-space of a bunch in a hard-edged homogeneous acceleration field for an initial bunch with a) a long length b) a short length. Two situations are shown, the static case (green) where the bunch transforms at the hard-edge of the field and the unipolar pulse case (red) where the field is switched off before it reaches the edge.
This equation shows that the lowest reachable energy spread, if it is not limited by space charge or inhomogeneous fields, is limited by a cross-term between the initial thermal energy and the final beam energy. In Fig. 6.5 this contribution to the energy spread is plotted as function of $U$ for different initial temperatures. Fortunately the initial temperature is low (around 200 µK) so the resulting energy spread is well below 10 meV for beam energies up to several kV.

To understand the physical mechanism behind Eq. (6.17), it is advantageous to think in terms of momentum gained during acceleration in switched fields, instead of kinetic energy. In the static case all ions with the same initial position receive the same amount of energy, independent of their initial velocity, simply because they travel the same distance. A particle with a positive initial velocity $v_0$ will exit the field at an earlier time, so less momentum is transferred. In the switched case however, such a particle will be accelerated over an extra distance of $v_0\tau$ before the field is turned off in comparison with a particle with zero initial velocity. The extra energy received from the field, the energy spread, can thus (alternative to Eq. (6.17) ) also be written as

$$\sigma_U = \sigma_{v_0} \tau E_0 q \quad (6.18)$$

with $\sigma_{v_0}$ the initial thermal velocity spread and $E_0$ the field strength of the homogeneous accelerator field.

### 6.4 Experimental Setup

To perform these ultra cold ion beam experiments with time varying fields, several different ingredients are required. First of all an atomic gas has to be laser-cooled and trapped, which
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is the basis of the UCIS. Secondly it has to be possible to photo-ionize a part of the cold atom cloud. This should all happen inside an accelerator structure of which the acceleration voltage can be adjusted in time. As final step charge particle diagnostics are needed to observe the ion bunches and to be able to extract the relevant information. In this section an overview of our system is given as used in the experiments.

A rubidium-85 Magneto-Optical Trap (MOT) is used to provide the required cold atoms. The trap is loaded from a low pressure rubidium background vapor. It consists of two perpendicular pairs of retro-reflected cooling beams that are positioned diagonally in the x-y plane and two separate counter propagating beams along the z-direction. The quadrupole magnetic field of about 10 G/cm, needed for the trapping, is produced by two coils in anti-Helmholtz configuration with a radius of 72 mm. They are placed inside the vacuum chamber around the z-axis, so the system stays cylindrically symmetric. The influence of this magnetic field on the trajectories of the ions is negligible, so the coils are not turned off while the ions were extracted. Properties of the trapped atomic cloud are measured by imaging the fluorescent light from two directions, so also the absolute position of the cloud can be obtained. Typically $10^8$ Rb atoms are trapped in a cloud with a $\text{rms}$ radius of 1 mm.

The atoms are ionized with use of a two-step process. They are first excited from the ground state to the $5p$ level with a focused 780 nm laser pulse propagating along the $z$-direction, using the same transition as used for the laser cooling. Subsequently they are photo-ionized with a 479 nm laser pulse propagating perpendicular to the excitation beam, that is tuned just above its ionization threshold. A fraction of the excited atoms is ionized in the overlap region of the excitation and ionization laser, as is schematically indicated in Fig. 6.1. An ion bunch with an initially gaussian distribution is created, with initial sizes $\sigma_z = 200 \pm 20 \mu m$ and $\sigma_r = 250 \pm 30 \mu m$.

For the experiments with a unipolar voltage pulse, a pulsed dye laser (Quanta-Ray PDL3, $\text{rms}$ pulse length 2.5 ns $\text{rms}$) was used at the maximal repetition rate of 10 Hz. For the transverse focusing experiments, where no time-of-flight data is required, a commercial frequency doubled diode laser system (Toptica TA-SHG 110) was used. The laser beam was chopped with an acousto optical deflector (Interaction ADm-70) to obtain pulses with an $\text{rms}$ duration of 100 ns and a repetition rate up to 100 kHz.

The ionization takes place at the heart of a cylindrically symmetric accelerator structure, in which the inner conductor, the anode, can be put at high voltage, see Ref. [17] for more details. The anode voltage $V_a$ can be switched between three states: zero, a positive high voltage level ($V_p$), and a negative high voltage level ($V_n$) with a switch time of 50 ns and a maximum pulse repetition rate of 30 kHz. If a time-dependent voltage is used, all ions should start accelerating at the same moment in time. If the ionization is performed when the accelerating field is already present, ions created in the beginning of the ionization laser pulse already start to accelerate while others have not yet been ionized. Therefore we have created the ions when the acceleration field is turned off, and turned it on several nanoseconds after the last ions were created.
The ion bunches are detected by a 40 mm diameter multi channel plate detector (MCP) with phosphor screen, which is mounted at a distance $L = 0.64$ m from the center of the accelerator. To increase the detection efficiency at low beam energies, the front plate of the MCP is placed at a voltage of $-900$ V. A metal grid is placed 10 mm in front of the detector to shield the electric field. A CCD camera (Apogee U9000) is used to capture images of the phosphor screen that contain the spatial information of the ion bunches. Simultaneously the temporal distribution of the ion bunch is recorded on an oscilloscope by using a transimpedance amplifier ($\approx 10$ ns resolution) connected to the phosphor screen.

From the recorded temporal signal of the amplifier the total charge $Q$ of the bunch, the time-of-flight $T$ to the detector and its $rms$ spread $\sigma_T$ are extracted by fitting the signal with a gaussian distribution function. It is important to know how this time-of-flight data can be translated to the longitudinal properties of the bunch, the average beam energy $U$ and the energy spread $\sigma_U$. If all ions would have been created at exactly the same position and thus all with exactly the same drift length $L$ to the detector, this would result in simple expressions. In that case the beam energy $U$ can be calculated using $U = (1/2) m (L/T)^2$, the longitudinal bunch length follows from $\sigma_z = L \sigma_T/T$, and the relative energy spread $\sigma_U/U$ is given by the relation $\sigma_U/U = 2 \sigma_T/T$.

If one looks closer into the details, complications arise. The ions start at different positions in the accelerator, the acceleration field is not homogenous and some post-acceleration occurs close to the detector. If a static acceleration field is used, as in Ref. [5], then an extra constant factor can be introduced to compensate for these effects. Namely, due to the longitudinal focusing effect of the accelerator, as discussed in Sec. 6.3.3, the bunch compresses in longitudinal direction due to the correlated velocity difference at a fixed position just outside the accelerator. This position with minimal bunch length can be used as a virtual cathode from where the simple formulas are valid again. For time-dependent acceleration fields such a single compensation factor does not work because the longitudinal focal strength changes, and therefore also the position of the minimal bunch length, the virtual cathode. Fortunately, the distance to the detector is long compared to the accelerator length and the initial bunch size. Numerical simulations show that the simple relations hold within 15 % for the situation used in the experiment.

### 6.5 Longitudinal manipulation

#### 6.5.1 Experimental results

We present results of the longitudinal phase-space manipulation in Fig. 6.6 where the longitudinal bunch length $\sigma_z$ and the relative energy spread $\sigma_U/U$ is plotted as a function of the beam energy $U$. First we discuss the static-measurements, indicated by the purple circles in Fig. 6.6. In this measurement series, the anode voltage $V_a$ is varied from 200 to 2500 V. As discussed, the bunch is compressed after leaving the accelerator. Using Eq. (6.10) the
Figure 6.6: Results of measurements with a unipolar voltage pulse. The beam energy \( U \) is varied by changing the pulse duration \( \tau \) from 100 ns up to 2 \( \mu \)s while keeping \( V_p \) constant. Three sets of measurements (black, red and blue squares) with respectively \( V_p = 1000, 500 \) and 250 V are shown. The longitudinal bunch length \( \sigma_z \) and the relative energy spread \( \sigma_U/U \) are plotted versus \( U \). Additionally static measurements (purple circles) are presented, where \( V_p \) is varied. Particle tracking simulations are depicted as solid curves (unipolar pulses) and dashed curves (static case). Simulations without space charge forces are depicted as dotted curves.
longitudinal focal length $f_l$ (in the static case) can be estimated to be $f_l = 26$ mm. The bunch length is minimal at this focal point. Then the bunch starts to expand again and subsequently hits the detector. The focal length $f_l$ is independent of the acceleration voltage. The resulting longitudinal magnification at the detector, i.e. the length of the bunch $\sigma_z$, is therefore independent of the beam energy as well. In the measurements we indeed observe a constant bunch length on the detector. The measured relative energy spread, indicated on the right axis in Fig. 6.6, is therefore automatically also nearly independent of the beam energy.

