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**Simulations of dynamics of ultra-cold  
quantum plasma**

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I would like to say thank you to my supervisor for not being mad at me, even though I am behind on schedule :).



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# Contents

<b>Introduction</b>	<b>3</b>
<b>1 Theoretical introduction</b>	<b>5</b>
1.1 Coulomb crystal . . . . .	5
1.2 Ion trapping . . . . .	5
1.2.1 Equation of motion . . . . .	5
1.2.2 Effective potential . . . . .	6
1.2.3 Adiabacity . . . . .	8
1.2.4 Trap geometry . . . . .	9
1.2.4.1 Multipole trap . . . . .	9
1.2.4.1.1 Quadrupole trap . . . . .	11
1.2.4.2 Real geometry of our trap . . . . .	11
1.2.5 Spring constant . . . . .	12
1.2.6 Mathieu equation . . . . .	13
1.2.7 Stability . . . . .	14
1.3 Laser cooling . . . . .	14
<b>2 Confinement of two species with radically different charge to mass ratio</b>	<b>17</b>
2.1 Two frequency quadrupole Paul trap . . . . .	17
2.2 Floquet theory . . . . .	19
2.3 Simulation . . . . .	21
2.3.1 Choice of time-step . . . . .	23
2.3.2 Treatment of laser cooling . . . . .	23
2.3.3 Simulating Coulomb crystal . . . . .	23
2.3.4 The code . . . . .	24
<b>3 Results and discussion</b>	<b>25</b>
3.1 Characteristics of $q_1 - q_2$ stability diagrams for one electron . .	25
3.1.1 Dependence on initial conditions . . . . .	27
3.2 Creating a Coulomb crystal . . . . .	28

3.3	Stability of electron in Coulomb crystal . . . . .	28
3.3.1	One electron - one ion . . . . .	28
3.3.2	One electron - twenty ions . . . . .	28
3.3.3	One electron - a hundred ions . . . . .	28
3.4	Design of the experiment . . . . .	28
3.5	Future . . . . .	28
<b>Conclusion</b>		<b>29</b>
<b>Bibliography</b>		<b>31</b>
<b>A Using software</b>		<b>33</b>

# Introduction

This thesis's practical aim is to contribute to developing an experiment initiated by my supervisor Mgr. Michal Hejduk, Ph.D. In this experiment, we wish to create and study the properties of a quite unusual type of plasma, Coulomb crystal. Coulomb crystals are mostly stationary structures of ions characterized by large coupling parameter  $\Gamma^1$ , representing the ratio between electrostatic and kinetic energy of ions. These structures have been extensively studied now for decades. Our ambition is to introduce electrons to such a crystal and cool everything down. We will be aiming for sub-kelvin temperatures when electrons de Broglie wavelength would be greater than the distance between them, forming so-called Fermi gas, which to my knowledge, has not been achieved yet inside a Coulomb crystal. Creating a Coulomb crystal means confining a certain number of charged particles in bounded space. The first thing standing in our way is Earnshaw's theorem [1], stating that there is no stable electrostatic configuration of charged particles. Of course, we are not about to give up just yet. Therefore we must try our luck outside the realm of electrostatics. Here we have already been presented with two well-established ways of storing charged particles. One utilizes an axial magnetic field to confine particles in a radial direction and a static electric field for confinement in an axial direction. This approach developed by H.G. Dehmelt is called the Penning trap. The second option to restrict the movement of charged particles in all directions is to solely use the dynamic electric field. Such a trap bears the name of Wolfgang Paul, hence the Paul trap. Both these gentlemen were awarded a shared Nobel prize for physics in 1989 for their efforts in this field. The ions in our experiment will be laser-cooled, which would be disturbed by a magnetic field due to Zeeman splitting. Ergo we are left with the latter method. Our job is to make a computer simulation of an ion crystal with electrons inside a Paul trap, optimizing its parameters to attain the lowest possible temperature of electrons, hopefully reaching the electron delocalization over multiple ions in the Coulomb crystal.

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<sup>1</sup>All the non-trivia will be further explained in the first chapter



# Chapter 1

## Theoretical introduction

In this chapter, we introduce concepts essential for understanding this thesis's concerns. This chapter is divided into several subsections.<sup>1</sup>

the sections in the first two chapters will probably be rearranged

### 1.1 Coulomb crystal

Things to write about: definition of plasma, characteristic parameters, coupling parameter  $\Gamma$ , better characterization of Coulomb crystal, point of crystallization, strongly coupled plasma in the nature, Rydberg atoms

### 1.2 Ion trapping

Here we introduce the concept of trapping a single ion by a quickly oscillating field. We will tightly follow a classic textbook [2] in the whole section, starting by writing the equation of motion.

#### 1.2.1 Equation of motion

Let us consider a particle with mass  $M$ , charge  $Q$ , and position denoted by vector  $r$ . We insert such a particle into the external time-dependent electromagnetic field described by  $E(t, r)$  and  $B(t, r)$ . The Lorentz force gives the equation of motion:

$$M\ddot{r} = Q [E(t, r) + \dot{r} \times B(t, r)]. \quad (1.1)$$

<sup>1</sup>In the first subsection, we are going to discuss the basic principles of plasma physics. In the following subsection, we will talk about the motion of a charged particle inside the Paul trap. Next, we will introduce the idea of laser cooling. And finally, in the last subsection, we will present our approach to simulating such a system, entering this thesis's practical component.

Since we are not using any external magnetic field, and while trapping a particle in a compact space, we usually deal with small velocities. Therefore we neglect<sup>2</sup> the effect of the term  $\dot{\mathbf{r}} \times \mathbf{B}$ , which means that the equation of motion simplifies to:

$$M\ddot{\mathbf{r}} = Q\mathbf{E}(t, \mathbf{r}). \quad (1.2)$$

We further assume that the electric field is composed of static and time-dependent parts. We are looking for a simple periodic time-dependency. A typical way to model such behavior would be  $\mathbf{E}(t) \sim \cos(\Omega_1 t)$ , giving us:

$$\mathbf{E}(t, \mathbf{r}) = \mathbf{E}_s(\mathbf{r}) + \mathbf{E}_0(\mathbf{r}) \cos(\Omega_1 t), \quad (1.3)$$

and following equation of motion:

$$M\ddot{\mathbf{r}} = Q [\mathbf{E}_s(\mathbf{r}) + \mathbf{E}_0(\mathbf{r}) \cos(\Omega_1 t)]. \quad (1.4)$$

### 1.2.2 Effective potential

Dealing with such rapidly changing non-autonomous differential equations can become a riot, although it is possible to solve them analytically for special boundary conditions, as will be discussed further. By a lucky chance, we are not always interested in exact solutions while trapping ions. The relevance often lies in the time-averaged effect of a swiftly changing field. With that in mind, we will now try to derive *effective potential* fulfilling precisely this role.

