Towards trapping of molecular ions in a linear Paul Trap

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PhD Progress Report

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Abstract

An abstract...

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Towards trapping of molecular ions in a linear Paul Trap

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Chapter 1

Introduction

In the 1950's Wolfgang Paul invented the so-called Paul trap, for trapping charged particles within a quadrupolar electromagnetic field.CITE. In 1989 he would go on to recieve the Nobel Prize in physics, alongside Hans Dehmelt, "for the development of the ion trap technique" CITE. With the many technological and scientific advancements since the Paul trap's inception, among which the laser is an especially important one, it is now possible to trap, and cool single ions to temperatures below 1mK CITE Wineland. Such cold ions pose many interesting possibilities for science, as they can make good candidates for atomic clocks CLOCK, or the basis for quantum computers Wineland, Cirac Zoller.

Paul traps are also used for the study of fluorescence of molecules in the gas phase CITE Steen?, where pulsed lasers can be used to excite large clouds of molecular ions, whose fluorescence spectrum may then be recorded and studied. However as most molecules lack the necessary energy level structure for laser cooling, the temperature of these experiments are limited by their cryogenic cooling environment.

The aim of my PhD thesis is to build an experiment where single molecular ions from an electrospray ionization source FENN can be trapped in a linear Paul trap alongside a Ba^+ ion and cooled to their motional ground state. In such a setup we would like to investigate the molecules using a method called photon recoil spectroscopy CITE EMILIE. This method functions by using the momentum kick associated with the molecules absorption of light as a measure of whether absorption has occured, and is explained further in chapter 5. Directly applying this method to two-ion systems with large mismatches in mass and charge is challenging, since the motions of the ions are only very weakly coupled, and thus the absorption kick will predominantly excite the motion of the molecule, which is not sensitive to the readout performed by a laser on the Ba^+ ion. Due to this issue I have been looking at CITE, and developing theory for how to transfer energy from one motional mode to another, to allow for efficient readout of the absorption kick.

Outline of the report

The report is divided into 6 different chapters. Chapter 1 is a brief introduction to the field, some of the challenges I face, and what I hope to accomplish with my PhD.

Chapter 2 describes the physics of trapping ions in a linear Paul trap and is split into two sections, the first describing the trapping of a single ion, while the latter derives the common motion of two ions in the trap.

Next is chapter 3 which describes the electrospray ionization source, which is the source of molecular ions for the experiment. The first section of this chapter is an overview of the setup and the second contains a characterization of one of the octopoles guides within the setup.

After that I move on to chapter 4 which describes the laser cooling necessary for eventually reaching the motional ground state of a two-ion system. The first section contains the theory for doppler cooling, which allows the ions to reach a temperature of ~1mK. The second section describes sideband cooling, which is necessary to cool the motion of the system to its quantum mechanical ground state. Finally the 3rd section of this chapter talks on how one can couple the motion of the ions by using fx. an external field, in order to improve the cooling of systems where the two ions have large differences in mass and charge.

Finally chapter 6 gives a short plan of the work I plan to do in the latter half of my PhD studies here at Aarhus.

Chapter 2

The Linear Paul Trap

2.1 Single ion in a linear Paul Trap

The linear Paul trap consists of four rods, each of which is split into three electrodes as is seen on fig. 2.1. The coordinate system for the trap is defined such that the z-axis runs down along the centre of the trap, while the x, y-axes go between diagonally opposed rods. Furthermore we define z_0 to be half the length of center electrodes, while we define r_0 as half the distance between diagoanlly opposed electrodes as seen on fig. 2.1. In order to trap an ion along the z-direction a static voltage V_{end} is applied to all of the electrodes on the end of the rods. By applying such a votlage to these endcap electrodes an electrical potential is generated, which in the region around the centre of the trap can be written as

$$\phi_{DC}(z) = \frac{\kappa V_{end}}{z_0^2} z^2, \tag{2.1}$$

where κ is a constant defined by the specific geometry of the trap, and z is the position of the ion along the z axis. Thus an ion of mass m and charge Q finds itself sitting in a harmonic potential

$$V_{DC}(z) = \frac{1}{2} m\omega_z^2 z^2, \quad \omega_z = \sqrt{\frac{2Q\kappa V_{end}}{m z_0^2}}, \tag{2.2}$$

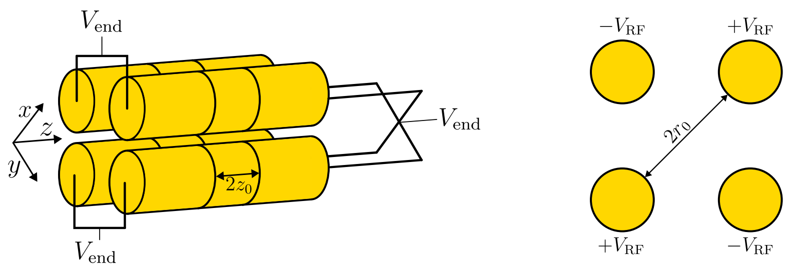

Figure 2.1: Example schematic of a linear paul trap showing: (left) a 3D model of the paul Trap with both the DC endcap voltages applied. (right) an end-view down the Paul trap, showing the phase of the RF voltages applied to the different rods..

where ω_z is the frequency of the ions oscillating motion along the z-axis.