In Fig. 6.6 also measurements are shown performed with a unipolar pulse, indicated by black, red and blue squares. The relative energy spread $\sigma_U/U$ is measured as a function of $U$ by varying $\tau$ from 100 ns up to 2 $\mu$s. The measurements have been done for three different voltages: $V_p = 2000$ V, 1000 V and 500 V; at a bunch charge of $\approx 0.5$ fC. The encircled points correspond to pulse durations for which the ions have already left the accelerator at $t = \tau$, and are therefore not influenced by the field switching. In that case the relative energy spread coincides with the static measurements. For shorter $\tau$, both $U$ and $\sigma_U/U$ are reduced. For even shorter $\tau$, $T$ becomes so long that space charge effects start to increase $\sigma_U$ again. This effect was also observed in Ref. [5]. In the region where space-charge effects are not important, the curves for different $V_p$ have the same shape and can in fact be made to overlap by scaling the $U$ axis proportionally to $V_p$. We conclude that a relative energy spread reduction of a factor three is obtained by switching the field off before the ion bunch has left the accelerator.

6.5.2 Simulations

To quantitatively understand the measurements, particle tracking simulations were performed with the GPT [18] code. The electric field inside the accelerator was calculated with the superfish poisson solver [19]. All the ions in the bunch are tracked individually with all mutual Coulomb interactions included. The initial conditions are the same for all simulations: The ions are started with a gaussian density distribution with experimentally determined values for the position and width. The simulation results are depicted as dashed (static case) and solid (unipolar switch) curves in Fig. 6.6. Good agreement with the data is obtained. Small deviations from the simulations occur in the low-energy region, where space-charge effects become significant.

In the simulations the space-charge forces between the ions can be turned off, without changing any other parameter. The resulting curves are plotted as the dotted lines. For these curves only the interaction with the accelerator field is important, so they can be directly compared to the results of the analytical model.
6.5.3 Analytical energy-spread models

We will now make a more detailed comparison between the simulations and the model presented in section 6.3.4. The calculated longitudinal focal length for the static case of \( f_l = 26 \text{ mm} \) matches within 1% with the simulation results. To compare the model for the time-dependent acceleration fields, the relative energy spread resulting from GPT simulations, without space-charge effects (black solid line), is shown in Fig. 6.7. It is plotted as function of the switch position \( z_{s1} \) instead of the bunch energy. In that case all three simulation curves (dotted lines) of Fig. 6.6 overlap and form the black solid line in Fig. 6.7. Small \( z_{s1} \) correspond to short durations, and large \( z_{s1} \) to long durations. If the field is switched off at large \( z_{s1} \), i.e. at a position where the field has almost reduced to zero, \( \sigma_U/U \) does not change anymore, so the curve levels off for large \( z_s \).

![Figure 6.7: Models of the energy spread of the bunch as function of the bunch center position. See text for more details about the different models.](image)

The relative energy spread calculated with the model of Eq. (6.15) is depicted by the blue dashed line. First of all, it can be improved (dashed green curve) by correcting for the changing beam energy \( U \) by multiplying the focal strength with the factor \( \Gamma \) defined in Appendix 6.A. This curve shows the same overall behavior as the simulation curve, but there is a clear difference for small \( z_{s1} \).

The largest part of the remaining discrepancy can be attributed to the assumption that the bunch length \( \sigma_z(z) \) does not change in the acceleration field, as used in Eq. (6.3b). Without this assumption we get

\[
\frac{\sigma_U}{U} = \Gamma |\sigma_z(z_{s1})e_z(z_{s1}) - \sigma_z(z_0)e_z(z_0)|, \tag{6.19}
\]

with \( \sigma_z(z) \) the bunch length as function of its center position. This bunch length can be approximated with a model described in Appendix 6.B. If \( \sigma_z(z) \) is approximated with a second order model in Eq. (6.19), this results in an energy spread curve (red dashed line) which agrees within 10% with the simulated curve.
From the comparison between model and simulations we learn that the energy spread can be understood quantitatively only by taking higher-order derivatives of the field into account at the initial position $z_0$ and at the position $z_{s1}$, where the field is switched off. The accelerator field can be designed in such a way that it is more uniform than in the present setup. A much larger energy spread reduction should then be obtainable.

6.6 Transverse focusing

So far we looked only at the longitudinal behavior. In this section we will discuss experiments where the transverse behavior is studied for different time-dependent voltage pulses. We will start by presenting and discussing the transverse results of the unipolar pulse experiments that have been described in the previous section and continue with more complex pulse shapes.

6.6.1 Results uni-polar pulse

The accelerator field also influences the ions in transverse direction, as discussed in section 6.3. To study this, the spatial ion bunch distribution on the detector was captured by the CCD camera, simultaneously with the time-of-flight signals that were used already in previous section. The transverse sizes $\sigma_x$ and $\sigma_y$ of the ion bunches were extracted from the images by performing a fit with a two-dimensional gaussian distribution. In Fig. 6.8 we present these transverse results of the same set of experiments that was used for the longitudinal measurements of Fig. 6.6. Both $\sigma_x$ and $\sigma_y$ are shown as function of the beam energy $U$.

We will first focus on the static case, the purple circles in the figure, where the divergent field at the exit hole of the accelerator structure acts as a negative lens for the ions. The focal strength of the lens can be approximated by Eq. (6.6), which results in $f_t = -51$ mm for our accelerator. Due to this lens the bunches will be transversely magnified when they arrive at the detector position. The focal length and therefore also the magnification is, according to the model, independent of the beam energy $U$. In the measurements we indeed observe a constant bunch size on the detector, except again at low beam energies where the spot blows up due to space charge forces.

In Fig. 6.8 the results of the unipolar experiments are shown. These unipolar pulsed experiments were performed at the same three voltages, $V_p = 2000$ V (black symbols), 1000 V (red symbols) and 500 V (blue symbols) as before. There is a clear resemblance between these results and the longitudinal results shown in Fig. 6.6. For long $\tau$ (encircled points), the ions have again already left the accelerator structure when the field is switched off, so they experience the full divergent part of the field. These data points are thus effectively just static measurements.

For shorter $\tau$, the field is switched off while the ions are still in the accelerator structure, and thus before they experienced the full divergent part of the field. Therefore not only
Figure 6.8: Measurements of transverse bunch sizes with a unipolar voltage pulse. The beam energy $U$ is varied by changing the pulse duration $\tau$ from 100 ns up to 2 $\mu$s while keeping $V_p$ constant. Three curves (black, red and blue squares) with respectively $V_p = 1000, 500$ and 250 V are shown. In a) the transverse size $\sigma_x$ on the detector is plotted versus $U$ and in b) the transverse size $\sigma_y$. Additionally static measurements (purple circles) are presented, where $V_p$ is varied. Particle tracking simulations are depicted as solid curves (unipolar pulses) and dashed curves (static case).
the beam energy $U$ decreases, but also the radial momentum spread $\Delta p_r$ they receive, as illustrated in the diagrams on top of Fig. 6.8. This reduces the negative lens strength of the accelerator, as described by Eq. (6.7). As a result of this, the transverse magnification of the bunch by the lens is reduced, so a smaller spot on the detector is obtained. This reduction is clearly visible in the experimental data. At even shorter $\tau$, and thus lower $U$, space-charge forces start to dominate again, causing the spot size to increase again.

The results of the particle tracking simulations, that were described in section 6.5.2, are also depicted in Fig. 6.8. The dashed curve represents the static measurements. With use of such a simulation with a static field, the transverse focal length has been obtained. A smaller focal length $f_t = -35$ mm has been found than predicted with the simple analytical model ($f_t = -51$ mm). This relatively large deviation is due to the fact that for our accelerator field, with an acceleration length comparable to the exit hole size, the assumptions made in the derivation of the model are partially violated. The beam expands already inside the field, and the velocity is not constant while passing through the divergent area. Both these effects increase the focal strength.

The three solid curves in the figure correspond to the simulation results of the unipolar pulsed experiments. The overall behavior of the simulation curves is comparable to the experimental data. The spot size of the pulsed measurements starts at the value of the static simulation, then decreases and eventually blows up because of space charge. The agreement between the simulation and the measured data is least satisfactory for the curve with the lowest pulse amplitude. The deviations are therefore most likely caused by the combination of space charge and uncertainties in the initial ion distribution.

Another interesting point are the striking similarities between the transverse measurements in this figure and the longitudinal measurements in Fig. 6.6. Not only the overall shape of the curves are comparable, but also the absolute values of the bunch sizes. The produced bunches have comparable sizes in all the three dimensions. Due to the factor $-2$ between the longitudinal and the transverse focal length in Eq. (6.6) both have a similar value. For our accelerator the difference is in absolute value even smaller in practice namely $f_t = 26$ mm and $f_r = -35$ mm. At distances $z >> |f_t|, |f_r|$ the sign of the focal length is not important anymore for the divergence of the bunch. So if one starts with a round ionization volume, as approximately done in this experiment, then a relative round ion bunch will be produced at the detector.