Let's consider initial conditions:  $\mathbf{r}(0) = \mathbf{r}_0$  and  $\dot{\mathbf{r}}(0) = 0$ . For the simplest case of homogeneous electric field  $\mathbf{E}_0(\mathbf{r}) = \text{const}$ , we obtain a trivial solution:

$$\mathbf{r}(t) = \mathbf{r}_0 - \mathbf{A} \cos(\Omega_1 t), \quad (1.5)$$

where the vector:

$$\mathbf{A} \equiv \mathbf{A}(\mathbf{r}) = \frac{Q\mathbf{E}_0(\mathbf{r})}{m\Omega_1^2}, \quad (1.6)$$

is an amplitude of oscillation around the initial position of the particle. The crucial consequence of this result is that we can further restrict the motion of a particle by increasing the frequency of field oscillation. Of course, the situation changes when we bring a small inhomogeneity into the field. Here comes our first leap of fate by assuming that the amplitude of oscillation  $\mathbf{A}$  won't be affected by this inhomogeneity. Instead, the particle will drift slowly towards the weaker field region. Motivated by this observation, we can try to find a solution to the equation of motion in the form:

$$\mathbf{r}(t) = \mathbf{R}_0(t) + \mathbf{R}_1(t), \quad (1.7)$$

---

<sup>2</sup>This and other approximations are further discussed in the section 2.3.

where  $\mathbf{R}_0(t)$  represents consequence of smooth drift and  $\mathbf{R}_1(t)$  stands for rapid oscillation, expressed as:

$$\mathbf{R}_1(t) = -\mathbf{A} \cos(\Omega_1 t). \quad (1.8)$$

If the field amplitude  $\mathbf{E}_0(\mathbf{r})$  varies smoothly with regards to the space dimension, we can get by just with its first-order Taylor expansion around  $\mathbf{R}_0$ :

$$\mathbf{E}_0(\mathbf{R}_0(t) - \mathbf{A} \cos(\Omega_1 t)) \approx \mathbf{E}_0(\mathbf{R}_0(t)) - (\mathbf{A} \cdot \nabla) \mathbf{E}_0(\mathbf{R}_0(t)) \cos(\Omega_1 t) + \dots \quad (1.9)$$

Substituting (1.7) and (1.9) into equation of motion (1.4) (*omitting currently uninteresting static term  $\mathbf{E}_s$* ), we get:

$$M(\ddot{\mathbf{R}}_0(t) + \ddot{\mathbf{R}}_1(t)) = Q \cos(\Omega_1 t) [\mathbf{E}_0(\mathbf{R}_0(t)) - (\mathbf{A} \cdot \nabla) \mathbf{E}_0(\mathbf{R}_0(t)) \cos(\Omega_1 t)]. \quad (1.10)$$

Presuming slow spacial variation of vectorfield  $\mathbf{E}_0(\mathbf{r})$  implies:

$|\ddot{\mathbf{A}}| \ll |\dot{\mathbf{A}}|\Omega_1 \ll |\mathbf{A}|\Omega_1^2$ , which we can exploit in time derivative of quickly oscillating term  $\mathbf{R}_1(t)$  (1.8), giving us:

$$\ddot{\mathbf{R}}_1 = -\ddot{\mathbf{A}} \cos(\Omega_1 t) + 2\Omega_1 \dot{\mathbf{A}} \sin(\Omega_1 t) + \mathbf{A}\Omega_1^2 \cos(\Omega_1 t) \approx \mathbf{A}\Omega_1^2 \cos(\Omega_1 t) \quad (1.11)$$

Further substituting for amplitude of oscillation  $\mathbf{A}$  from (1.6) continuing in the spirit of time-averaging:

$$\mathbf{A} = \frac{q\mathbf{E}_0(\mathbf{r})}{M\Omega_1^2} \approx \frac{q\mathbf{E}_0(\mathbf{R}_0(t))}{M\Omega_1^2}, \quad (1.12)$$

which transfers into  $\mathbf{R}_1$  as:

$$\mathbf{R}_1(t) = -\frac{QE_0(\mathbf{R}_0(t))}{M\Omega_1^2} \cos(\Omega_1 t). \quad (1.13)$$

Terms in the equation of motion with dependence on  $\cos(\Omega_1 t)$  cancel each other out and by using a vector identity:

$$(\mathbf{E}_0 \cdot \nabla) \mathbf{E}_0 = \frac{1}{2} \nabla E_0^2 - \mathbf{E}_0 \times (\nabla \times \mathbf{E}_0) = \frac{1}{2} \nabla E_0^2, \quad (1.14)$$

where the second equality follows from Maxwell equation for quasistatic field:  $\nabla \times \mathbf{E}_0 = 0$ . By replacing term  $\cos^2(\Omega_1 t)$  with its mean value  $\overline{\cos^2(\Omega_1 t)} = 1/2$  we finally obtain:

$$M\ddot{\mathbf{R}}_0 = \frac{Q^2}{4M\Omega_1^2} \nabla E_0^2. \quad (1.15)$$

Now by resurrecting the static field term as  $\mathbf{E}_s = -\nabla\Phi_s$ , we can define the effective potential:

$$V^*(\mathbf{R}_0) = \frac{Q^2 E_0^2(\mathbf{R}_0)}{4M\Omega_1^2} + q\Phi_s, \quad (1.16)$$

describing the time-averaged force on a charged particle:

$$M\ddot{\mathbf{R}}_0 = -\nabla V^*(\mathbf{R}_0). \quad (1.17)$$

This equation is much easier to solve and discuss than the original equation of motion (1.4) as it does not involve any explicit time-dependency. After solving it, we can quickly obtain the term  $\mathbf{R}_1(t)$  from (1.13) and get an approximative solution to the original equation of motion. From the Fourier analyses of numerically exact solutions [2] we know about the presence of higher-order terms:

$$\mathbf{r}(t) = \mathbf{R}_0(t) + \mathbf{R}_1(t) + \mathbf{R}_2(t) + \dots,$$

where  $\mathbf{R}_2(t) + \dots$  are referred to as micro oscillations. We must be careful about keeping the space variation of  $\mathbf{E}_0(r)$  sufficiently small. Otherwise, these micro oscillations can become large enough to disturb the trajectory of a particle significantly.

### 1.2.3 Adiabacity

Let us examine the motion of a charged particle in derived effective potential. The first integral of the equation (1.17) is:

$$\frac{1}{2}MR_0^2 + \frac{Q^2 E_0^2}{4M\Omega_1^2} + Q\Phi_s = E_m, \quad (1.18)$$

where  $E_m = \text{const}$  is the total energy of a charged particle inside the trap. Furthermore, if we consider the average kinetic energy of the rapidly oscillatory motion:

$$\left\langle \frac{1}{2}MR_1^2 \right\rangle = \frac{1}{2}M \frac{Q^2 E_0^2}{M^2 \Omega^4} \Omega^2 \langle \sin^2(\Omega t) \rangle = \frac{Q^2 E_0^2}{4M\Omega_1^2}, \quad (1.19)$$

we see that equation (1.18) implies:

$$\frac{1}{2}MR_0^2 + \left\langle \frac{1}{2}MR_1^2 \right\rangle + Q\Phi_s = E_m, \quad (1.20)$$

which means that if the necessary assumptions in the derivation of the effective potential are met, then the total time-averaged energy of the system is an adiabatic constant. This raises the question of whether there is a way to quantify a range of

validity for the effective potential. There are more ways to approach this problem, but we will follow the one demonstrated in [2], kicking off the necessary condition for keeping just the first two terms in Taylor expansion (1.9) of the field  $\mathbf{E}(\mathbf{r})$ . This condition is met if the change of the field is much smaller than the field itself over the scope of one rapid oscillation, meaning:

$$|2(\mathbf{A} \cdot \nabla)\mathbf{E}_0| < |\mathbf{E}_0|. \quad (1.21)$$

Inspired by this condition we define a new parameter  $\eta$ :

$$\eta = \frac{|2(\mathbf{A} \cdot \nabla)\mathbf{E}_0|}{|\mathbf{E}_0|} = \frac{2Q|\nabla\mathbf{E}_0|}{M\Omega_1^2}, \quad (1.22)$$

where the last equality follows after implementing (1.6) and (1.14).

