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**BACHELOR THESIS**

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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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# 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 rapidly changing 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, for their efforts in this field, awarded a shared Nobel prize for physics in 1989. 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 will be to make a computer simulation of an ion crystal with electrons inside a Paul trap trying to optimize the parameters of the trap to attain the lowest possible temperature of electrons, hopefully reaching the point of crystallization for such a system.

---

<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 What is plasma?

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

### 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  $Q$  with it's position denoted by vector  $\mathbf{r}$ . We insert such a particle into the external time-dependent electromagnetic field described by  $\mathbf{E}(t, \mathbf{r})$  and  $\mathbf{B}(t, \mathbf{r})$ . The Lorentz force gives the equation of motion:

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

<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 can neglect 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:

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

### 1.2.2 Effective potential

Solving such a differential equation with a rapidly changing right-hand side can be troublesome, albeit not impossible. It will be examined in the section 2.2. When trapping ions, we are not always interested in exact trajectories. 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:

$$\mathbf{r}(t) = \mathbf{r}_0 - \mathbf{A} \cos(\Omega_1 t), \quad (1.4)$$

where the vector:

$$\mathbf{A} \equiv \mathbf{A}(\mathbf{r}) = \frac{Q\mathbf{E}_0(\mathbf{r})}{m\Omega_1^2}, \quad (1.5)$$

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 <sup>2</sup>. 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:

$$\mathbf{r}(t) = \mathbf{R}_0(t) + \mathbf{R}_1(t), \quad (1.6)$$

---

<sup>2</sup>Frequencies used for trapping ions (or even electrons) are in the range of radio frequencies (RF). Therefore, we can treat the electric field in the quasistatic approximation.

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

$$\mathbf{R}_1(t) = -\mathbf{A} \cos(\Omega_1 t). \quad (1.7)$$

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  $\mathbf{R}_0$ :

$$\mathbf{E}_0(\mathbf{R}_0(t) - \mathbf{A} \cos(\Omega_1 t)) \approx \mathbf{E}_0(\mathbf{R}_0(t)) - (\mathbf{A} \cdot \nabla) \mathbf{E}_0(\mathbf{R}_0(t)) \cos(\Omega_1 t) + \dots \quad (1.8)$$

Substituting (1.6) and (1.8) into equation of motion (1.2) (*omitting currently uninteresting static term  $\mathbf{E}_s$* ), we get:

$$m(\ddot{\mathbf{R}}_0(t) + \ddot{\mathbf{R}}_1(t)) = Q \cos(\Omega_1 t) [\mathbf{E}_0(\mathbf{R}_0(t)) - (\mathbf{A} \cdot \nabla) \mathbf{E}_0(\mathbf{R}_0(t)) \cos(\Omega_1 t)]. \quad (1.9)$$

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  $\mathbf{R}_1(t)$  (1.7), giving us:

$$\ddot{\mathbf{R}}_1 = -\ddot{\mathbf{A}} \cos(\Omega_1 t) + 2\Omega_1 \dot{\mathbf{A}} \sin(\Omega_1 t) + \mathbf{A}\Omega_1^2 \cos(\Omega_1 t) \approx \mathbf{A}\Omega_1^2 \cos(\Omega_1 t) \quad (1.10)$$

Further substituting for amplitude of oscillation  $\mathbf{A}$  from (1.5) continuing in the spirit of time-averaging:

$$\mathbf{A} = \frac{q\mathbf{E}_0(\mathbf{r})}{m\Omega_1^2} \approx \frac{q\mathbf{E}_0(\mathbf{R}_0(t))}{m\Omega_1^2}, \quad (1.11)$$

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

$$\mathbf{R}_1(t) = -\frac{QE_0(\mathbf{R}_0(t))}{m\Omega_1^2} \cos(\Omega_1 t). \quad (1.12)$$

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

$$(\mathbf{E}_0 \cdot \nabla) \mathbf{E}_0 = \frac{1}{2} \nabla E_0^2 - \mathbf{E}_0 \times (\nabla \times \mathbf{E}_0) = \frac{1}{2} \nabla E_0^2, \quad (1.13)$$