### 6.6.2 Results multi-polar pulses

By using more complex pulses it is possible to change the negative lens in a positive focusing lens, as discussed in section 6.3.2. In Fig. 6.9 this is demonstrated with a bipolar pulse, which can be interpreted as a tripolar pulse with $\tau_n = \infty$. The transverse size $\sigma_x$ has been plotted as function of the negative voltage $V_n$, ranging from 0 V to $-1000$ V. The positive part of the pulse is kept constant, $V_p = 1000$ V and $\tau = 633$ ns. In the figure it can be clearly observed that when $V_n$ gets more negative the bunch starts to focus, so the spot size decreases at the
Figure 6.9: Focusing using bipolar voltage pulses with \( V_p = 1000 \) V and \( \tau = 633 \) ns. The transverse size in \( x \)-direction \( \sigma_x \) of the bunch on the detector is measured as function of \( V_n \). Phosphor images of the beam are shown at the bottom. The solid curve corresponds to particle tracking simulations.

detector. The minimal spot size is observed at \( V_n = -540 \) V, when the focus lies on the detector. In that case the bunch is accelerated to \( U = 280 \) \( \text{eV} \) with the positive pulse and decelerated to \( U = 180 \) \( \text{eV} \) by the negative pulse. At even lower \( V_n \) the beam over-focuses so the spot size increases again at the detector. Phosphor screen images have been added in the bottom of the image to illustrate the effect. Particle tracking simulations (solid curve) agree well with the measurements.

To enable direct measurements of the focal length of the time-dependent lens, independent of aberrations, another set of experiments has been performed: instead of relating the focal length to the measured spot size, the transverse position \( x \) of the center of the spot on the detector was measured as function of the position \( x_0 \) of the initial ionization volume. When the lens is ideal, the relation between \( x_0 \) and \( x \) is simply linear: \( x = Ax_0 \). From the linear coefficient \( A \) the focal length can be obtained.

The position \( x_0 \) was changed by moving the ionization laser focus. In the experiments described in the previous sections we used two focused laser beams, an excitation and an ionization laser beam, to ionize only a fraction of the cold atoms in the overlap region. For experimental convenience we now keep the MOT cooling beams on, instead of the separate focused excitation beam to excite all the atoms to the required intermediate level. Precise alignment is then not required to overlap both lasers at the right position. In this way a vertical cylinder (in the \( y \)-direction) of ions is produced coinciding with the waist of the ionization laser.

The focal behavior of bipolar voltage pulses, similar to those used in Fig. 6.9, is studied with this method. In Fig. 6.10 the transverse ion bunch position \( x \) at the detector is plotted as
Figure 6.10: Direct measurement of the focal behavior of a bipolar pulse with $V_p = 1000$ V and $\tau = 633$ ns while $V_n$ was varied from $-50$ to $-1000$ V. The transverse ion bunch position $x$ at the detector is plotted as function of the initial position $x_0$. The curves are fitted with $x = Ax_0 - Cx_0^3$ (solid lines). See text for more details.

function of the initial position $x_0$. The bipolar pulse has a fixed positive part with $V_p = 1000$ V and $\tau = 633$ ns, while $V_n$ was varied from $-50$ to $-1000$ V. At all these different voltage pulses, the ionization laser position $x_0$ was scanned over a range of $-2$ to $4$ mm, limited by the size of the atomic cloud. Every dot in the figure correspond to an analyzed phosphor screen image from which the center cylinder position $x$ was determined. In this set of measurements, the focal strength of the lens is now derived from the slope $A$ of the curves, instead of the bunch size as in Fig. 6.9.

The relation between the slope $A$ and the focal length is $f_t = -L/(A - 1)$. For small values of $V_n$ the lens is still negative so $A > 1$; as the amplitude of $V_n$ increases a parallel beam is created which corresponds to $A = 1$. At further increased amplitude the beam starts to focus ($A < 1$), up to the point where the focus lies at the detector position ($A = 0$). This happens at $V_n \approx -550$ V, which is consistent with the position of the smallest waist in Fig. 6.9. For even larger values the focus lies in front of the detector ($A < 0$).

A more extensive measurement series has been performed to study the focal behavior of the tripolar pulses. The parameters $V_n$ and $\tau_n$ were varied, while $V_p$ was kept constant at 1000 V and $\tau = 633$ ns. Again the initial position $x_0$ was varied for each of these different voltage pulses. By fitting the curves, the $A$ parameter was determined. The resulting focal strengths $1/f_t$ of this parameter scan are presented in Fig. 6.11b.

The horizontal axis represents the negative pulse duration $\tau_n$ and the vertical axis the
Figure 6.11: Measurements and simulations of the focal strength $1/f_t$ as function of two parameters of a tri-polar pulse. The parameters $V_n$ and $\tau_n$ are varied, while $V_p = 1000$ V and $\tau = 633$ ns are kept constant. a) Schematic of the voltage pulse and field b) Experimental data c) GPT Particle tracking simulation.
negative voltage $V_n$. Every colored dot corresponds to a measurement with the color scale indicating the focal strength. Several lines of constant $f_t$ are added as a guide to the eye. Two regions are visible, a blue area that represents a negative focal strength and a red area that represents a positive focal strength. For small values of $\tau_n$ nothing is changed in comparison with the static case and the values are thus close to the expected $1/f_t = -28 \text{ m}^{-1}$. When $\tau_n$ is increased, the influence of the negative voltage becomes stronger, up to the point where $\tau_n$ is so long that the tri-polar voltage pulse is effectively the same as a bi-polar pulse, and therefore the focal strength $1/f_t$ becomes independent of $\tau_n$.

By increasing the magnitude of the negative voltage $V_n$ the focal strength increases. The beam starts at $V_n = 0 \text{ V}$ as a divergent beam ($1/f_t < 0$), and it gets less divergent up to the point were a parallel beam is produced ($1/f_t = 0$). Subsequently, for even more negative $V_n$, the beam starts to focus ($1/f_t > 0$).

6.6.3 Simulations

For better understanding, again particle tracking simulations have been performed with use of GPT. In the simulations the same procedure is followed as in the experiment; for every voltage pulse shape a simulation is performed with particles starting from different initial $x_0$ positions while recording the positions $x$ where the trajectories intersect the detector. Again the linear coefficient $A$ is determined for every voltage pulse shape to calculate $1/f_t$. The results are depicted in Fig. 6.11c.

The simulations are in good agreement with the measured data. The overall shape is very similar. There are some deviations, mostly in the negative voltage needed for some particular focal strength. These deviations can probably be attributed to small errors in the electric field shape of the accelerator as used in the simulations and in the initial bunch position.

6.6.4 Analytical model

The analytical model described in section 6.3.2 can also be used to describe the focusing. To compare this with the results of simulations, the pulse durations ($\tau$ and $\tau_n$) have to be converted to switch positions ($z_{s1}$ and $z_{s2}$). This is done by using a numerically calculated trajectory of a particle started in the center of the bunch. Equation (6.8) is corrected for the change in final beam energy, due to switching, by multiplying with the factor $\Gamma$ defined in appendix 6.A.

The results, $1/f_t$ versus $\tau_n$ and $V_n$, are plotted in Fig. 6.12. The overall shape and behavior is very similar, showing that focusing with a time-dependent voltage pulse can be approximated with this simple model. Again, there is a difference with the simulation curves, specially in the region where the lens has a negative focal length, as we discussed for the static case. This is mainly caused by the assumption that $v_z(z)$ is constant while passing through the field and the assumption of a constant bunch size.

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Figure 6.12: Plot of the focal strength \(1/f_t\) (solid lines) as calculated with Eq. (6.8) multiplied by the factor \(\Gamma\) defined in appendix 6.A. The result differs slightly from the particle tracking simulations (dotted lines).

6.7 Spherical aberrations

6.7.1 Experimental results

Up to now, we have shown that we can control the linear term in Eqs. (6.3a) and (6.3b) with the time-dependent fields, but control of higher orders is also possible. To demonstrate this, we change the spherical aberration due to the exit fields of the accelerator. Importantly, we circumvent Scherzer’s theorem [12, 20], a major restriction in conventional static cylindrical systems, which states that spherical aberration coefficients are always positive. This makes it impossible to simply cancel this aberration by combining lenses with both positive and negative coefficients. With time-dependent fields there is no such restriction.

To determine the amount of spherical aberration we use the same method as used in section 6.6.2 to determine the focal length, namely measuring the transverse position \(x\) on the detector as a function of the initial position \(x_0\). When the exit lens is aberration free, as illustrated in Fig. 6.13a, the relation between \(x_0\) and \(x\) is strictly linear (\(x = Ax_0\)). When spherical aberrations are present, shown in Figs. 6.13b and c, an additional third order term appears (\(x = Ax_0 - Cx_0^3\)). The aberration are the result of the \(e''''\) term in Eq. (6.3a). By changing \(V_a(t)\), and thus \(\tilde{V}_a(z)\), the integral of this term can be controlled as illustrated in the diagrams of Fig. 6.14.

A deviation from the linear behavior can already be observed in the measurements in
Fig. 6.10. By fitting the data with \( x = Ax_0 - Cx_0^3 \) (solid curves), the parameters \( A \) and \( C \) are obtained. If the bunch is focused at the position of the detector \( (f_t = L) \), the third-order coefficient \( C \) is related to the \( C_s \) coefficient by \( C_s = f_t^3C \). The spot size \( \delta_s \) due to spherical aberrations in a focusing system is given in general by \( \delta_s = C_s\alpha^3 \), with \( \alpha \) the lens acceptance angle [12].