### 1.2.4 Trap geometry

Previously derived equations indirectly feature the potential  $\Phi = \Phi_{rf} + \Phi_s$  as the dynamic and static electric intensities are  $\mathbf{E}_0 \cos(\Omega_1 t) = -\nabla\Phi_{rf}$  and  $\mathbf{E}_s = -\nabla\Phi_s$ . So to give these general equations some concrete shape, we need to find this potential. In our quasistationary treatment of the electric field, it means solving the Laplace equation for a given boundary condition. Writing a general solution to the Laplace equation is possible only for certain symmetries. One of them is cylindrical symmetry, for which we get a solution by a Fourier method of separation of variables in polar coordinates ( $x = r \cos \varphi$ ,  $y = r \sin \varphi$ ) as:

$$\Phi(r, \varphi) = C_0 + D_0 \ln(r) + \sum_{n \in \mathbb{N}} \left( [A_n r^n + B_n r^{-n}] [C_n \sin(n\varphi) + D_n \cos(n\varphi)] \right), \quad (1.23)$$

where  $C_0$ ,  $D_0$ ,  $A_n$ ,  $B_n$ ,  $C_n$  and  $D_n$  are coefficients that need to be determined from boundary conditions.

#### 1.2.4.1 Multipole trap

A multipole is one of an RF trap's classical, well-studied geometries used mainly for two-dimensional confinement.  $N$ -th order multipole consists of  $2n$  linear electrodes arranged in a discretely symmetrical manner. We define a characteristic length of the multipole  $\ell_0$ , indicating the distance from the trap's center to an electrode. It is possible to obtain a potential of a multipole with infinitely long linear electrodes by applying boundary conditions (1.24) to a solution of Laplace

equation with cylindrical symmetry (1.23).

$$\Phi(r, \varphi)|_{r=0} = 0, \quad (1.24a)$$

$$\Phi(r, \varphi)|_{r=\ell_0} = \Phi_0 \cos(n\varphi), \quad (1.24b)$$

where  $\Phi_0 = V_0 + V_1 \cos(\Omega_1 t)$  is a potential applied on electrodes. Most of the coefficients in (1.23) get wiped out, and we end up with the potential of n-th order multipole ( $n > 0$ ) as:

$$\Phi(r, \varphi) = \Phi_0 \hat{r}^n \cos(n\varphi), \quad (1.25)$$

where  $\hat{r} = r/\ell_0$ . We get an electric intensity in polar coordinates as:

$$\mathbf{E}(r, \varphi) = -\nabla_{r\varphi}\Phi(r, \varphi), \quad (1.26)$$

where  $\nabla_{r\varphi} = \left[ \frac{\partial}{\partial r}, \frac{1}{r} \frac{\partial}{\partial \varphi} \right]^\top$ . We get:

$$\mathbf{E}(r, \varphi) = \frac{\Phi_0}{\ell_0} n \hat{r}^{n-1} \begin{bmatrix} -\cos(n\varphi) \\ \sin(n\varphi) \end{bmatrix}, \quad (1.27)$$

which in the Cartesian representation takes the form [2]:

$$\begin{bmatrix} E_x \\ E_y \end{bmatrix} = \frac{\Phi_0}{\ell_0} n \hat{r}^{n-1} \begin{bmatrix} -\cos((n-1)\varphi) \\ \sin((n-1)\varphi) \end{bmatrix}. \quad (1.28)$$

After substituting for  $\Phi_0$  we get equation of motion in variable  $\hat{\mathbf{r}} = [x/\ell_0, y/\ell_0]^\top$ :

$$\frac{d^2 \hat{\mathbf{r}}}{dt^2} + F(t) \hat{r}^{n-1} \begin{bmatrix} -\cos((n-1)\varphi) \\ \sin((n-1)\varphi) \end{bmatrix} = \mathbf{0}, \quad (1.29)$$

where we, for abbreviation, introduced the function:

$$F(t) = n \frac{QV_0}{M\ell_0^2} + n \frac{QV_1}{M\ell_0^2} \cos(\Omega_1 t). \quad (1.30)$$

We see that for  $n = 2$  the equation of motion (1.29) is linear. The same is clearly not true for the case of  $n > 2$ . That is why the motion in a quadrupole trap is easiest to describe, and we chose this geometry to study simultaneous electron-ion trapping in this thesis.

### 1.2.4.1.1 Quadrupole trap

We have already derived a equation of motion for single charged particle in a quadrupole trap  $\rightarrow n = 2$  in (1.29). This equation gets further simplified by replacing linear electrodes with perfect hyperbolical ones. With this change, the electric field loses the spatial dependence on the angle  $\varphi$ . In that case, the motion in the x and y directions stays decoupled, and we obtain an equation of motion in a variable  $\mathbf{r} = (x, y)^\top$  for an idealized quadrupole trap:

$$\ddot{\mathbf{r}} = -\frac{2Q}{M\ell_0^2} [V_0 + V_1 \cos(\Omega_1 t)] \mathbf{r}. \quad (1.31)$$

The same equation describes motion in the z-direction, but with a rescaled right-hand side by the factor of  $-2$ . We will take a closer look at the equation (1.31) in the section 1.2.6. Another essential subject we are interested in is the effective potential for this geometry. For that, we need to evaluate for  $E_0$  in the equation (1.16). The value of  $E_0$  can be easily derived from (1.27) as:

$$E_0 = \frac{2V_1}{\ell_0^2} r, \quad (1.32)$$

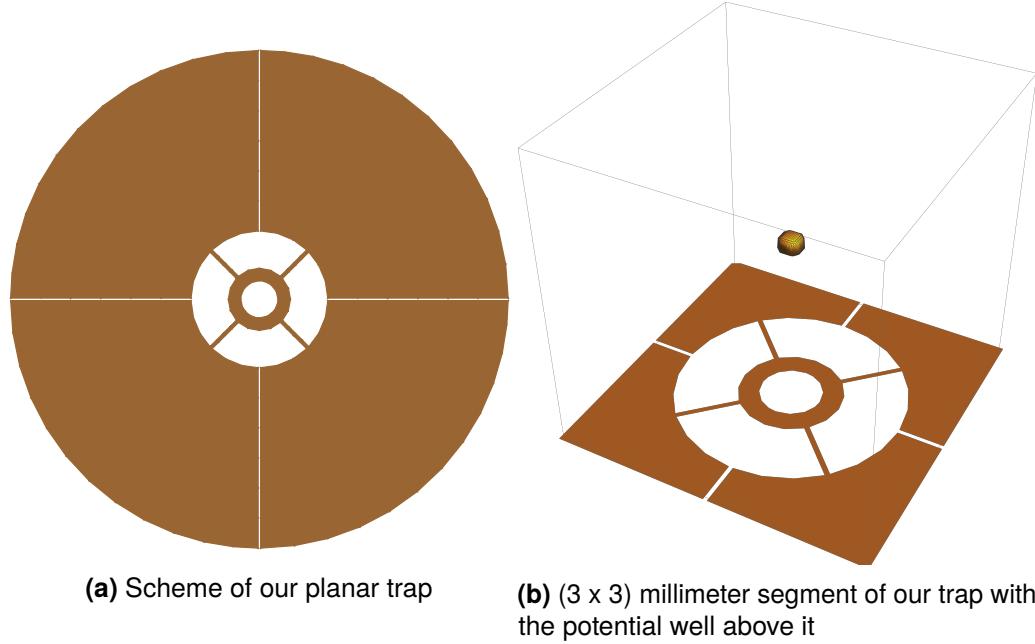
which means that the effective potential is:

$$V^*(\mathbf{r}) = \frac{Q^2 V_1^2}{\ell_0^4 M \Omega_1^2} r^2 + q \Phi_s. \quad (1.33)$$

### 1.2.4.2 Real geometry of our trap

Since we want to implement laser cooling in our experiment, the linear Paul trap is not a viable option, as its apparatus would stand in the way of laser beams. For this reason, we will use surface electrodes where the particles levitate above the trap so that the ions will be accessible to us.

need to add pictures throughout the whole thesis



**Figure 1.1** Planar trap geometry

Nevertheless, we will conduct our research in this thesis by examining the situation with the geometry of the ideal quadrupole trap with hyperbolic electrodes.

### 1.2.5 Spring constant

If we focus on the dynamic component of an effective potential (1.33), we can see that it is formally equivalent a potential of a harmonic oscillator<sup>3</sup>. This encourages us to define a spring constant:

$$\kappa \equiv \frac{2Q^2V_1^2}{\ell_0^4M\Omega_1^2}, \quad (1.34)$$

characterizing the strength of trapping potential. The spring constant is closely related to a frequency of oscillation in a harmonic potential. Such frequency is called secular, denoted:

$$\omega \approx \sqrt{\kappa/M} = \sqrt{2QV_1/\ell_0^2M\Omega_1}. \quad (1.35)$$

The good news is that the spring constant does not depend on the charge sign, making it possible to trap electrons as well as ions. The bad news is that the

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<sup>3</sup>Meaning a potential in the form:  $V(\xi) = \frac{\kappa}{2}\xi^2$

spring constant depends on the charge-to-mass ratio  $Q/M$ , making it practically very difficult to trap electrons and ions simultaneously. For our case of trapping  $\text{Ca}^+$  ions together with electrons, we get  $\kappa_{\text{electron}}/\kappa_{\text{ion}} = M_{\text{ion}}/M_{\text{electron}} \approx 73000$  while we would like to achieve  $\kappa_{\text{electron}}/\kappa_{\text{ion}} \approx 1$  so that electron trajectories fill up a similar region as ion's. It seems that we have hit upon a huge snag with our approach. Fortunately, this does not mean we have to abandon the idea of RF trapping itself. Instead, we can improve on it by adding a second frequency, giving us the freedom to treat the stability of both species individually and making it possible to manage the desired ratio of spring constants. Two frequency Paul trap will be further discussed in section 2.1.

### 1.2.6 Mathieu equation

Let us reexamine our original equation of motion (1.4) for the case of a quadrupole trap with ideal hyperbolical electrodes. After time transformation  $\tau = \Omega_1 t/2$ , the equation (1.31) molds into:

$$\ddot{\mathbf{r}}(\tau) = [a - 2q_1 \cos(2\tau)] \mathbf{r}, \quad (1.36)$$

where:

$$a = \frac{8QV_0}{M\ell_0^2\Omega_1^2}, \quad (1.37a)$$

$$q_1 = -\frac{4QV_1}{M\ell_0^2\Omega_1^2}. \quad (1.37b)$$

The equation (1.36) bears a name after E.L. Mathieu, who was the first to extensively study it in the context of vibrating membranes. It has an analytical solution [3] in terms of special functions called Mathieu functions, denoted  $c_{n\ell}$  and  $s_{n\ell}$ , sometimes referred to as cosine-elliptic and sine-elliptic. The secular is given by [2] the Dehmelt approximation:

$$\omega \approx \frac{\Omega_1}{2} \sqrt{a + \frac{q_1^2}{2}}. \quad (1.38)$$

If we apply no static field  $a = 0$  the secular frequency is:

$$\omega \approx \frac{\Omega_1}{2} \sqrt{\frac{q_1^2}{2}} = \frac{\sqrt{2}QV_1}{\ell_0^2 M \Omega_1}, \quad (1.39)$$

which is in accordance with the result we attained with the spring constant of the harmonic pseudopotential.

### 1.2.7 Stability

For a linear system such as (1.36), we can examine the stability of its solutions with the Floquet theory, which we do in section ???. Nevertheless, we eventually want to study the trapping of multiple charged particles, and their mutual interaction razes the linearity of our equations. There is no single outright mathematical way to define the stability of a non-linear, non-autonomous system. Mathematical approaches might demand the boundedness of the solution in the phase space. Then we would talk about Lagrange stability [4]. Another approach would be to seek stable points and study what happens to the solutions starting in their proximity. This approach is referred to as Lyapunov stability [5]. We will use a simple but practical criterion for identifying stable solutions. A stable particle cannot vacate the internal dimension of the trap, meaning:

$$\max_{x \in \mathcal{L}}(r) \leq r_m < \ell_0, \quad (1.40)$$

where  $\mathcal{L}$  is the whole trajectory of the particle and  $r_m$  is maximal allowed distance from the center of a trap. The drawback of this definition is that we must keep the simulation going long enough to account for the slowly diverging particles, and we are yet to determine the value of  $r_m$ . However, we can also characterize the mode for stable confinement in a more general manner [2]. First, we limit ourselves to work within the condition for adiabaticity to ensure that the dynamic field does not continually augment the particle's energy. Then we can exploit the equation (1.20) in the following way. A stable particle must have no secular momentum  $\dot{\mathbf{R}}_0 = 0$  at the point  $r_m$  to avoid collision with the electrode. The effective potential near the electrode must be greater than the adiabatic constant  $E_m$ . Otherwise, the potential will not be powerful enough to prevent rapid oscillatory motion from ejecting the particle out of the trap. Giving us the applicable inequality for stable confinement:

$$\frac{Q^2 E_0^2(r_m)}{4M\Omega^2} + Q\Phi_s > E_m. \quad (1.41)$$

We still need to find the right value for  $r_m$ . It has been established [2] that  $r_m = 0.8 \ell_0$  accomplishes adiabaticity for most cases, which we will also use as a stability condition in our simulations:

$$\max_{x \in \mathcal{L}}(r) \leq 0.8 \ell_0. \quad (1.42)$$

## 1.3 Laser cooling

The Ca+ ion has an energy gap between the ground ( $s_{1/2}$ ) and one of its excited ( $p_{1/2}$ ) states with the value corresponding to the wavelength of 397 nm [6]. By

tuning the wavelength of our laser slightly below this transition energy, we can exploit the Doppler effect so that only ions moving towards the laser can experience radiation with the right frequency to excite them. After a brief time, the atom will deexcite, emitting a photon in a random direction. The only way the ion would still have the same momentum as before the absorption is if the photon was emitted exactly in the same direction as it was absorbed (as if the photon did not interact with the atom at all). But since the photon emission is isotropic, the ion will effectively slow down. This type of laser cooling is also known as *Doppler cooling*. Detailed explanation can be found in [7].