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:

$$m\ddot{\mathbf{R}}_0 = \frac{Q^2}{4m\Omega_1^2} \nabla E_0^2. \quad (1.14)$$

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

$$V^*(\mathbf{R}_0) = \frac{Q^2 E_0^2(\mathbf{R}_0)}{4m\Omega_1^2} + q\Phi_s, \quad (1.15)$$

describing the time-averaged force on a charged particle:

$$m\ddot{\mathbf{R}}_0 = -\nabla V^*(\mathbf{R}_0). \quad (1.16)$$

This equation is much easier to solve and discuss than the original equation of motion (1.2) as it does not involve any explicit time-dependency. After solving it, we can quickly obtain the term  $\mathbf{R}_1(t)$  from (1.12) 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  $\mathbf{E}_0(\mathbf{r})$  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 (1.16) is:

$$\frac{1}{2}mR_0^2 + \frac{Q^2 E_0^2}{4m\Omega_1^2} + Q\Phi_s = E_m. \quad (1.17)$$

Furthermore, if we consider the average kinetic energy of the rapidly oscillatory motion:

$$\left\langle \frac{1}{2}mR_1^2 \right\rangle = \frac{Q^2 E_0^2}{4m\Omega_1^2}, \quad (1.18)$$

we see that equation (1.17) implies:

$$\frac{1}{2}mR_0^2 + \left\langle \frac{1}{2}mR_1^2 \right\rangle + Q\Phi_s = E_m, \quad (1.19)$$

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.

### 1.2.4 Trap geometry

Previously derived equations indirectly feature the potential  $\Phi = \Phi_{\text{rf}} + \Phi_s$  as the dynamic and static electric intensities are  $\mathbf{E}_0 \cos(\Omega_1 t) = -\nabla \Phi_{\text{rf}}$  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 as:

$$\Phi(r, \varphi) = C_0 + D_0 \ln(r) + \sum_{n \in \mathbb{N}} \left( [A_n r^n + B_n r^{-n}] [C_n \sin(n\varphi) + D_n \cos(n\varphi)] \right), \quad (1.20)$$

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 can obtain a potential of an ideal multipole with infinitely long electrodes by applying boundary conditions (1.21) to a solution of Laplace equation with cylindrical symmetry (1.20).

$$\Phi(r, \varphi)|_{r=0} = 0, \quad (1.21a)$$

$$\Phi(r, \varphi)|_{r=\ell_0} = \Phi_0 \cos(n\varphi), \quad (1.21b)$$

where  $\Phi_0 = V_0 + V_1 \cos(\Omega_1 t)$  is a potential applied on electrodes. Most of the coefficients in (1.20) get wiped out, and we end up with the potential of  $n$ -th order multipole ( $n > 0$ ) as:

$$\Phi(r, \varphi) = \Phi_0 \hat{r}^n \cos(n\varphi), \quad (1.22)$$

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

$$\mathbf{E}(r, \varphi) = -\nabla_{r\varphi} \Phi(r, \varphi), \quad (1.23)$$

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

$$\mathbf{E}(r, \varphi) = \frac{\Phi_0}{\ell_0} n \hat{r}^{n-1} \begin{bmatrix} -\cos(n\varphi) \\ \sin(n\varphi) \end{bmatrix}, \quad (1.24)$$

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

$$\begin{bmatrix} E_x \\ E_y \end{bmatrix} = \frac{\Phi_0}{\ell_0} n \hat{r}^{n-1} \begin{bmatrix} -\cos((n-1)\varphi) \\ \sin((n-1)\varphi) \end{bmatrix}. \quad (1.25)$$

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

$$\frac{d^2 \hat{r}}{dt^2} + F(t) \hat{r}^{n-1} \begin{bmatrix} -\cos((n-1)\varphi) \\ \sin((n-1)\varphi) \end{bmatrix} = \mathbf{0}, \quad (1.26)$$

where we introduce the function:

$$F(t) = n \frac{QV_0}{m\ell_0^2} + n \frac{QV_1}{m\ell_0^2} \cos(\Omega_1 t). \quad (1.27)$$