To make the deviations from linear behavior more visible, an enlarged plot of the center curves \( (f_t \simeq L) \) are given in Fig. 6.14a. Again the position at the detector \( x \) is plotted versus the initial position \( x_0 \). The data fits well with the third order fitting function (solid curves). This bipolar pulse results in \( C_s = -1.1\pm0.1 \times 10^4 \text{ m} \). By changing only to a tripolar pulse, as is shown in Fig. 6.14b, the sign of the aberration coefficient is reversed to \( C_s = 4.0\pm0.2 \times 10^4 \text{ m} \). This shows that manipulation with time-dependent fields can be used to achieve aberration corrected systems.

To study the dependence of the spherical aberrations on the voltage pulse shape in more detail, the \( C \) coefficients have been determined for all the measurements performed with the tripolar pulses, described in section 6.6, in Fig. 6.11a. Points in parameter space which did not allow a reliable fit of the third order coefficient were left out. The results are depicted in Fig. 6.15a. Two distinct regions are visible: on the left (small \( \tau_n \)) a region of positive \( C \) and on the right (large \( \tau_n \)) a region of negative \( C \). In between the regions the \( C \) coefficient goes through zero. The positions in parameter space corresponding to the measurements shown in Fig. 6.14 are indicated by an asterisk.

The black solid curve in Fig. 6.15a corresponds to combinations of \( V_n \) and \( \tau_n \) which give
Figure 6.14: Demonstration of the sign reversal of the spherical aberration coefficients. The position $x$ of the ion bunch on the detector is recorded as function of the position $x_0$ of the initial ionization volume (scatter plots). In all measurements $V_p = 1000$ V. The curves are fitted with the relation $x = Ax_0 - Cx_0^3$ (solid curves). Results are shown of measurements using a) a bipolar pulse ($C < 0$) and b) a tripolar pulse ($C > 0$).
Figure 6.15: Plot of the third-order coefficient $C$ as function of the tri-polar voltage pulse parameters $V_n$ and $\tau_n$, while $V_p$ is kept constant at 1000 V and $\tau = 633$ ns. a) measurement results. The black solid curve corresponds to $f_t = L$. b) Results of particle tracking simulations.
rise to a focal length of \( f_t = 0.63 \) m, i.e. a focus on the detector surface. The curve is extracted from the measured data in Fig. 6.11b. By moving over this curve of constant focal length \( f_t \), however, the C coefficients can be changed. For small \( \tau_n \) the C value is positive. When \( \tau_n \) is increased, the C value goes through zero and eventually becomes negative. This demonstrates that the spherical aberrations can be adjusted without changing the focal strength.

### 6.7.2 Simulations

From the particle tracking simulations performed in Fig. 6.11c, also the third order coefficient \( C \) can be obtained by fitting the \( x \) vs \( x_0 \) curves with an additional third order term. These results are presented in Fig. 6.15b. The overall behavior of \( C \) in the parameter space in the simulations matches with the measurements. Both have a region of positive \( C \) and a region of negative \( C \) with comparable magnitudes and the regions are separated at about \( \tau_n = 700 \) ns by a region of small \( |C| \). Furthermore the \( C \) coefficient increases for large \( \tau_n \) and negative \( V_n \).

Again, there are also differences in the exact shape of the distribution, such as the increase in magnitude in the top left corner. The simulations are quite sensitive to the initial positions and the exact shape of the field used. This is likely the cause of the deviations between the simulations and the measurements.

Describing the spherical aberrations reliably with a simple analytical model, as was done in section 6.6 for the focal strength, is difficult. Calculating the \( C \) coefficient by only using the third order term of Eq. (6.3b) does not work, because in practice the change in \( \sigma_r(z) \) cannot be neglected. Moreover, cross terms between the linear and third order field terms start to get important. In addition, in many situations different contributions nearly cancel each other making precise modeling harder. Developing an analytical model that can accurately predict the spherical aberrations is outside the scope of this paper.

### 6.8 Conclusion

In conclusion, we have experimentally demonstrated that manipulation of ion bunches extracted from an laser-cooled gas with use of time-dependent fields is possible. More specifically we have shown that by using a unipolar pulse the relative energy spread in longitudinal direction can be reduced. In transverse direction we demonstrated that by using more complex pulses, such as tripolar pulses, the negative lens effect of an accelerator structure can be converted in a versatile adjustable lens. The sign and strength of this lens, as well as the sign and strength of the spherical aberrations coefficient can be adjusted by only changing the applied time-dependent voltage.
Appendix 6.A  Beam energy

As a side effect of a time-dependent acceleration pulse, the ions are only accelerated over a smaller distance, or with multi-polar pulses, decelerated because the field in z-direction is also reversed. This is illustrated in Fig. 6.16, where the final beam energy $U$, following from the particle tracking simulation performed for Fig. 6.11b, are shown. At low $\tau_n$ the beam energy is close to the beam energy $U_s$ of the static case. The beam energy $U$ decreases for increasing $\tau_n$ and more negative $V_n$.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure6_16.png}
\caption{Final beam energy $U$ from particle tracking simulation after applying a tri-polar voltage pulse. The parameters $V_n$ and $\tau_n$ are varied, while $V_p$ is kept constant at 1000 V and $\tau = 633$ ns.}
\end{figure}

The final beam energy resulting from a time-dependent voltage can be analytically written as

$$U = \int_{z_0}^\infty \alpha \tilde{V}_a(z) e_z(z) dz,$$

which results for a tri-polar pulse, such as in the simulation, in an energy of

$$U = qV_p\varphi(z_0) + q \left(V_p - V_n\right) \left(\varphi(z_{s2}) - \varphi(z_{s1})\right),$$

with $\varphi(z)$ the normalized static potential defined as $\varphi(z) = \phi(z)/\phi(z_0)$. In the static case only the first term remains, so the energy is then

$$U_s = qV_p\varphi(z_0).$$
In Eq. (6.6) and Eq. (6.9), which are used to derive the equations in section 6.3, the final beam energy $U$ is assumed to be equal to $U_s$. In some situations $U$ can be much lower than $U_s$, so the focal strength will be enhanced in comparison with the assumed situation. To correct for this effect, we introduce the energy correction factor $\Gamma$:

$$\frac{1}{\Gamma} = \frac{U}{U_s} = 1 + \left(1 - \frac{V_n}{V_p}\right) \left(\frac{\varphi(z_{s2}) - \varphi(z_{s1})}{\varphi(z_0)}\right).$$

(6.23)

The focal strength can be corrected in first order for the energy change by multiplying with $\Gamma$.

### Appendix 6.B Bunch length model

To model the relative energy spread in the bunch, the bunch length as function of bunch position is needed. In this section a simple approximation model is derived.

The length $\sigma_z$ immediately starts to change due to non-homogenous fields present at the initial position $z_0$. To approximate the bunch length change we Taylor expand the field at the initial position:

$$e_z(z) = e_z(z_0) + e'_z(z_0)(z - z_0) + 1/2 e''_z(z_0)(z - z_0)^2 + \cdots.$$  

The difference in field between a particle in the center and at position $\sigma_z$ is then $\Delta e_z(z) = \sigma_z (e'_z(z_0) + e''_z(z_0)(z - z_0) + 1/2 e'''_z(z_0)(z - z_0)^2)$ to first order in $\sigma_z$. The difference in velocity can be calculated (similar as in expression Eq. (6.3b) ) as

$$\Delta p_z(z) = q \int_{z_0}^{z} \frac{\Delta e_z(z')}{v_z(z')} dz'.$$

(6.24)

By keeping track of the length change due to this velocity differences in the bunch while accelerating, results in

$$\Delta z(z) = \frac{1}{m} \int_{z_0}^{z} \frac{\Delta p_z(z')}{v_z(z')} dz'.$$

(6.25)

If only the constant term of the field is used to calculate the center velocity $v_z(z)$ this results in an polynomial approximation of the bunch length as

$$\sigma_z(z) = \sigma_{z_0} \left(1 + \frac{e'_z(z_0)}{e_z(z_0)}(z - z_0) + \frac{1}{6} \frac{e''_z(z_0)}{e_z(z_0)}(z - z_0)^2 + \cdots\right).$$

(6.26)

In Fig. 6.17 $\sigma_z(z)$ is plotted as function of the center bunch position. The particle tracking simulation (black solid line) shows the pulse is already significantly compressed while still traveling inside the field ($z_{s1} < 20$ mm). In our specific acceleration field the ions start close to a field maximum so the linear field term is small, which results in only a minor correction by the first term in Eq. (6.26), depicted as the gray dashed curve. But if also the second order term is used (red dashed curve), the analytical bunch length expression inside the accelerator agrees within 5% with the simulation.
Figure 6.17: Models of the bunch length as function of the bunch center position. See text for more details about the different models.