# Chapter 2

## Confinement of two species with radically different charge to mass ratio

In this chapter we will build on theory from the first chapter and introduce some new theory as well

### 2.1 Two frequency quadrupole Paul trap

As was mentioned in the section 1.2.5, we can use two frequencies, each targeting to optimize the trapping of one species. Higher frequency  $\Omega_2$  for trapping electrons, with the potential  $V_2$  applied to the electrode. A lower frequency  $\Omega_1$  with potential  $V_1$  for trapping ions. We proceed in setting up a two-frequency trap as described in [8, 9]. First, we must acknowledge that while higher frequency will have no significant impact on heavier ions, a light electron will experience the slower field to the full extent. Therefore we have to ensure that the trapping of electrons due to the higher frequency field is strong enough to withstand misguiding by the field with a lower frequency. This potential instability is referred to as *parametric excitation*. We can secure that to some extent by feeding potentials on electrodes in such a way that  $V_1 \ll V_2$ . We can provide potentials up to  $V_2 \sim 100$  V, and  $V_1 \sim 5$  V, in the conditions of our experiment. Assuming that this allows us to look at each frequency setup independently, using (1.34), we get a ratio of spring constants:

$$K = \frac{\kappa_{\text{electron}}(\Omega_2)}{\kappa_{\text{ion}}(\Omega_1)} \approx \frac{M_{\text{ion}}}{M_{\text{electron}}} \left( \frac{V_2}{V_1} \frac{\Omega_1}{\Omega_2} \right)^2. \quad (2.1)$$

The correct way to create a stable configuration of a two-frequency trap is to begin by finding the optimal parameters for the confinement of lighter species. Optimal trapping in a single frequency trap corresponds to [2]  $q_2 \approx 0.4$ . Using (2.5c), with the choice of  $V_2 = 100$  V, we obtain optimal frequency for electron trapping as  $\Omega_2 = 1.88 \times 10^{10}$  rad s $^{-1}$ . Now, we must choose the  $\Omega_1$  and  $V_1$  for ion trapping in a way that suppresses parametric heating of electrons. It is crucial to keep the electron's secular frequency higher than the driving frequency for ion confinement. Otherwise, the  $\Omega_2$  frequency field would be too slow to save an electron from parametric excitation. So another condition that must be satisfied in two frequency trapping is:

$$\Omega_1 \ll \omega_2 = \frac{\sqrt{2}QV_2}{M_{\text{electron}}\ell_0^2\Omega_2}, \quad (2.2)$$

where the second equality follows from (1.35).

**Same criterion for optimal trapping  $q_1 \approx 0.4$  gives us frequency  $\Omega_1 = 1.55 \times 10^7$  rad s $^{-1}$ .** For such setting we obtain the ratio of spring constants for both species  $K = 20$ , which is already a great improvement compared to a single frequency trap.

... build a little bridge from the section explaining a single frequency trap. We need two frequencies for particles with widely different charge to mass ratios:  $Q_m \equiv Q/m$  [8]. In the case of a linear quadrupole with perfectly hyperbolical electrodes with cylindrical symmetry we have a electric potential in the form [10] :

$$V(t, \mathbf{r}) = \left[ V_0 + V_1 \cos(\Omega_1 t) + V_2 \cos(\Omega_2 t) \right] \frac{x^2 + y^2 - 2z^2}{2\ell_0^2}, \quad (2.3)$$

where  $V_0$  is an amplitude of static potential,  $V_1$  of slower potential and  $V_2$  is an amplitude of rapidly oscillating potential on the electrode. The equations of motion for a particle in such potential, after change of variable:  $\tau = t\Omega_2/2$  are:

$$\ddot{x}(\tau) = x(\tau) \left[ a - 2q_1 \cos(2\tau\Omega_1/\Omega_2) - 2q_2 \cos(2\tau) \right], \quad (2.4a)$$

$$\ddot{y}(\tau) = y(\tau) \left[ a - 2q_1 \cos(2\tau\Omega_1/\Omega_2) - 2q_2 \cos(2\tau) \right], \quad (2.4b)$$

$$\ddot{z}(\tau) = -2z(\tau) \left[ a - 2q_1 \cos(2\tau\Omega_1/\Omega_2) - 2q_2 \cos(2\tau) \right], \quad (2.4c)$$

where  $a$ ,  $q_1$  and  $q_2$  are dimensionless parameters:

$$a = 4 \frac{QV_0}{M\Omega_2^2 \ell_0^2}, \quad (2.5a)$$

$$q_1 = -2 \frac{QV_1}{M\Omega_2^2 \ell_0^2}, \quad (2.5b)$$

$$q_2 = -2 \frac{QV_2}{M\Omega_2^2 \ell_0^2}. \quad (2.5c)$$

## 2.2 Floquet theory

Since the particle experiences the weakest confinement in the  $z$ -direction, we will examine this equation's properties. Floquet theory is a theory covering linear first-order ODEs with periodic coefficients. These are equations of the form:

$$\dot{\mathbf{u}}(\tau) = \mathbb{F}(\tau)\mathbf{u}(\tau), \quad (2.6)$$

where  $\mathbb{F}$  is a matrix valued function with minimal period  $T$ . Let's illustrate this theory for the case of our differential equation. We begin by rewriting the equation (2.4c) as a system of two first-order differential equations written in the matrix form:

$$\frac{d}{d\tau} \begin{bmatrix} z(\tau) \\ \dot{z}(\tau) \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -2 \left( a - 2q_1 \cos(2\tau\Omega_1/\Omega_2) - 2q_2 \cos(2\tau) \right) & 0 \end{bmatrix} \begin{bmatrix} z(\tau) \\ \dot{z}(\tau) \end{bmatrix}, \quad (2.7)$$

which already has a structure of (2.6). Without the necessity of finding a solution to this system, we can acquire knowledge about its stability. The information we are interested in is whether a solution is bounded for a given set of parameters or not. In this section, we will limit ourselves to the driving frequencies, which can be represented as:  $\Omega_2/\Omega_1 \equiv m/n$ , where  $m$  and  $n$  are integers and  $m/n$  is an irreducible fraction. Then the matrix in equation (2.7) is  $T = m\pi$  periodic. As in [10], we identify the edge of stability regions as a set of parameters for which a solution of (2.4c) is a  $2T$  periodic function<sup>1</sup> to our problem (2.7). This allows us to seek a solution to our problem in the form:

$$z(\tau) = \sum_{k=-\infty}^{\infty} c_k \exp\left(i \frac{k}{m}\tau\right), \quad (2.8)$$