For the radial directions it is necessary to take a slightly different approach, indeed Earnshaw's theorem Earnshaw states that it is impossible to trap a charged particle in all three directions, solely through the use of electrostatic forces. If we look at the electrical potential in the x, y-plane from the DC endcaps we also find

$$\phi_{DC}(x, y) = -\frac{\kappa V_{end}}{2z_0^2}(x^2 + y^2), \tag{2.3}$$

which is clearly repulsing the ion from the center of the trap.

To counteract this repulsive effect, we employ an RF voltage, oscillating at frequency Ω_{RF}, with an amplitude V_{RF} on all four rods. Neighbouring rods have opposites phases while, diogantly opposing rods share a phase, as seen on fig. 2.1. We can then write the total time dependant electrical potential in the x, y-plane as KARIN

$$\phi(x, y, t) = -\frac{\kappa V_{end}}{2z_0^2}(x^2 + y^2) - \frac{V_{RF}}{2r_0^2}(x^2 - y^2)\cos(\Omega_{RF} t), \tag{2.4}$$

where the first term comes from the repulsing DC potential, and the second term comes from the RF voltages applied to the rods.

The equations of motion in the radial plane can be rewritten on a more compact form by adopting the notation

$$\tau = \frac{\Omega_{RF} t}{2}, \quad a = -\frac{4Q\kappa V_{DC}}{m z_0^2 \Omega_{RF}^2}, \quad q_x = -q_y = \frac{2QV_{RF}}{m r_0^2 \Omega_{RF}^2}, \tag{2.5}$$

which allows for the equations of motion to be written as

$$\frac{\mathrm{d}^2\rho}{\mathrm{d}\tau^2} + (a - 2q_\rho \cos(2\tau))\rho, \quad \rho \in \{x, y\}. \tag{2.6}$$

Equation (2.6) is known as the Mathieu equation CITE, the Mathieu equation has bounded solutions for several sets of (a, q_ρ) parameters, however, the conditions usually used in experiment state that for a given value of q_ρ, a must be found between the two curves approximated by CITE

$$a_0(q_\rho) \approx -\frac{1}{2}q_\rho^2 + \frac{7}{128}q_\rho^4 - \frac{29}{2304}q_\rho^6 + \frac{68687}{18874368}q_\rho^8, \tag{2.7}$$

$$b_1(q_\rho) \approx 1 - q_\rho - \frac{1}{8}q_\rho^2 + \frac{1}{64}q_\rho^3 - \frac{1}{1536}q_\rho^4 - \frac{11}{36864}q_\rho^5. \tag{2.8}$$

Together these two lines form what is known as a stability diagram. Since a positive DC voltage is needed for the confinement in the axial direction, we usually confine ourselves to considering stability in the $a < 0$ region. A plot of the stable region for the linear Paul trap can be see on fig. 2.2

In the case where $|a|, |q_\rho| \ll 1$ the solution to eq. (2.6) can be approximated to

$$\rho(t) = \rho_0\left(1 - \frac{q_\rho}{2}\cos(\Omega_{RF} t)\right)\cos(\omega_r t), \quad \omega_r = \frac{\Omega_{RF}}{2}\sqrt{\frac{q_\rho^2}{2} + a}. \tag{2.9}$$

Since $|q_\rho| \ll 1$ we see that there is a large-amplitude motion of the ion at frequency ω_r. This motion is typically referred to as secular motion in the litterature. The

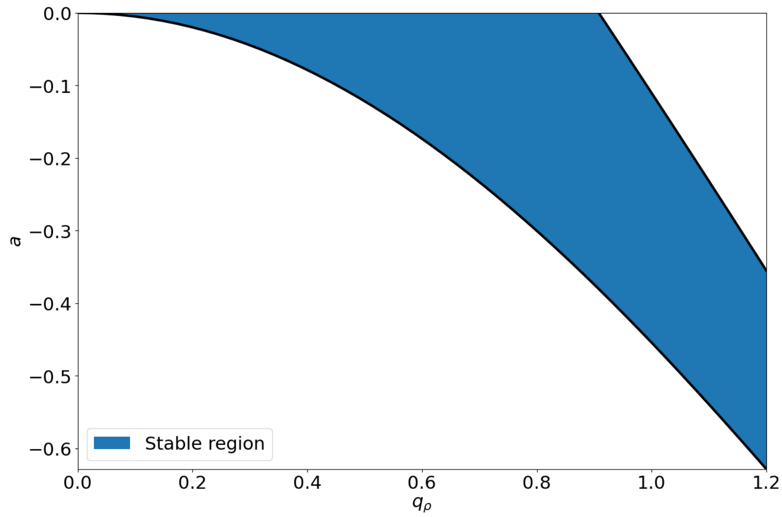

FIGURE 2.2: Plot of the Mathieu stability diagram for negative values of a. The blue colored area contains the set of bounded, and thus stable solution to the Mathieu equation of eq. (2.6).