We see that for  $n = 2$  the equation of motion (1.26) is linear, and motion in the  $x$  and  $y$  directions stays decoupled. 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  $\rightarrow$  substitute  $n = 2$  in (1.26). This equation can be simplified further by replacing linear electrodes with perfect hyperbolical ones. With this change, the potential loses the spatial dependence on the angle, and we obtain an equation of motion in the  $x$ - $y$  direction for an idealized quadrupole trap:

$$\ddot{\mathbf{r}} = -\frac{2Q}{m\ell_0^2} [V_0 + V_1 \cos(\Omega_1 t)] \mathbf{r}. \quad (1.28)$$

The same equation describes motion in the  $z$ -direction with rescaled right-hand side by a factor of  $-2$ . We will take a closer look at this equation in the section 1.2.6. Another essential subject we in is an effective potential for this geometry. For that, we need to substitute for something in the equation. Another essential subject is the effective potential for this geometry. For that, we need to substitute for  $E_0$  in the equation (1.15). Where we can get the norm of  $\mathbf{E}_0$  for example from (1.24) as:

$$E_0 = 2 \frac{V_1}{\ell_0} \hat{r}, \quad (1.29)$$

which means that the effective potential is:

$$V^*(\mathbf{r}) = \frac{Q^2 V_1^2}{\ell_0^4 m \Omega_1^2} r^2 + q \Phi_s. \quad (1.30)$$

#### 1.2.4.2 Real geometry of our trap

need to add pictures throughout the whole thesis

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. 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(1.30), 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  $\kappa \equiv 2Q^2V_1^2/(\ell_0^4m\Omega_1^2)$ , characterizing the strength of trapping potential. 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 spring constant depends on the charge-to-mass ratio  $Q/m \equiv Q_m$ , making it practically very difficult to trap electrons and ions simultaneously. For our case of trapping 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 trapped electrons occupy on average a similar region as ions. 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 look at the stability of both species individually. Making it possible to manage the desired ratio of spring constants. Two frequency Paul trap will be further discussed in section 2.1. The spring constant is closely related to a frequency of oscillation in a harmonic potential. Such frequency is called secular, denoted  $\omega \approx \sqrt{\kappa/m} = \sqrt{2QV_1/\ell_0^2m\Omega_1}$ .

#### 1.2.6 Mathieu equation

should cite [3] as well Let us reexamine our original equation of motion (1.2) for the case of a quadrupole trap with ideal hyperbolical electrodes. After time transformation  $\tau = \Omega_1 t/2$ , the equation (1.28) molds into:

$$\ddot{\mathbf{r}}(\tau) = [a - 2q_1 \cos(2\tau)] \mathbf{r}, \quad (1.31)$$

---

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

where:

$$a = \frac{8QV_0}{m\ell_0^2\Omega_1^2}, \quad (1.32a)$$

$$q_1 = -\frac{4QV_1}{m\ell_0^2\Omega_1^2}. \quad (1.32b)$$

The equation (1.31) 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 [4] in terms of special functions called Mathieu functions, denoted  $ce_n$  and  $se_n$ , sometimes referred to as cosine-elliptic and sine-elliptic. The secular is given by the Dehmelt approximation:

$$\omega \approx \frac{\Omega_1}{2} \sqrt{a + \frac{q_1^2}{2}}. \quad (1.33)$$

When  $a \approx 0$  the secular frequency is:

$$\omega \approx \frac{\Omega_1}{2} \sqrt{\frac{q_1^2}{2}} = \frac{\sqrt{2}QV_1}{\ell_0^2 m \Omega_1}, \quad (1.34)$$

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

### 1.2.7 Stability

The concept of stability is not straightforward to define for our system. We have Lagrange stability, Liapunov stability...First, we want to be working within the condition for adiabaticity so that the dynamic field will not augment the particle's energy. Inside this restriction, we will further search for characterization of stability.

The linear Paul trap has its characteristic length  $\ell_0$  defined by the distance from the middle of the trap to the electrode. We will use a criterion of stability established in [2] declaring a solution stable if it satisfies the condition:

$\max_{x \in \mathcal{L}}(r) \leq 0.8 \ell_0$ , where  $\mathcal{L}$  is the whole trajectory of a particle, is declared stable.

The drawback of this definition is that we must keep the simulation going long enough to account for the slowly diverging particles.