---

<sup>1</sup>Note that such stability condition differs from the one we demand while simulating the motion of a particle. The periodic solution of equation of motion implies boundedness, but the value of this boundary might lie outside the physical dimensions of the trap. That is why we ought not to be surprised when we find some differences in stability diagrams, even for the simplest case of a single particle in the trap.

where  $c_k$  are constant coefficients. Substituting this into equation (2.7) yields an identity:

$$\sum_{k=-\infty}^{\infty} \left[ \left( a - \frac{k^2}{m^2} \right) c_k - q_1 (c_{k-2n} + c_{k+2n}) - q_2 (c_{k-2m} + c_{k+2m}) \right] \exp\left(i \frac{k}{m} \tau\right) = 0, \quad (2.9)$$

which holds for every  $\tau$  only if each element of the sum is equal to zero. This relation can be written as:

$$\mathbb{F} \cdot \begin{bmatrix} \vdots \\ c_{k-1} \\ c_k \\ c_{k+1} \\ \vdots \end{bmatrix} = \mathbf{0}, \quad (2.10)$$

where  $\mathbb{F}$  is an infinite matrix with elements:

$$\mathbb{F}_{ij} = \left[ \left( a - \frac{k^2}{m^2} \right) \delta_{ij} - q_1 (\delta_{ij-2n} + \delta_{ij+2n}) - q_2 (\delta_{ij-2m} + \delta_{ij+2m}) \right], \quad (2.11)$$

where:

$$\delta_{ij} = \begin{cases} 1 & i = j, \\ 0 & i \neq j. \end{cases} \quad (2.12)$$

The equation (2.10) is equivalent to:

$$\det(\mathbb{F}) = 0. \quad (2.13)$$

So the determination of stability boils down to computing a determinant of a matrix  $\mathbb{F}$ . We approximate  $\mathbb{F}$  by sufficiently large  $\rightarrow (10m + 1) \times (10m + 1)$  finite matrix. For the index  $k$  in previous equations it means:

$$k \in \{-5m, -5m + 1, \dots, 5m - 1, 5m\} \subset \mathbb{Z},$$

neglecting solutions with smaller periods. Parameters for which  $\det(\mathbb{F}) > 0$  were identified as stable and for  $\det(\mathbb{F}) < 0$  as unstable.

## 2.3 Simulation

Let us begin this section by summarizing our approximations, some of which we have already applied while deriving the equation of motion. We follow mainly the overview from [11]. Starting with insignificant neglections and moving towards more problematic ones.

**Gravitational interaction:** neglecting gravitational interaction goes without saying since, for Ca<sup>+</sup> ions, it is weaker than electrostatic force by order of  $\sim 10^{32}$ .

**Relativistic effects:** we did not involve any relativistic corrections since we usually deal with small velocities while trapping particles. Ca<sup>+</sup> ions are Doppler cooled down to energies of  $\sim 10^{-4}$  eV. The fastest simulated electrons had a kinetic energy of  $\sim 1$  eV, for which the relativistic gamma factor is still  $\gamma \approx 1$  up to the fifth decimal place.

**Ion radiation:** a well-known consequence of Maxwell equations is that accelerating charged particle emits electromagnetic radiation. We did not account for this energetic loss due to the relatively small force applied to particles in a trap. The power [P] = [Watt] of such radiation can be for our non-relativistic case calculated using [12] the Larmor formula:

$$P = \frac{Q^2 a_c^2}{6\pi\epsilon_0 c^3},$$

where  $c$  is a speed of light,  $a_c$  denotes the acceleration of a particle at the given time, and  $\epsilon_0$  is the vacuum permittivity. We can easily estimate the upper bound of acceleration by considering the maximal reasonable value of each term in the equation (2.4)<sup>2</sup>:  $r = \ell_0$ ,  $\cos = 1$ ,  $a = 0$ ,  $q_1 = 0.1$  and  $q_2 = 0.5$ . We get:

$$a_c^{\max} \approx 1.8 \times 10^{-3} \text{ m s}^{-2},$$

which means that the maximal power of radiation was:

$$P^{\max} = 2 \times 10^{-59} \text{ W}.$$

Considering such a constant energy loss, it would take an electron  $\sim 3 \times 10^{33}$  years to radiate the energy of 1 eV.

---

<sup>2</sup>Note that for this set of parameters are all solutions already fully unstable

**Magnetic field:** Let us begin by writing full form Maxwell's equations in the vacuum:

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}, \quad (2.14a)$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}, \quad (2.14b)$$

$$\nabla \cdot \mathbf{B} = 0, \quad (2.14c)$$

$$\nabla \times \mathbf{B} = \frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t}. \quad (2.14d)$$

We are using quasistatic form instead:

$$\nabla \cdot \mathbf{E} = 0, \quad (2.15a)$$

$$\nabla \times \mathbf{E} = \mathbf{0}, \quad (2.15b)$$

$$\nabla \cdot \mathbf{B} = 0, \quad (2.15c)$$

$$\nabla \times \mathbf{B} = \mathbf{0}. \quad (2.15d)$$

finish this

**Induced charge on the electrodes:** charged particles induce surface charge density on the electrodes. This causes attraction of a particle toward the electrode, which can contribute to vacation of the particle from the trap. For reference we can look at simplified situation of a charged particle near an infinite conductive plane. An average acceleration of an electron throughout the stable simulated trajectory was in the order of  $\bar{a}_c \sim 10^{17}$ . For an infinite conductor to cause an acceleration  $\sim \bar{a}_c/100$ , the electron would have to approach the electrode up to the distance of  $\approx 0.25 \mu\text{m}$ , which would already be outside our definition of stable trajectory. Hence we can omit such an effect.

**Creation of Rydberg atoms:** An electron can get caught in some highly excited ion orbital creating a Rydberg atom. The electron can subsequently drop to a lower but still very unstable orbital and vacate from it, losing energy by the associated photon emission. It might be necessary to add such a process to our simulation in the future.

**Phase shift:** induced by the finite speed of electric signal delivered to the electrode. This could be problematic since the characteristic dimension of our trap is  $\ell_0 = 0.5 \text{ mm}$ , and we are using frequencies up to the orders of  $\Omega_2 \sim 10^{10} \text{ rad s}^{-1}$ . Suppose we optimistically assume that the signal travels through the electrode with the speed of light. In that case, the signal

in one period  $1/\Omega_2$  spans over the distance of  $\sim 0.03$  mm, which is getting close to our characteristic length. We tackle this problem by dividing our electrodes into eight sections, see 1.1a, each with its own feeding from the power source.