Bibliography


First steps to future prospects

In the course of the project several new ideas have surfaced which are interesting for future experiments with cold ions. In this chapter two of these ideas will be briefly discussed. In the first section we present calculations which show that the observation of coulomb interaction, in bunches with only a few ions, should be experimentally feasible and may lead to the direct observation of statistical Coulomb effects such as stochastic heating. In the second section a design for a next generation UCIS is presented based on photo-ionization of a laser-cooled and intensified atomic beam which should make an even higher brightness possible.

7.1 Single ion interactions

Coulomb interactions in an ion bunch start to play a significant role at low beam energies. At these energies the time-of-flight is long, thus more time is available for interactions. Furthermore, the average longitudinal velocity is low so coulomb forces result in larger angular deviations. Even at a low number of ions per bunch, about 150, space charge effects were observed in the time-of-flight energy spread measurements described in chapter 4. When the ion bunch is focused, these effects become more visible. In this section we present calculations that show that interactions between only two ions already result in interesting behavior that should be detectable in our setup and may subsequently be used to study other effects like stochastic heating.

The effect of the coulomb interactions on the bunches is studied with particle tracking simulations, similar to those used in chapter 6. In this example a small ionization volume with a gaussian probability distribution with \( \sigma_x = \sigma_y = \sigma_z = 20 \, \mu m \) is used, placed in the center of the accelerator structure. A temperature of 200 \( \mu K \) is assumed for the ions. Bunches with 1,2 and 3 particles have been created, accelerated, and subsequently focused with a bipolar
Figure 7.1: Results of particle tracking simulations of space charge effects in bunches with several ions. The transverse ion distribution at the focus and the cross section of the distribution are shown for bunches with 1, 2 and 3 ions.
time-dependent pulse at a position 1.5 m from the accelerator center, while taking the mutual
coulomb interactions into account. The ions receive an energy of 19 eV and arrive after 220 µs
at the focal position where the transverse position is recorded. Many different bunches have
been simulated, each with their own random initial positions and thermal velocities, so the
probability distribution on the detector was obtained.

The results of these simulations are depicted in Fig. 7.1. On the top row, Fig. 7.1a, the
results of bunches with a single ion are presented, with on the left the normalized density
distribution and on the right a cross section of the distribution with the corresponding in-
tensity. These ions are focused to a small spot of about 40 µm rms, limited by the initial
temperature.

The results of the simulations with two ions per bunch in Fig. 7.1b show a completely
different behavior. The coulomb interaction resulted in a ring like distribution of the ions at
the focal position. The ring has a diameter of about 2 mm, which should be easily detectable
in the experiment. The origin of this distribution is simple: the coulomb potential energy
of the two ions is almost completely converted to kinetic energy. If the thermal velocities
are neglected, this results in both ions obtaining the same outward radial velocity, but in
opposite directions. At the focal position, the spatial distribution is completely determined
by the velocity distribution.

The initial potential energy only depends on the distance between the two particles. Due
to the small size of the ionization volume, almost all particles get an outward velocity so they
do not hit the center. Similarly, there is a most likely distance between the initial particles,
which results in the ring. For simpler initial distributions, such as a homogeneous sphere, an
analytical expression for the probability distribution of the distance between the particles can
be obtained [1]. With use of this expression, the shape of the rings, and the dependence on
different parameters such as the initial volume size can be explained. For bunches with more
than two ions, such as depicted in Fig. 7.1c, a simple model is more difficult. If the number
of ions are increased further, the ring structure gets less pronounced and the distribution
starts to transform to a broadened peak. At a value of \( n \approx 20 \) the ring structure disappears
completely for these bunch parameters.

The ionization of the cold atoms is a probability process, and therefore follows poisson
statistics. The average number of ions per bunch \( \lambda \) can be adjusted by changing the intensity
or pulse length of the ionization laser. The number of ions per bunch will fluctuate, which
will be most significant at low average number of ions. This is illustrated in Fig. 7.2 where
the probability to create a bunch with a specific number of ions \( (n) \) is plotted as function of
the average number of ions in the bunches. At zero intensity of the ionization laser, no atoms
will be ionized. At an increased intensity and thus larger \( \lambda \), the chance of a bunch with a
single ion increases. At even larger \( \lambda \) also the chance of creating bunches with multiple ions
rapidly increases. Beside that, also the contribution to the total beam current scales with the
number of ions present in a bunch. At \( \lambda = 1 \) for example, the beam current already exists of
63 % of bunches with more than one ion.
Figure 7.2: Plot of the occurrence of a specific number of $n$ ions per bunch as function of the average number of ions per bunch $\lambda$ due to the poisson distribution of the ionization process.

To obtain the distribution that would also be observed in the experiment, the density distributions for the different number of ions per bunch have to be combined. First these distributions have to be weighted with the probability from the poisson distribution, which depends on $\lambda$, before they are added. The ratio of the different contributions can thus be changed by varying the ionization laser intensity. This is illustrated in Fig. 7.3 where the resulting density profile cross sections are plotted for different laser intensities, corresponding to $\lambda = 1, 2, 4$ and 6 ions per bunch. The separate contributions of bunches with a specific number of ions to the complete cross section is visualized with different colors. All the profiles consist of a bright peak at the origin due to bunches with only a single ion. The intensity of this peak decreases for $\lambda > 1$ but is still much higher than the plotted range for all these examples.

For low intensity ($\lambda = 1$) the profile consists, besides the center peak, of a ring-like structure. It is mainly due to bunches with two ions. At an increased intensity, the fraction of bunches with more than two ions increases, which have a less pronounced ring profile. This results in a broadening of the ring shape that at even higher intensities completely disappears. By measuring these distributions and analyzing the profiles, information about the interaction between individual ions can be obtained. This is interesting to study the microscopic behavior in ion bunches directly, and thus also the stochastic behavior that is not present in the mean-field macroscopic description of space charge effects.

It might be possible to directly relate these results to the stochastic heating that occurs in ion beams. This heating is mainly caused by the interaction of the nearest neighboring ions in a beam. If one would be able to stop the creation of ions that are initially close together, it is expected that the heating will be severely decreased. This may be accomplished by using
the dipole blockade mechanism \cite{2, 3}. In this effect the dipole coupling between Rydberg atoms shifts the energy level of the atoms such that it prevents the excitation of two atoms that are close together with the same laser frequency. If the excited Rydberg atoms can be subsequently field ionized, the chance of producing two ions close together would be greatly reduced. It should be investigated if the dipole interaction can be used in practice to prevent excitations at close distance, which would be needed to effectively reduce the heating. If this is not the case, it might also be possible to find a related scheme, where the local field of an already ionized ion is used to block the ionization path of neighboring atoms.

If this method would work in practice, this would directly result in an observable change in the distribution of the rings. A reduction of the number of bunches with more than one ion is then expected. Additionally, a change in the distribution of the outer part of the ring might be observable. Overall, we showed that coulomb interactions in the cold ion beams can

**Figure 7.3:** Plot of the cross sections of the density distributions resulting from different laser intensities, corresponding to $\lambda = 1, 2, 4$ and $6$ ions per bunch. The different colors correspond to the contribution of bunches with a specific number of ions $n$. 
produce interesting behavior that should be studied in more detail. In the future it might be used to study the stochastic heating and test a scheme that might even prevent it from happening, resulting in even brighter beams.

7.2 Next generation ultra-cold ion source

In this section a brief overview of a new promising alternative source to produce ultra cold ions will be presented. So far in this thesis the cold ions are created by ionizing atoms trapped in a three dimensional magneto optical trap. To enhance the atomic density and loading rate of the 3D-MOT, required to improve the brightness and maximum current, atoms can be loaded from an atomic beam instead of a vapor background as done in the experiments described in this thesis. For this purpose a two dimensional MOT was added to our setup [4], which cools and traps the atoms only in two directions, so an intense atomic beam can be produced. We made it operational and obtained a factor of 10 improvement of the loading rate [5] of the 3D-MOT in comparison with the old situation of using a vapor background. If experimental difficulties are solved, allowing it to be operated at higher rubidium pressure, another factor of 10 improvement is expected [5].

Calculations show that by leaving out the 3D-MOT completely and directly ionizing the atom beam, an even brighter continuous ion beam can be created. This is a further improvement of the idea presented in Ref. [6]. The reason for this is that in the case of such an atomic beam, the influx of atoms is not limited by the low thermal velocities of the cooled atoms as in a 3D-MOT. The longitudinal velocities can be higher, and thus also the influx at the same density. Longitudinal cooling of the atoms is not that important to create a high-brightness ion source. The thermal velocities of the atoms, even at relatively high temperatures, result only in a minor energy spread. For example a longitudinal temperature of 500 °C corresponds to an energy spread below 0.1 eV, still much lower than the competing liquid metal ion source (LMIS) with an energy spread of about 4.5 eV FWHM. This makes it possible to use an oven as a atomic beam source, a so-called Knudsen cell. Because it operates above room-temperature, the vapor density can be fairly high inside, so a relative high flux beam can be extracted from a small hole.