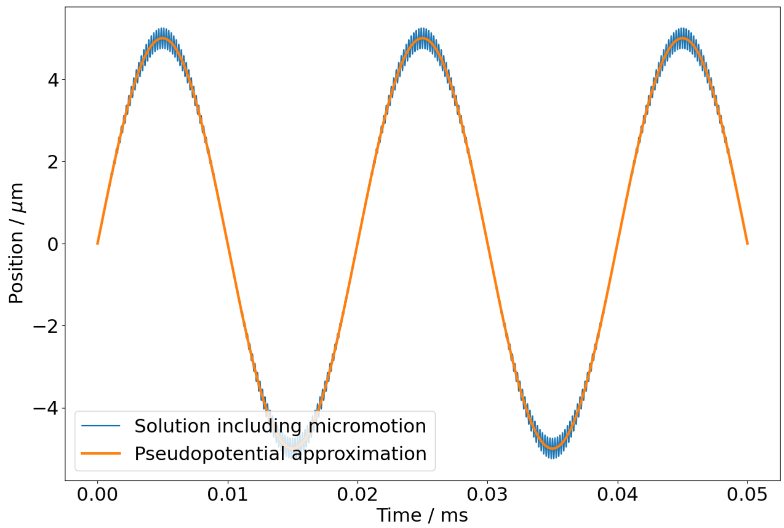

FIGURE 2.3: Trajectories including (blue) micromotion or calculated through the pseudopotential approximation (orange), for $\rho_0 = 5\mu$m, $\omega_r = 2\pi \times 50$kHz, $\Omega_{RF} = 2\pi \times 5.2$MHz..

frequency ω_r is much slower than the RF frequency of the trap (typically 10's-100's of kHz vs. 5MHz in the case of our trap).

In addition there is a small-amplitude motion superimposed on top, oscillating at the RF frequency. This motion is typically referred to as micromotion. Thus the full picture we now get, is one of the ion performing slow, but large oscillations in the radial plane, with an additional micromotion on top. An example trajectory can be seen on fig. 2.3, where the micromotion is clearly visible.

It is common to average over the micromotion of the ion, keeping only the term oscillating at ω_r. If this is done, it is clear that the ion then moves as if in an effective potential (often referred to as pseudopotential in the litterature) given by

$$V_{Pseudo}(\rho) = \frac{1}{2}m\omega_r^2\rho^2, \quad \rho \in \{x, y\}. \tag{2.10}$$

The pseudopotential approximation is especially useful when working with trapped ions in a quantum mechanical regime, since their Hamiltonian is then simply that of a harmonic oscillator, which is one of the most well-studied examples in all of quantum mechanics.

2.2 Two ions in a linear Paul trap

We now move on to the topic of two co-trapped ions in a Paul trap. We shall denote the ions 1 and 2 respectively, with masses m_1, m_2, and charges Q_1, Q_2. Remembering to include the Coulomb interaction between the two ions, the potential energy of the system, in the pseudopotential approximation, can then be written as

$$\begin{aligned} V(\boldsymbol{r_1}, \boldsymbol{r_2}) = &\frac{1}{2}m_1\left(\omega_{1,z}^2 z_1^2 + \omega_{1,r}^2(x_1^2 + y_1^2)\right) + \frac{1}{2}m_2\left(\omega_{2,z}^2 + \omega_{2,r}^2(x_2^2 + y_2^2)\right) \\ &+ \frac{Q_2 Q_2}{4\pi\epsilon_0}\frac{1}{|r_1 - r_2|}, \end{aligned} \tag{2.11}$$

where $\omega_{j,(r/z)}$ is calculated as in eqs. (2.2) and (2.9), using the mass and charge of ion j. For the rest of the derivations in this report we are, unless otherwise noted, going to ignore the y part of motion of the ions since our system exhibits a radial symmetry, and thus any equations that hold for x will hold for y as well.

Chapter 3

Electrospray ionization source

3.1 Overview of the electrospray and its components

3.2 Experiments on the first octopole

Chapter 4

Cooling

4.1 Doppler cooling

4.2 Sideband Cooling

4.3 Coupling of motional modes to enhance cooling

Chapter 5

Photon Recoil Spectroscopy (WHERE SHOULD THIS GO?)

Chapter 6

Future Work

In the following, I will outline the topics I will work on in the final part of my PhD …