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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 intend to 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?

definition of plasma, characteristic parameters, coupling parameter  $\Gamma$ , characterisation of Coulomb crystal, strongly coupled plasma in the nature

### 1.2 Ion trapping

#### 1.2.1 Equation of motion

This section follows the derivation from [2]. Let us consider a particle with mass  $m$ , charge  $q$  with it's position denoted by vector  $\mathbf{r}$ . We insert such 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:

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

Since we are not using any external magnetic field, and while trapping a particle in a bounded 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 equation of motion simplifies to:

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

---

<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.

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  $\mathbf{E}(t) \sim \cos(\Omega t)$ , giving us:

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

### 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:

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

where the vector:

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

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 smooth 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:

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

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

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

If the field amplitude  $\mathbf{E}_0(\mathbf{r})$  won't change too quickly, we can get by just with its first order Taylor expansion:

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

---

<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.

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

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

Presuming slow spacial variation of vectorfield  $\mathbf{E}_0(\mathbf{r})$  implies:  
 $|\ddot{\mathbf{A}}| \ll |\dot{\mathbf{A}}|\Omega \ll |\mathbf{A}|\Omega^2$ , which we can exploit in time derivative of quickly oscillating term  $\mathbf{R}_0(t)$  (1.7), giving us:

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

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

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

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

$$\mathbf{R}_1(t) = -\frac{q\mathbf{E}_0(\mathbf{R}_0(t))}{m\Omega^2} \cos(\Omega t), \quad (1.12)$$

terms with dependence on  $\cos(\Omega t)$  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  $\cos^2(\Omega t)$  with its mean value  $\overline{\cos^2(\Omega t)} = 1/2$  we finally obtain:

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

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

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

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 than the original equation of motion (1.2) as it does not involve any explicit time-dependency.

### 1.2.3 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 this apparatus would stand in the way. For this reason, we will use surface electrodes where particles will levitate above the trap so that we can access the ions with laser beams. Nevertheless, we will start our research by examining the situation with the geometry of the ideal linear Paul trap.

### 1.2.4 Linear multipole Paul trap

main source [2]

### 1.2.5 Stability

The concept of stability is not straightforward to define for our system. We have Lagrange stability, Liapunov stability...

The linear Paul trap has its characteristic length  $r_0$  defined by the distance from the middle of the trap to the electrode. We will use criterion of stability established in [2] stating that solutions that satisfy  $\max_{x \in \mathcal{L}} \leq 0.8 r_0$ , 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 [3]. 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. Making this arrangement in all three directions creates so-called optical molasses. This type of laser cooling is also known as *Doppler cooling*. More detailed explanation can be found in [4].

## 1.4 Simulation

Let us begin this section by summarising our approximations (inspired by [5]) 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)

**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>3</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)

---

<sup>3</sup>[https://github.com/rendeka/Bachelor\\_thesis.git](https://github.com/rendeka/Bachelor_thesis.git)

# Chapter 2

## More advanced chapter

Applying theory from the first chapter

### 2.1 Two frequency linear Paul trap

[6] [7]

### 2.2 Floquet theory

### 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 [8]. 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  $1/(2 f)$ . 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>1</sup> for numerical solving of ODEs [9]. For the case of a single electron in the trap with the expected initial conditions *thisOne.dat* had

---

<sup>1</sup>All tried methods can be found in the file *intMethods.py*

the best performance a predictor-corrector method, which we have defined as *StepEulerAdvanced*. The sufficient time-step for this method was  $\Delta t = 1/(10 f)$ .

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 summarising our approximations (inspired by [5]) 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 minimal temperature, which can be obtained by laser cooling (about 0.01 Kelvin). **could have implemented some simplex based algorithm with the molecular dynamics**

---

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

---

```
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])
```

---

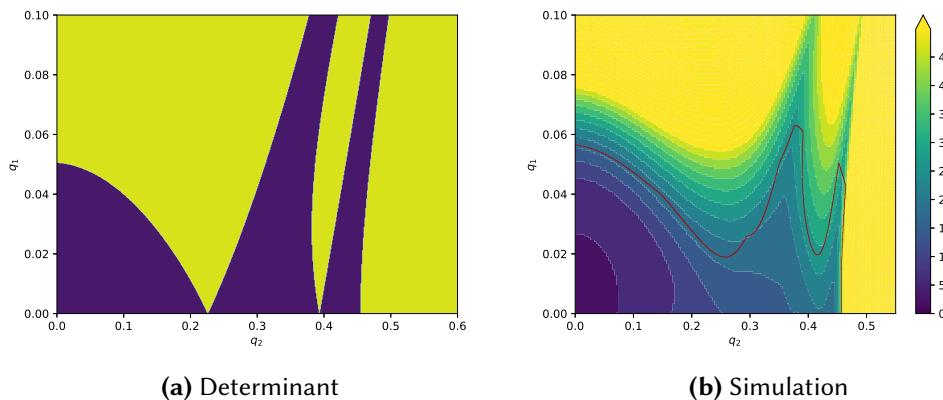


# Chapter 3

## Results and discussion

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

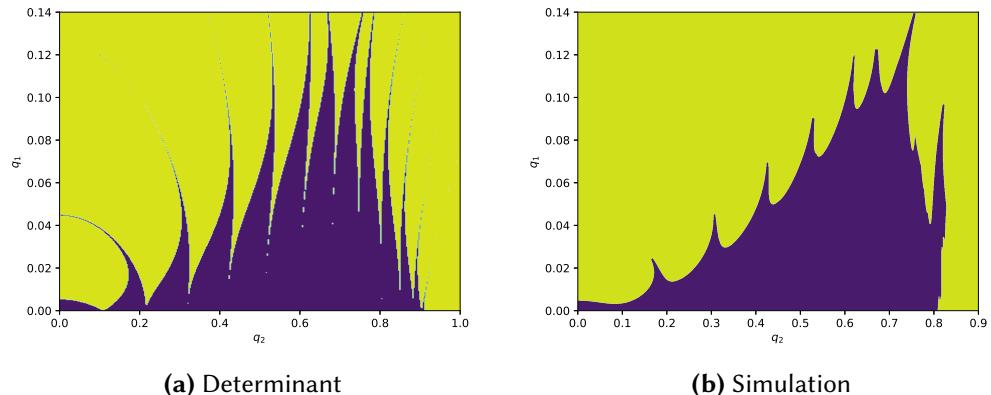
We will start by looking at the stability diagrams for different  $\Omega_2/\Omega_1$  ratios. Starting with 3.2.



**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 red 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.

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



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

### 3.1.1 Dependence on initial conditions

## 3.2 Creating a Coulomb crystal

## 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

## **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()
```

---