An overview of the proposed setup is given in Fig. 7.4. A high-flux alkali-metal atomic beam is formed by skimming the effusive flow from a heated Knudsen cell. In the next stage, the atomic beam is transversely laser-cooled and compressed. This is done in a 2D-magneto-optical-trap configuration with wide laser beams to enhance the interaction time and a quadrupole magnetic field to compress the beam. The beam can be cooled to sub-millikelvin transverse temperatures and a spot size with sub-millimeter diameters. Subsequently the atomic beam is photo-ionized in a relative low extraction field, so only a small longitudinal energy spread is added by the field. This is completely analogous to the extraction of ions from a 3D-MOT as discussed in this thesis. Simple estimation shows that energy spreads below 0.1 eV can be obtained for extractions fields up to 100 kV/m. Due to the higher
longitudinal velocities of the atoms, and thus shorter interaction time, more ionization laser power is required in comparison with the 3D-MOT source. An optical cavity can be used to reduce the required ionization laser power, as illustrated in the figure. Finally the ion beam can be post-accelerated to the required energy used in a focused ion beam (FIB) system, where it is focused to a small spot. The simple design of this source should make it possible to build it relatively compact with a length of about 25 cm. Optical fibres can be used for both the cooling beams as well as the ionization laser to make the device more robust, so less optical alignment is needed. The laser systems can then be placed at a convenient distance from the source.

The performance of this source can be estimated with a simple model given in [5]. We will not go into the details here, but in this model the brightness is estimated by starting with the flux of the skimmed Knudsen cell. The skimming angle is chosen such that the majority of the atoms has a radial velocity below the capture velocity[7]. By using standard laser cooling relations [7], the final transverse temperature and compressed beam size can be estimated. If it is assumed that all atoms in the atomic beam are ionized, the final ion beam brightness can be calculated. For a rubidium ion source, with a laser-cool section of only 50 mm and a fairly low oven temperature of 100 °C, a reduced brightness is estimated of approximately $10^9 \text{A/(m}^2\text{sr)V}$ with a current up to 1 nA, 3 orders of magnitude higher brightness than a LMIS. Which would make this source also about 3 to 4 orders of magnitude brighter than our previous source.

The brightness in this estimation can even be further increased if other parameters are chosen, such as higher oven temperatures. It is clear that at some point the model breaks down and will produce unrealistic results. In practice the setup is more complicated, and one should study the parts in detail to find their limitations. For example the oven temperature is mainly limited by the requirements that no atom collisions take place in the atomic beam near the exit opening of the cell.

Another important limitation is given by the laser cooling and compression step. The
relatively short interaction time for fast moving atoms limits the attainable cooling and compression. More importantly, if the beam gets more compressed, the density increases up to the point where it gets optically dense, and laser cooling does not work efficiently anymore. Finally, the brighter the ion beam created, the stronger the coulomb interactions that degrade the beam quality due to disorder induced heating.

For parameters of the example above, these effects have been studied in some more detail \[5\]. Basic particle tracking simulations have been performed to estimate the performance of the laser cooling and compression stage, using simplified continuous force equations for the laser cooling. The resulting atomic beam is subsequently ionized, and the resulting ion beam has been simulated with all the mutual coulomb interactions between the ions, taking the disorder-induced heating into account. A reduced brightness of at least $10^8 \text{A}/(\text{m}^2\text{sr}\text{V})$ has been found for currents up to 10 pA. This new generation source is therefore a much better idea for continuous sources than the 3D-MOT source. It may result in very high-brightness, compact and robust sources for different ion species with a brightness about 2 orders of magnitude higher than the LMIS and comparable with the helium field emission source, all in combination with a low longitudinal energy spread. More systematic research should be performed to look into the realistic possibilities and limitations, but we can definitely conclude that ultra cold ion sources have a bright future.

**Bibliography**


Concluding remarks

The goal of the project was to build and investigate the properties of an ultra-cold ion source (UCIS) and, in particular for this thesis, to study the energy spread. In this chapter the main results of this thesis will be discussed and put in a somewhat broader context regarding the current status of this research field. We started with a simple model of the source to describe the properties of the ion beams resulting from the ionization of the cold atoms. For the development of a usable source it is important to know how three crucial properties of the model behave in practice. First of all, under which conditions is it possible to extract ions with effective transverse temperatures comparable with the laser-cooled atoms. Secondly, whether sufficient current can be extracted from the ionization volume. This current depends on the influx of atoms into the volume. Finally, it should be checked under what conditions it is possible to extract the ions with a low energy spread. It is this low energy spread which makes this source interesting for focused ion beam (FIB) applications, since chromatic aberrations in the ion optics are presently limiting the resolution. In this chapter we will briefly discuss what already has been done to answer these questions and other related properties that should be investigated.

8.1 Brightness

Experiments have been performed by the group of McClelland at NIST \cite{1} on a chromium UCIS to measure the effective transverse source temperature. They found an effective source temperature which, as expected, matches with the temperature of the cold atoms. In our lab we also investigated the effective source temperature and found a value of \(1 \pm 2\) mK \cite{2}, which agrees with the expected ion temperature of 0.4 mK. These results show that it is indeed possible to maintain the low temperature, at least at low beam currents.
Chapter 8.

The group at NIST also obtained a brightness of \(2.3 \times 10^4\) A/(m\(^2\)srV) at a current of 1.4 pA, limited by the low density of the chromium atom cloud in the magneto-optical trap. They demonstrated linear scaling of the current, and thus also of the brightness on the atomic density. This scaling is subsequently used over two orders of magnitude to show that higher brightness, comparable to the liquid-metal ion source (LMIS), should be possible when different elements are used which can be trapped with sufficient density. In our experiment we already extracted up to 60 pA continuous current by ionizing a relatively large volume in the atomic cloud. This shows that the loading rate of the whole MOT is already adequate for FIB applications. However, we have not yet optimized the density of the trapped cloud of atoms to extract the same current from a smaller volume, to achieve higher brightness.

We performed realistic particle tracking simulations of the extraction process of the source to investigate the influence of the coulomb interactions on the ion beam. Our simulations show that at higher currents (> 1 pA) the stochastic coulomb interactions start to play a significant role and will increase the effective beam temperature, and therefore lower the brightness. Linear scaling of the brightness with the current over two orders of magnitude, as done by the group at NIST [1], is therefore overoptimistic. Nevertheless we still conclude, based on the simulations, that a brightness of a factor of three lower than the LMIS should be practically achievable. Fortunately, this brightness comes together with a much lower energy spread compared to the LMIS, making it still an interesting alternative, even at the expense of some brightness.

8.2 Longitudinal Energy spread

In this thesis we investigated the longitudinal energy spread more closely. We concluded, based on time-of-flight measurements, that very low energy spread is indeed possible. Bunches with an energy spread as low as 20 meV have been extracted, which is two orders of magnitude lower than with a LMIS. Simultaneously it was demonstrated that well-defined beams of only several eV are possible. This is a completely new regime for ion beams, which might open up new applications such as for example direct ion deposition on a sample.

In these experiments the UCIS was operated in a pulsed manner, mainly because this allowed energy analysis by time-of-flight measurements. The transition from high beam energies, where the ion bunches behave ballistically, to a region with low beam energy where they are space-charge dominated, have been studied. Even at small bunch charge the effects of space charge have been observed, limiting the lowest attainable energy spread. If the source is operated in a continuous fashion, which is desirable for FIB applications, the charge density in the beam will be much lower so space charge is less of an issue. The peak currents of the pulsed measurements, even with the lowest charge \((Q \approx 0.026\) fC) already exceeds 100 pA. As mentioned before, we already have produced quasi-continuous beams, but we did not have the diagnostics to measure their energy spread. It is expected that they have the same energy spread as pulsed beams that are not space-charge limited.
While the overall mean-field space charge effects thus only play a minor role in continuous beams, the stochastic coulomb interaction can still severely degrade the beam quality. This effect has only been studied in simulations for an extraction field of 100 kV/m. For lower extraction fields, used to reach the lowest energy spread and beam energies in the experiment, this has not yet been studied. A much larger degradation effect, at the same current, is expected from the fact that at lower energy the charge density is higher and the timescales are longer. It is therefore still an open question which combination of brightness and energy spread are feasible in the lowest energy regime. There will always be a trade-off between beam energy and brightness. This trade-off and the maximum achievable brightness of this source will be investigated further in the thesis of N. Debernardi.

An interesting alternative application of these low energy ion bunches is to use them as a model system to study complex space charge behavior in charged particle bunches. The initial conditions of the ion bunches, such as the initial ion distribution, can be precisely controlled. For even more control additional techniques such as spatial light modulators (SLMs) can be added to shape the ionization and excitation laser profiles. The timescale of the dynamics in the bunches is relatively long, and can therefore easily be studied in experiments. This is in contrast to dynamics in electron bunches which occurs at sub-nanosecond timescales. Therefore these experiments can help to understand the dynamics of pulsed electron beams, in which deteriorating effects by non-linear space charge forces play an important role. With the cold ions it should, for example, be possible to study in detail the idea of creating a perfectly homogenous ellipsoidal bunch by shaping the initial density distribution [3, 4] in order to overcome these non-linear effects.