## 1.3 Laser cooling

The Ca+ ion has an energy gap between the ground and one of its excited states with the value corresponding to the wavelength of 397 nm [5]. 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*. More detailed explanation can be found in [6].

rephrase this sentence

## 1.4 Simulation

Let us begin this section by summarizing our approximations (inspired by [7]) already used when deriving the equation of motion → starting with insignificant ones.

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

**Induced charge on the electrodes:** charged particles will induce surface charge density on the electrodes made from electrically conductive material. This causes attraction of a particle toward the electrode, which can contribute to vacation of the particle from the trap. We will neglect this effect since our definition of stable trajectory does not allow the particle to approach to the electrode close enough for this effect to be significant.

**Relativistic effects:** we did not involve any relativistic corrections since while trapping particles we are dealing with small velocities.

**Ion radiation:** well known consequence of Maxwell equations is that accelerating charged particle emits electromagnetic radiation. We did not account for this energetic loss.

**Magnetic field:** created by presence of quickly changing electric field and moving charges is neglected since we work with weak fields and slow particles.

Here ends the list of phenomena whose oversight should not have any significant effect on our results. It could be the case that to get realistic results we might need to account for some of the following effects.

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

if I have understood from today's meeting correctly, then we handle this problem by dividing our electrodes into eight sections, each with its own feeding.

**Phase shift:** induced by the finite speed of electrons inside an electrode and the final speed of light since we will use quite a small trap and high frequencies.  
not sure if it can bring significant complications

### 1.4.1 The code

The practical part of this thesis consists of developing the code simulating the motion of ions and electrons in 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 (will probably be free to use) 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

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 2

## More advanced chapter

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

...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 [9] :

$$V(t, \mathbf{r}) = \left[ V_0 + V_1 \cos(\Omega_1 t) + V_2 \cos(\Omega_2 t) \right] \frac{x^2 + y^2 - 2z^2}{2\ell_0^2}, \quad (2.1)$$

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:  $\tau = t/(2\Omega_1)$  are:

$$\ddot{x}(\tau) = x(\tau) \left[ a - 2q_1 \cos \left( 2\frac{\Omega_1}{\Omega_2} \tau \right) - 2q_2 \cos(2\tau) \right], \quad (2.2a)$$

$$\ddot{y}(\tau) = y(\tau) \left[ a - 2q_1 \cos \left( 2\frac{\Omega_1}{\Omega_2} \tau \right) - 2q_2 \cos(2\tau) \right], \quad (2.2b)$$

$$\ddot{z}(\tau) = -2z(\tau) \left[ a - 2q_1 \cos \left( 2\frac{\Omega_1}{\Omega_2} \tau \right) - 2q_2 \cos(2\tau) \right], \quad (2.2c)$$

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

$$a = 4Q_m \frac{V_0}{\Omega_2^2 \ell_0^2}, \quad (2.3a)$$

$$q_1 = -2Q_m \frac{V_1}{\Omega_2^2 \ell_0^2}, \quad (2.3b)$$

$$q_2 = -2Q_m \frac{V_2}{\Omega_2^2 \ell_0^2}. \quad (2.3c)$$

## 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:

$$\dot{\mathbf{u}}(\tau) = \mathbb{F}(\tau)\mathbf{u}(\tau), \quad (2.4)$$

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 (2.2c) as a system of two first-order differential equations written in the matrix form:

$$\frac{d}{d\tau} \begin{bmatrix} z(\tau) \\ \dot{z}(\tau) \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -2 \left( a - 2q_1 \cos \left( 2 \frac{\Omega_1}{\Omega_2} \tau \right) - 2q_2 \cos(2\tau) \right) & 0 \end{bmatrix} \begin{bmatrix} z(\tau) \\ \dot{z}(\tau) \end{bmatrix}, \quad (2.5)$$

which already has a structure of (2.4). 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 (2.5) is  $T = m\pi$  periodic. As in [9], we identify the edge of stability regions as a set of parameters for which a solution of (2.2c) is a  $2T$  periodic function<sup>1</sup> to our problem (2.5). This allows us to seek a solution to our problem in the form:

$$z(\tau) = \sum_{k=-\infty}^{\infty} c_k \exp \left( i \frac{k}{m} \tau \right), \quad (2.6)$$