**Collisions with neutrals:** we will be able to make a vacuum with pressure of (no idea and not sure it it can produce significant problems)

### 2.3.1 Choice of time-step

We have tried several integration methods when numerically solving our equations of motion, whether with exact or effective potential. Choice of time-step is always a delicate issue. For the case of solving the Mathieu-type equation, we followed the Nyquist criterion [13]. Nyquist criterion is used mainly in signal processing for compact signals with convergent Fourier series. It states that for the signal with the highest frequency  $f$ , the largest possible sample size so that the discretization of the signal will carry equivalent information as the continuous one is  $1/(2f)$ . We started numerically solving the equation of motion with this time step, gradually increasing its size until the numerical solution with the denser sampling would give us the same result for the given tolerance. Repeating this process for several methods<sup>3</sup> for numerical solving of ODEs [14]. For the case of a single electron in the trap with the expected initial conditions *thisOne.dat* had the best performance a predictor-corrector method, which we have defined as *StepEulerAdvanced*. The sufficient time-step for this method was  $\Delta t = 1/(5f)$ .

verb doesn't work for some reason that's why are names of the files are currently in italics

### 2.3.2 Treatment of laser cooling

In our simulation, we treated the effect of laser cooling of ions by introducing a new frictional force, meaning it is proportional to  $\propto -\dot{\mathbf{r}}$ . The strength of this force is characterized by the parameter  $\beta \in (0, 1)$ . Let us begin this section by summarizing our approximations (inspired by [11]) when deriving the equation of motion.

### 2.3.3 Simulating Coulomb crystal

We simulated Coulomb crystal by molecular dynamics, meaning we solved the equation of motion for each ion in effective potential with Coulomb interaction. We simulated the creation of a Coulomb crystal by molecular dynamics while keeping an eye on the total potential energy. We solved an equation of motion for each ion in effective potential with Coulomb interaction and laser cooling

---

<sup>3</sup>All tried methods can be found in the file *intMethods.py*

represented by the damping factor. We have used damping parameter  $\beta$  large enough to decelerate the particles within a computationally reasonable time. To ensure that the ions had enough time to find a potential minimum, they were given a synthetic boost in kinetic energy every time they were slowed down to the minimal temperature, which can be obtained by laser cooling (about 0.01 Kelvin).

might be good idea to implement some simplex based algorithm with the molecular dynamics

### 2.3.4 The code

The practical part of this thesis consists of developing the code simulating the motion of ions and electrons in a two frequency Paul trap. We have chosen the programming language python for its current popularity allied with an abundance of highly optimized libraries and a good combination of computational and development costs. The source code can be found at github<sup>4</sup>. Main features of the program are:

- Creating a Coulomb crystal.
- Making stability diagram in dependence on  $q_1$  and  $q_2$  parameters.
- Parallelizing the computation of stability diagram.
- Optimizing the algorithm to compute stability only on the edge of stability regions.
- Tracking the information about the system: positions, velocities, energies
- Producing graphical outcomes.

I think it would be beneficial to explain, for example what I mean by "optimizing," but I do not think it belongs here. I will probably put it into the appendix.

---

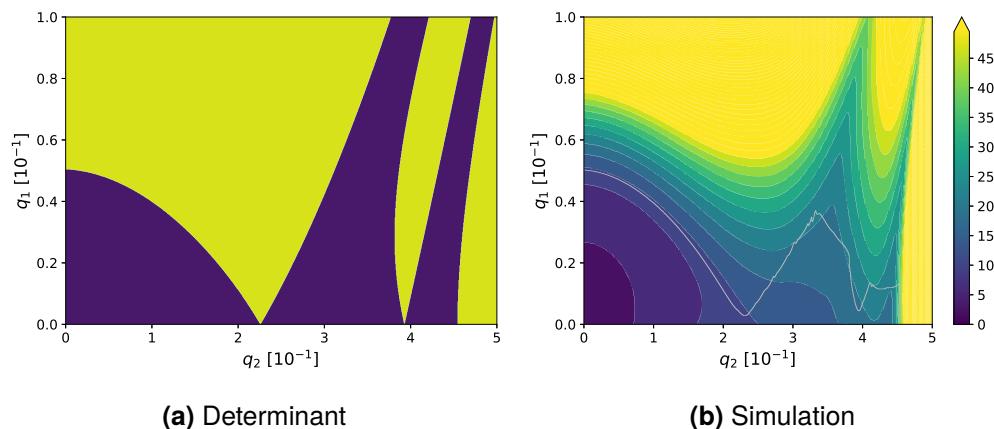
<sup>4</sup>[https://github.com/rendeka/Bachelor\\_thesis.git](https://github.com/rendeka/Bachelor_thesis.git)

# Chapter 3

## Results and discussion

### 3.1 Characteristics of $q_1$ - $q_2$ stability diagrams for one electron

We will start by looking at the stability diagrams for different  $\Omega_2/\Omega_1$  ratios. Starting with 3.1.

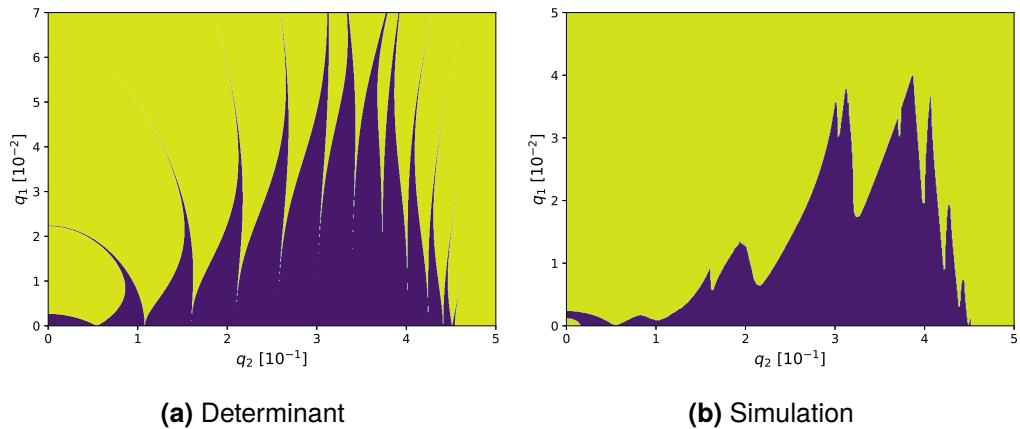


**Figure 3.1** Stability diagrams for  $\Omega_2/\Omega_1 = 3$

In the sub-figure 3.1a we can see stable(*dark*) and unstable(*light*) regions of the studied differential equation. The image 3.1b combines two pictures. The white curve indicates the edge of stability regions → the region under the curve is stable. In the background is a contour plot of the average electron velocity throughout the trajectory relative to the initial velocity. The color bar to the right indicates the value of this ratio. The figures such as 3.1b can help us find the stable trap parameters while keeping electron temperature as low as possible,

which is our ultimate goal. In contrast with the determinant solution, we can see that the two stable areas for a simulated particle are cut off in the field with higher amplitudes. In the following figure, we increase the total simulation time and the diameter for identifying stable particles. And it doesn't work...

