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BACHELOR THESIS

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Simulations of dynamics of ultra-cold quantum plasma

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Author's signature

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

Title: Simulations of dynamics of ultra-cold quantum plasma

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Introduction

The practical aim of this thesis is to contribute to the development of 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 Γ, 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, which to my knowledge, hasn't been achieved yet. We will be aiming for sub-kelvin temperatures when electrons de Broglie wavelength would be bigger than the distance between them, forming so-called Fermi gas. Creating a Coulomb crystal means confining a certain number of charged particles in bounded space. The first thing standing in our way is the Earnshaw theorem, 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 use the dynamic electric field solely. 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. My 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 crystalization for such a system.

Chapter 1

Theoretical introduction

In this chapter, we intend to introduce concepts essential for understanding this thesis's concerns. This chapter is divided into three subsections. In the first subsection, we are going to discuss the vital principles in plasma physics. In the following subsection, we will talk about the motion of a charged particle inside the Paul trap. Finally, in the last subsection, we will present our approach to simulating such a system, entering this thesis's practical component.

1.1 What is plasma?

1.2 Ion trapping

1.2.1 Equation of motion

This section follows the derivation from [**gerlich1992inhomogeneous**]. 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 $\mathbf{E}(\mathrm{t}, \mathbf{r})$ and $\mathbf{B}(\mathrm{t}, \mathbf{r})$. The Lorentz force gives the equation of motion:

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

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 the effect of the term $\dot{\mathbf{r}} \times \mathbf{B}$, which means that equation of motion simplifies to:

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

We further assume that the electric field is composed of the static and time-dependent part. We are looking for periodic time-dependency; therefore, the obvious ansatz would be $\mathbf{E}(\mathrm{t}) \sim \cos(\Omega \mathrm{t})$, giving us:

$$\mathbf{E}(\mathrm{t}, \mathbf{r}) = \mathbf{E_s}(\mathbf{r}) + \mathbf{E_0}(\mathbf{r})\cos(\Omega \mathrm{t}). \tag{1.3}$$

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 next section of this chapter 1.3. 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 $\mathbf{E_0}(\mathbf{r}) = \mathrm{const}$, we obtain a trivial solution:

$$\mathbf{r}(\mathrm{t}) = \mathbf{r_0} - \mathbf{A}\cos(\Omega \mathrm{t}), \tag{1.4}$$

where the vector:

$$\mathbf{A} \equiv \mathbf{A}(\mathbf{r}) = \frac{\mathrm{q}\mathbf{E_0}(\mathbf{r})}{\mathrm{m}\Omega^2}, \tag{1.5}$$

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 [1]. 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:

$$\mathbf{r}(\mathrm{t}) = \mathbf{R_0}(\mathrm{t}) + \mathbf{R_1}(\mathrm{t}), \tag{1.6}$$

where $\mathbf{R_0}(\mathrm{t})$ represents consequence of smooth drift and $\mathbf{R_1}(\mathrm{t})$ stands for rapid oscillation, expressed as:

$$\mathbf{R_1}(\mathrm{t}) = -\mathbf{A}\cos(\Omega \mathrm{t}). \tag{1.7}$$

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:

$$\mathbf{E_0}(\mathbf{R_0}(\mathrm{t}) - \mathbf{A}\cos(\Omega \mathrm{t})) \approx \mathbf{E_0}(\mathbf{R_0}(\mathrm{t})) - (\mathbf{A} \cdot \nabla)\mathbf{E_0}(\mathbf{R_0})\cos(\Omega \mathrm{t}) + \dots . \tag{1.8}$$

[1] 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:

$$m\Big(\ddot{\mathbf{R}}_\mathbf{0}(\mathbf{t})+\ddot{\mathbf{R}}_\mathbf{1}(\mathbf{t})\Big) = q\cos(\Omega t)\Big[\mathbf{E_0}(\mathbf{R_0}(\mathbf{t}))-(\mathbf{A}\cdot\nabla)\mathbf{E_0}(\mathbf{R_0}(\mathbf{t}))\cos(\Omega t)\Big]. \quad (1.9)$$

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:

$$\ddot{\mathbf{R}}_\mathbf{1} = -\ddot{\mathbf{A}}\cos(\Omega t) + 2\Omega\dot{\mathbf{A}}\sin(\Omega t) + \mathbf{A}\Omega^2\cos(\Omega t) \approx \mathbf{A}\Omega^2\cos(\Omega t) \quad (1.10)$$

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:

$$m\ddot{\mathbf{R}}_\mathbf{0} = \frac{q^2}{4m\Omega^2}\nabla E_0^2. \quad (1.14)$$

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

$$V^*(\mathbf{R_0}) = \frac{q^2E_0^2(\mathbf{R_0})}{4m\Omega^2} + q\Phi_s, \quad (1.15)$$

describing the time-averaged force on a charged particle:

$$m\ddot{\mathbf{R}}_\mathbf{0} = -\nabla V^*(\mathbf{R_0}). \quad (1.16)$$

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 Stability

1.3 Simulation

1.3.1 Laser cooling

Let us begin this section by summarising our approximations (inspired by [**Friedman_1982**]) when deriving the equation of motion—starting with insignificant ones.

Gravitational interaction: we the neglecting completely since gravitational effects are several orders of magnitudes smaller then electrostatic.

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 by significant.

Relativistic effects: while trapping particles we are dealing with velocities of orders $\mathrm{v}/\mathrm{c} \approx 10^{-\mathrm{something}}$ making relativistic effects irrelevant.

Ion radiation: well know consequence of Maxwell equations is that accelerating charged emits electromagnetic radiation, effectively loosing energy that we will not account for.

Here ends the list of phenomena whose oversight should not have any significant effect on our results

Chapter 2

Applying theory from the first chapter

explain my choices while writing the python script

Chapter 3

Results and discussion

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

3.1.1 Dependence on initial conditions

3.1.2 Comparison of simulation and determinant stability criterion

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 - 20 ions

3.3.3 One electron - 100 ions

Conclusion

We were perhaps able to optimize parameters of two frequency Paul trap for storing ions and electrons together…

Bibliography

Appendix A

Using software

This appendix intends to explain to the reader how to use the python script.

To unpack and compile the software, proceed as follows:

```
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 Example program.

```
if __name__ == '__main__':

    prayForItToWork()
```