---

<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 (2.5) yields an identity:

$$\sum_{k=-\infty}^{\infty} \left[ \left( a - \frac{k^2}{m^2} \right) c_k - q_1 (c_{k-2n} + c_{k+2n}) - q_2 (c_{k-2m} + c_{k+2m}) \right] \exp\left(i \frac{k}{m} \tau\right) = 0, \quad (2.7)$$

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

$$\mathbb{F} \cdot \begin{bmatrix} \vdots \\ c_{k-1} \\ c_k \\ c_{k+1} \\ \vdots \end{bmatrix} = \mathbf{0}, \quad (2.8)$$

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

$$\mathbb{F}_{ij} = \left[ \left( a - \frac{k^2}{m^2} \right) \delta_{ij} - q_1 (\delta_{ij-2n} + \delta_{ij+2n}) - q_2 (\delta_{ij-2m} + \delta_{ij+2m}) \right], \quad (2.9)$$

where:

$$\delta_{ij} = \begin{cases} 1 & i = j, \\ 0 & i \neq j. \end{cases} \quad (2.10)$$

The equation (2.8) is equivalent to:

$$\det(\mathbb{F}) = 0. \quad (2.11)$$

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, otherwise unstable.

## 2.3 Simulation

### 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 [10]. 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>2</sup> for numerical solving of ODEs [11]. 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 [7]) 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 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

<sup>2</sup>All tried methods can be found in the file *intMethods.py*

minimal temperature, which can be obtained by laser cooling (about 0.01 Kelvin).

---

**Listing 1** The system of ODEs used for simulating Coulomb crystal.

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

```
def ODESSystemEffectiveDamping(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])
```

---

There is no real intention to keep this block of code here. I am just not sure if it is a good idea to have such blocks of code in the thesis at all

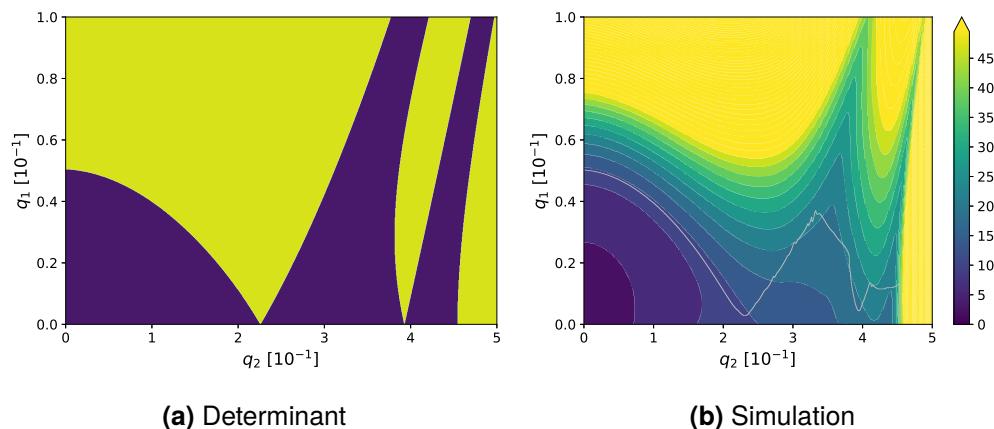


# Chapter 3

## 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.

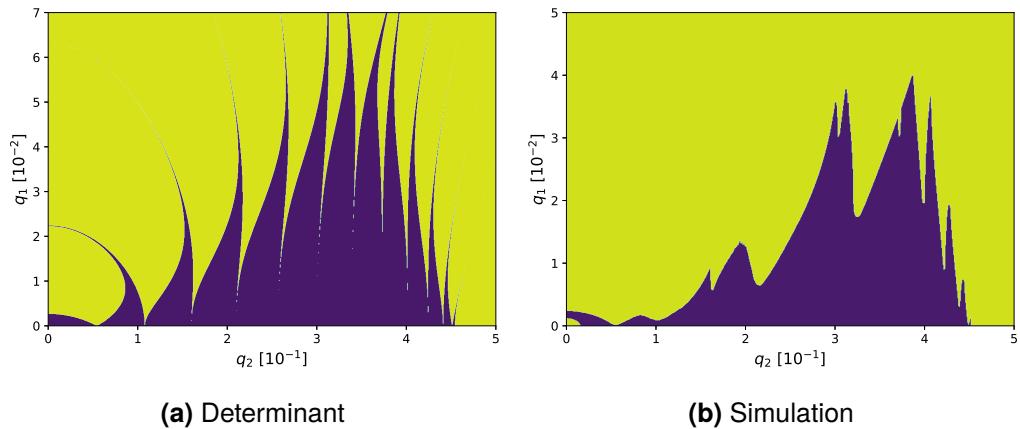


**Figure 3.1** Stability diagrams for  $\Omega_2/\Omega_1 = 3$

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...