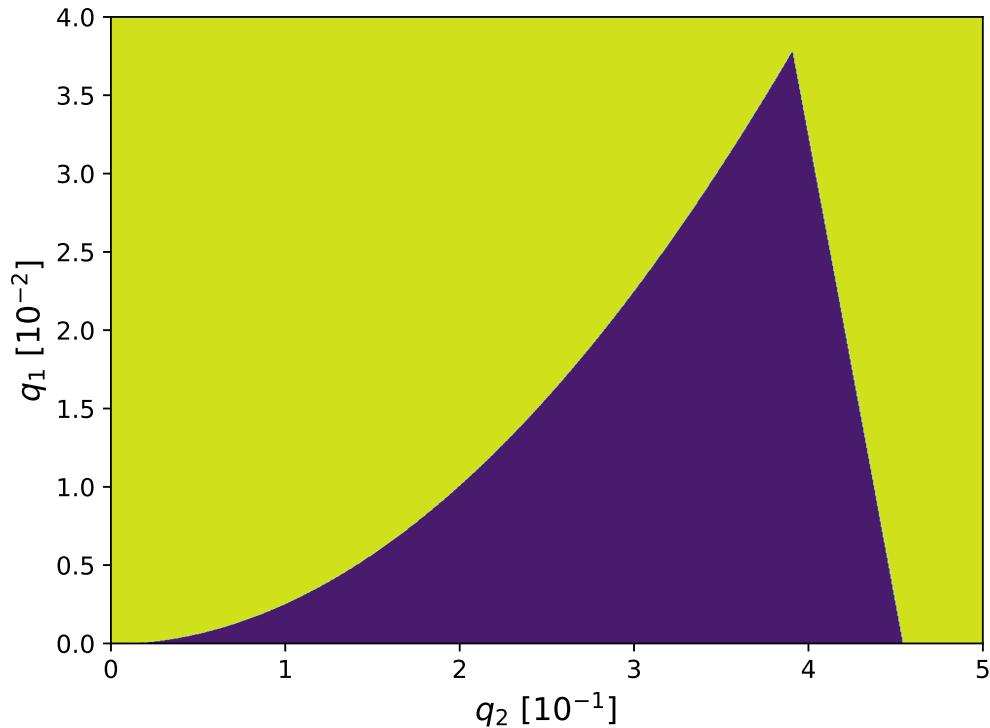
Moving to larger frequency ratio  $\rightarrow \Omega_2/\Omega_1 = 13$  we can start to notice some patterns.



**Figure 3.2** Stability diagrams for  $\Omega_2/\Omega_1 = 13$

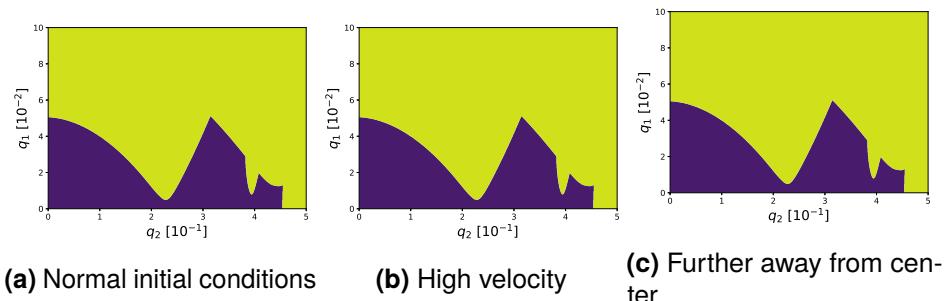
There emerges one stable triangle with many tongues of instability. With an increasing ratio  $\Omega_2/\Omega_1$  we can see a gain in the number of these tongues, but their width promptly shrinks as well. We expect that by further increasing the frequency ratio, the unstable tongues will be realistically affecting only the regions near the edge of stability, leaving the regions further inside a stable triangle safe to work with.

Continuing to the frequency ratio compatible for trapping electrons and Ca+ ions



**Figure 3.3** Simulated stability diagram for  $\Omega_2/\Omega_1 = 833$

### 3.1.1 Dependence on initial conditions



**Figure 3.4**  $\Omega_2/\Omega_1 = 3$ , different initial conditions

High initial velocity 3.4b makes the region with the weakest field (around  $q_1 \approx q_2 \approx 0$ ) unstable, which is understandable since the stability condition [reference](#) is not satisfied. A wider distance from the trap's center combined with the initial

velocity pointing away from the trap 3.4c distorts the stability diagram's shape significantly.

as a sanity check we try to reproduce a result from [10].

## 3.2 Creating a Coulomb crystal

currently making some useable pictures

## 3.3 Stability of electron in Coulomb crystal

### 3.3.1 One electron - one ion

### 3.3.2 One electron - twenty ions

### 3.3.3 One electron - a hundred ions

## 3.4 Design of the experiment

## 3.5 Future

Our concerns in the future will be reproducing results of this thesis for the real planar geometry of the trap used in our experiment. The potential of such a trap can be formulated in integral form utilizing Bessel functions, which will make our simulations much more computationally expensive. We need to derive equation of motion and identify parameters analogous to  $a$ ,  $q_1$  and  $q_2$  which we had for ideal quadrupole trap. After that we can use our exiting program to study stability of particles in dependence on such parameters exactly as we did in this thesis.

# Conclusion

We were perhaps able to optimize parameters of two frequency Paul trap for storing ions and electrons together... Next step will be applying obtained observations and updating the software to reproduce results of this thesis for the real geometry



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# Appendix A

## Using software

This appendix intends to explain to the reader how to use the python script. The program starts by running the `main.py` file. In this file there are definition of function which uses more complex functionalities from the other modules. When running the `main.py` one should uncomment all the lines he/she want to be executed (see 1).

This is an example code.

```
def StepVerlet(ODESystem, rv, t, dt, aCoulomb, mass, charge, trapParams):  
  
    r, v = rv  
    v, a = ODESystem(rv, t, aCoulomb, mass, charge, trapParams)  
  
    r1 = r + v * dt + 0.5 * a * dt**2  
  
    a1 = ODESystem(np.array([r1, v]), t, aCoulomb, mass, charge, trapParams)[1]  
  
    v1 = v + 0.5 * (a + a1) * dt  
    t1 = t + dt  
  
    rv1 = np.array([r1, v1])  
  
    return rv1, t1
```

---

**Listing 1** Main program.

---

```
if __name__ == '__main__':
    prayForItToWork()
```

---

---

**Listing 2** The system of ODEs used for simulating Coulomb crystal.

---

```
def ODESystemEffectiveDamping(rv, aCoulomb, mass, charge, trapParams):
    if (mass == electronMass):
        a, q1, q2 = trapParams
        q1 = 0
    else:
        a, q1, q2 = trapParams * (electronMass / mass)

    # unpacking position and velocity components
    r, v = rv
    x, y, z = r
    vx, vy, vz = v

    # defining the system of first order ODEs
    x1 = vx
    vx1 = aCoulomb[0] - x / 4 * (a + 2 * q1**2 / 2 * (f2 / f1)**2
        + q2**2 / 2) - 2 * beta * vx

    y1 = vy
    vy1 = aCoulomb[1] - y / 4 * (a + 2 * q1**2 / 2 * (f2 / f1)**2
        + q2**2 / 2) - 2 * beta * vy

    z1 = vz
    vz1 = aCoulomb[2] - z / 2 * (a + 2 * q1**2 / 2 * (f2 / f1)**2
        + q2**2 / 2) - 2 * beta * vz

    # defining derivatives of position and velocity
    r1 = np.array([x1, y1, z1])
    v1 = np.array([vx1, vy1, vz1])

    return np.array([r1, v1])
```

---