### 8.3 Time-dependent fields

In this thesis we also investigated the interesting possibility of operating the ultra cold ion source in pulsed mode. We have demonstrated that this source is well suited for manipulation of the phase-space distribution of the ion bunch with time-dependent fields, both for longitudinal and transverse degrees of freedom. We were able to adjust the longitudinal-focal length which results - in combination with the finite bunch length - in an (correlated) energy spread. Experimentally a reduction of the relative energy spread of the ion bunches was obtained, in comparison to the case of a static acceleration field. Calculations showed that a much larger reduction can be achieved if an optimized, more homogenous accelerator field had been used.

Reducing the energy spread with a time-dependent acceleration field can be interesting because the final energy spread is, in principle, no longer determined by the initial size or acceleration field strength. This makes it possible to start with a longer initial spatial ion distribution, to reduce the coulomb interactions, and still end up with a low energy spread. Also stronger extraction fields can be used, without causing an increased energy spread. This may result in a better trade-off between energy spread and brightness in some situations than when using static fields.
Concerning the transverse direction, it has been shown that the acceleration field can be turned into a fully adjustable lens with control over the focal strength and its sign as well as the sign and strength of the spherical aberrations. Negative spherical aberrations are possible using time-dependent fields. In that case the aberration is not limited by the Scherzer’s theorem, stating that only positive spherical aberrations are possible for cylindrically symmetric fields. This lens may be used to create an aberration-corrected focusing column, without the need of using cumbersome non-rotationally symmetric geometries.

As a complication, the longitudinal and transverse phase-space manipulations are coupled by the zero-field divergence in the Maxwell equations. For the linear focusing this means that if the accelerator acts as a positive transverse lens, the longitudinal focal strength will be automatically negative and vice versa. Similar things will happen for the higher-order terms. If for example a voltage pulse is used that results in a negative spherical aberration in the transverse direction, an unwanted third-order aberration will occur in the longitudinal phase-space distribution.

Additionally, to make it even more challenging, cross terms between the longitudinal and transverse phase-space will be present. In the model of the time-dependent manipulation presented in this thesis, we only used test particles that were displaced in one direction; to describe longitudinal manipulation only a longitudinal displacement was used, and for transverse direction only a transverse displacement. If one uses test particles displaced in both directions simultaneously, one will find that the higher-order transverse manipulation also depends on the initial longitudinal position.

Whether these higher order cross term are a problem in practice, depends on the exact application and geometry. A possible solution to minimize these effects would be to start with a non-round initial ionization volume. For transverse manipulation a pancake-like initial ion distribution, with the smallest size in the $z$-direction, would be ideal, while for longitudinal manipulation a cigar distribution with radially the smallest dimension would be favorable. A more detailed study of a design for a specific application should be performed to conclude if this time-dependent technique can indeed be used in practice.

### 8.4 Cold electron source

In this thesis we limited ourself to ion experiments, but the same experimental setup has been used as a cold electron source; Only the polarity of the applied acceleration voltages has to be changed. We performed several experiments [5, 6] and demonstrated an effective source temperature of 15 K, which is several orders lower than photo-emission sources. Simulations [7] have shown that this source should enable orders of magnitude higher brightness electron bunches than state-of-the-art photo-emission sources. Time-dependent manipulation of electrons, very similar to the techniques demonstrated for ions in this thesis, become possible if radio-frequency (rf) cavities are used. Longitudinal focusing of 100 keV electron bunches with rf cavities makes bunches as short as 100 fs possible [8]. By performing electron diffrac-
Concluding remarks

ion with such short bunches, it should become possible to measure the molecular dynamics of crystals at these timescales. Recent calculations [9] performed in our group show that the combination of our cold plasma source with radio-frequency (rf) cavities, makes this a very interesting source for such Ultra-fast Electron Diffraction (UED) experiments. The low initial velocities of the cold electrons result in a long coherence length, so ultra-fast single-shot electron diffraction on large bio-molecules should become possible [9].

Bibliography


Summary - Ion Beams from Laser-cooled Gases

High-brightness ion sources are important for several applications such as focused ion beam (FIB) systems, in which an ion beam is focused on a sample to a spot size of a few nanometers. These systems have become an important tool in a wide array of material science and technological applications, because they offer both high-resolution imaging as well as micro-machining capabilities. The resolution in the most common FIB system, the Gallium-Liquid Metal Ion Source (Ga-LMIS) based FIB, is limited by chromatic aberrations in the lens column due to the energy spread of $\approx 2$ eV. To reach a higher resolution, a high-brightness ion source is needed with a lower energy spread.

In this thesis such a new source is presented, the ultra-cold ion source (UCIS) based on the photo-ionization of a laser-cooled atomic gas confined in a magneto-optical trap. The low temperature ($\approx 150 \mu$K) of the source makes it possible to reach high-brightness with an extended source size. The charge density at the source is thereby reduced compared to sources with a sharp tip, such as the LMIS, and thus also the Coulombic interactions that deteriorate the beam and increase the longitudinal energy spread. Additionally, many different atomic species can be laser-cooled, making the UCIS a versatile source for both heavy and light ion species. Light ion species such as Li are very suitable for imaging purposes without directly damaging the sample. Heavy ion species on the other hand, can be used for manipulation of a sample by sputtering away material at a small scale.

An analytical model has been developed to estimate the initial source performance. The extractable current from the ionization volume is estimated based on the influx of atoms, which depends on temperature and atomic density. According to the model, the energy spread $\sigma_U$ is proportional to the finite length of the ionization volume, limited by the size of the laser focus waist, and the acceleration field $E_0$. To study the influence of the ionic interactions in the beam in more detail, particle tracking simulations have been performed which take all mutual coulombic interactions into account under realistic experimental conditions. From these simulations we learned that when the current is increased, the brightness is lowered due to increased stochastic heating. Beam currents between 1 and 100 pA are feasible, with an energy spread much lower than that of the LMIS. At 1 pA the source has a peak brightness up to $B_r = 8 \times 10^4$ Am$^{-2}$sr$^{-1}$ with an energy spread $\sigma_U = 0.08$ eV. At 10 pA it has a brightness up to $B_r = 2 \times 10^4$ Am$^{-2}$sr$^{-1}$ with an energy spread $\sigma_U = 0.14$ eV.

An experimental setup has been built, consisting of a rubidium magneto-optical trap...
inside a cylindrically symmetric accelerator structure. By using a two-step photo-ionization process, a small fraction of the cold atoms in the cross-section of two laser beams is ionized. A pulsed ionization laser was used to produce ion bunches. A short beam line with a multi-channel plate detector was used to obtain both the temporal and the transverse spatial profile of the bunches.

Time-of-flight measurements have been performed to characterize the longitudinal energy spread of the beam as function of the beam energy $U$. We have demonstrated, as predicted by the model, that the energy spread $\sigma_U$ is indeed due to the length of the ionization volume in the acceleration field. By lowering the extraction field, well defined beams with an average energy of only 1 eV have been produced with an energy spread as low as 20 meV, more than two orders of magnitude lower than the LMIS. A transition from ballistic behavior at high beam energies, where $\sigma_U \propto U$, to a space-charge dominated regime at low beam energies, where $\sigma_U \propto \sqrt{U}$, has been observed. In the cross-over region an interesting new effect has been observed in which the space charge forces reduce the energy spread. The experimental results agree well with detailed particle tracking simulations.

The combination of well-defined ion beams at low energy and time-dependent acceleration fields opens new possibilities. Precise manipulation of the bunch distribution in both longitudinal and transverse phase-space has been demonstrated. Reduction of the longitudinal energy spread has been realized by switching the accelerator field off before the ions have had a chance to leave the accelerating structure. A reduction by a factor 3 is achieved, which is limited by the inhomogeneity of the field. Calculations show that a much stronger reduction is achievable in a more homogenous acceleration field. This would make low-energy spread possible without the need to go to small $\sigma_z$ and $E_0$, enabling even lower energy spread.

We also demonstrated that the accelerator structure, which normally acts as a fixed negative lens, can be transformed into a versatile lens by using time-dependent fields. Control over the focal length and sign, as well as the sign and strength of the spherical aberrations can be obtained by tailoring the applied time-dependent acceleration voltage. The possibility to create a negative spherical aberration may be used to correct for the spherical aberrations in the focal columns which are presently limiting the spatial resolution of FIBs. The dependence of the properties of this lens on the parameters of the applied tri-polar pulse has been studied in detail, both experimentally and with particle tracking simulations, which are in good agreement.