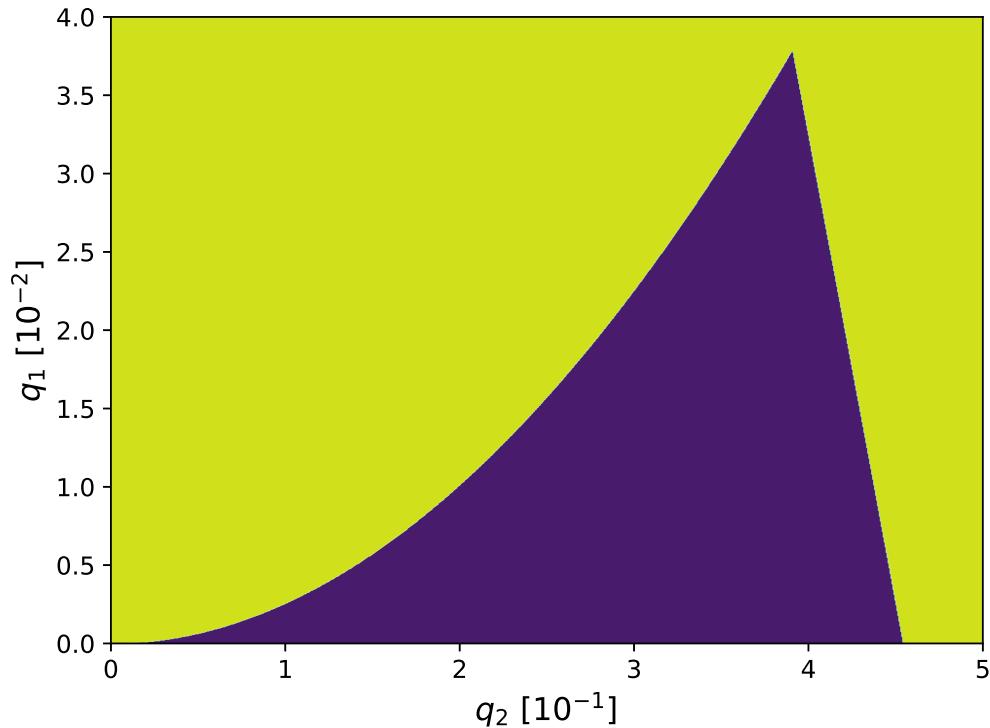
Moving to larger frequency ratio  $\rightarrow \Omega_2/\Omega_1 = 13$  we can start to notice some patterns.



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

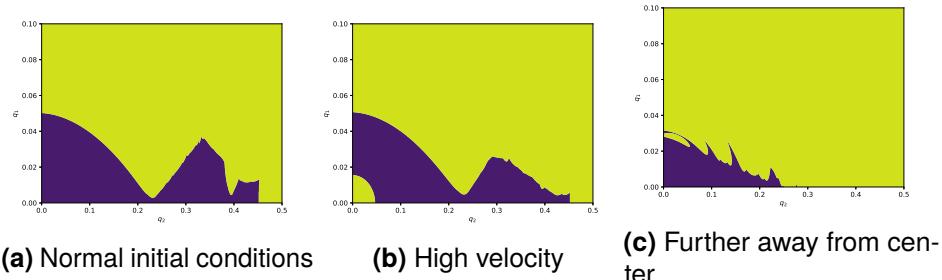
There emerges one stable triangle with many tongues of instability. With an increasing ratio  $\Omega_2/\Omega_1$  we can see a gain in the number of these tongues, but their width promptly shrinks as well. We expect that by further increasing the frequency ratio, the unstable tongues will be realistically 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** Stability diagrams 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.

## **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**

## **Chapter 4**

### **Future work**



# 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 2).

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 2** Main program.

---

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

---