Finally, based on lessons learned, the design of a next generation UCIS is briefly discussed, based on photo-ionization of a laser-cooled and intensified atomic beam. The principle is similar as an UCIS based on a MOT, but with a higher current density. Calculations show that this source should be able to produce orders of magnitude brighter beams in a more compact configuration. With this new design it should be possible to beat the LMIS not only in energy spread but now also in brightness.
Samenvatting - Ionenbundels op basis van lasergekoelde gassen

Om een atoom cirkelen net zoveel negatief geladen elektronen als het aantal positief geladen kerndeeltjes, zodat de totale lading van het atoom op nul uitkomt. Als er een elektron verwijderd wordt, ontstaat er een positief geladen deeltje, een ion. Doordat een ion geladen is, kan het relatief eenvoudig door middel van elektrische en magnetische velden beïnvloed worden. Dit maakt ionen, en geladen deeltjes in het algemeen, uitermate geschikt voor precisie toepassingen.

Een belangrijk voorbeeld hiervan is een zogenaamd 'focused ion beam' (FIB) systeem, waarin een bundel ionen gefocuseerd kan worden tot een kleine spot op een te onderzoeken of te bewerken sample. De spot kan een afmeting hebben van enkele nanometers, ongeveer 1000x zo klein als de dikte van een menselijke haar. Afhankelijk van de massa en de energie van de ionen, zal bij een botsing van de ionen op het sample materiaal verwijderd worden. Dit maakt het mogelijk om op deze kleine nanometer schaal gaten te boren, te snijden en ingewikkelde structuren te frezen in het sample. Naast het bewerken van het sample is het ook mogelijk om de ionenbundel te gebruiken om een afbeelding te maken van het sample oppervlak. Dit lijkt sterk op elektronen microscopy, waarin een bundel elektronen wordt gebruikt in plaats van ionen. Een van de voordelen van het gebruik van ionen is dat er een beter onderscheid gemaakt kan worden tussen materialen en dat er in principe een hogere resolutie behaald kan worden. Deze maximale resolutie hangt samen met de minimale spot grootte van de ionenbundel die in zo’n systeem bereikt kan worden.

Deze minimale spot grootte hangt vervolgens af van de kwaliteit van de gebruikte ionenbron. De ionenbron produceert het werkelijke ionenbundeltje dat in de rest van het apparaat door middel van elektrische en magnetische velden wordt gefocuseerd. FIB systemen worden veel gebruikt in de halfgeleiderindustrie voor het ontwikkelen van nieuwe computerschips. Structuren in deze nieuwe computer chips worden steeds kleiner en daarom moet ook de resolutie van FIB systemen verbeterd worden om bruikbaar te blijven. Meestal wordt als bron een 'vloeibaar metaal ionenbron' (VMIB) gebruikt, waarin een bundel van gallium ionen wordt geproduceerd op de punt van een scherpe naald. Alle ionen komen oorspronkelijk dus uit een klein oppervlakte (≈ 10 nm²) en zitten in het begin dus vaak dicht bij elkaar. Omdat de ionen elkaar afstoten, resulteert dat in een slechtere kwaliteit van de bundel, wat zich vooral
uit in een spreiding in de voorwaartse richting van de ionen, de zogenaamde energiespreiding. Deze energiespreiding (≈ 5 eV) veroorzaakt op zijn beurt weer een grotere gefocussederde spot doordat ionen met verschillende snelheden anders worden gefocussederd. Om toch hogere resolutie mogelijk te maken is een nieuw type ionenbron nodig met een lage energiespreiding.

Dit proefschrift beschrijft het onderzoek naar zo'n nieuwe soort ionenbron. Deze bron is gebaseerd op een compleet ander principe dan bestaande bronnen, zoals de VMIB. Deze proberen een ideale puntbron te benaderen door de ionen uit een zo klein mogelijk oppervlakte te halen. In dit project wordt een bron gebouwd die zoveel mogelijk een perfecte parallelle bundel benaderd. Dit laatste is mogelijk door gebruik te maken van hele koude atomen. Met behulp van laserkoeling kan een wolkje atomen afgekoeld worden tot ongeveer 0.0001 graad boven het absolute nulpunt. Bij deze lage temperatuur (≈ 100 µK) staan de atomen bijna stil. Als deze atomen geïoniseerd en versneld worden, ontstaat er een mooie parallelle bundel. De afstanden tussen de ionen zijn in dit geval groter, en onderlinge afstoting heeft daardoor minder nadelige effecten op de kwaliteit. Een eenvoudig analytisch model van dit nieuwe bron concept is gemaakt om de eigenschappen af te schatten voor verschillende keuze van parameters. Het model voorspelt dat een heldere ionenbundel met lage energiespreiding inderdaad mogelijk moet zijn. De energiespreiding wordt bepaald door de grootte van het te ioniseren volume en de sterkte van het aangelegde elektrische veld in de versneller. Naast dit model zijn door middel van deeltjes simulaties, waarin de banen van alle individuele ionen zijn berekend, ook de invloed van de interactie tussen de verschillende ionen op de helderheid van de bundel bekeken.

We hebben een experimentele opstelling gebouwd waar in het hart van een versnellend elektrisch veld rubidium atomen gekoeld kunnen worden in een magnetisch optische val. De atomen zijn in het experiment geïoniseerd door een gepulste laser. De ionen versnellen in het elektrisch veld en worden dan uiteindelijk waargenomen door een detector. Zowel de verdeling in aankomsttijd als in plaats wordt geregistreerd.

De spreiding in de snelheden in de voortbewegingsrichting, de energiespreiding, is onderzocht door te kijken naar de spreiding in aankomsttijd van de ionen. Dit is gedaan voor verschillende bundelenergieën door het versnelveld te variëren. We hebben laten zien dat de energiespreiding inderdaad zoals in het model veroorzaakt wordt door de begingrootte in het elektrische veld. Door naar lagere versnelvelden te gaan zijn goed gedefinieerde bundels met een gemiddelde energie van slechts 1 eV geproduceerd met een energiespreiding van maar 0.020 eV. Deze spreiding is meer dan twee ordes van grootte lager dan bij de VMIB. Een overgang van een regime bij hoge bundelenergie waar onderlinge afstotende krachten geen rol spelen naar een regime bij lage energie waar de onderlinge krachten domineren is waargenomen. In het overgangsgebied is een nieuw effect waargenomen waar de ruimteladingskrachten de energiespreiding reduceren. De experimentele data komt goed overeen met gedetailleerde deeltjessimulaties.

De combinatie van goed gedefinieerde laag energetische ionenbundels en tijdafhankelijke versnelvelden biedt nieuwe mogelijkheden. Precisie manipulatie van de ionenpens in zowel
de voortplantingsrichting als de breedterichting is gedemonstreerd. Vermindering van de energiespreiding is gerealiseerd door middel van het snel uitschakelen van het versnelveld voordat de ionen de kans hebben gehad om de versnelstructuur te verlaten. Een reductie met een factor 3 is aangetoond, gelimiteerd door de vorm van het gebruikte versnelveld. Berekeningen laten zien dat sterkere reductie mogelijk is in een homogene, beter geo-optimaliseerde versneller. Dit zou het mogelijk maken om lage energiespreiding te verkrijgen zonder naar (onpraktische) kleine ionizatierevolumes of lage versnelvelden te moeten gaan.

Hiernaast hebben we ook gedemonstreerd dat tijdafhankelijke velden gebruikt kunnen worden om de versnelstructuur, die normaal werkt als een vaste negatieve lens voor de ionen, getransformeerd kan worden in een veelzijdige instelbare lens. Volledige controle over de focuslengte en de (sferische) lensafwijkingen kan verkregen worden door het tijdafhankelijke versnelveld bij te stellen. De mogelijkheid om met behulp van tijdafhankelijke velden nu ook negatieve lensafwijkingen te maken kan mogelijk gebruikt worden om te corrigeren voor (sferische) afwijkingen in een FIB systeem. Dit kan bijdragen aan het verbeteren van de maximale resolutie. De afhankelijkheid van de focuseigenschappen van de lens als functie van de verschillende parameters die de vorm van de tijdafhankelijke pulse beschrijven is in detail onderzocht. De resultaten uit de experimenten en van de deeltjesimulaties komen goed overeen.

Als laatste is de opgedane kennis gebruikt voor het ontwerpen van een volgende generatie koude ionenbron. Die is gebaseerd op het ioniseren van een met laserkoeling intenser gemaakte atoombundel in plaats van een wolkje met atomen. Het principe is hetzelfde, maar hiermee kan een hogere stroomdichtheid gehaald worden. Berekeningen aan deze bron laten zien dat het in principe mogelijk is om meerdere ordes van grootte in helderheid te winnen. Met dit nieuwe ontwerp zou de bron de VMIB verbeteren op zowel energiespreiding als helderheid.
List of publications

- *Phase-Space Manipulation of Ultracold Ion Bunches with Time-Dependent Fields*,

- *Low-Energy-Spread Ion Bunches from a Trapped Atomic Gas*,

- *Design and validation of an accelerator for an ultracold electron source*,

- *Simulated performance of an ultracold ion source*,

- *Cold electron and ion beams generated from trapped atoms*,

To be published

- *Time-dependent manipulation of ultracold ion bunches*,

- *Ultracold ion source temperature measurement with a time-dependent electric field*,

- *Ultracold electron source for single-shot diffraction studies*,
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