Paul's Trap

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Being able to have particles isolated without the need to be physically touching them allows a much more precise study of their behaviour. In order to achieve that electrodynamic traps such as Paul's trap confine particles inside them using only a varying electric field. In this paper a trap of such characteristics will be simulated in order to observe the behaviour of the ions inside it.

I. INTRODUCTION

Paul Trap, is a type of ion trap that uses three plates and a dynamic electric field to trap ions inside. It is named after Wolfgang Paul, who won the Nobel Price in Physics for the invention of this device in 1989. The particular shape of the Paul Trap, and a varying electric field with the right frequency, traps the particle inside the device. In this project we generate a full simulation of the Paul Trap and find the right frequency for different types of charged particles.

In order to do so, the aim of the first part of the project is to define the geometry of the trap, and triangularize it in small parts so that we can define the charge variation, the potential and the electric field in every single small piece of the trap separately. With the mesh as the surface the integral Poisson equation can be discretized as a linear system of equations that will lead to the calculation of the potential and the electric field. Once the geometry of is well defined, the second part of the project consists on computing the time-varying potential and charge in the plates of the Paul Trap, so that particles can be trapped inside. Finally, the last part, simulates the movement of the trapped particle inside the Paul Trap due to the electric field generated in the plates, by defining the equations of the motion of any charged particle inside the trap for any initial position inside the ion trap.

The goal of the project is then, to make a full simulation of the time-varying electric field in the ion trap, and thus be able to simulate the movement of any charged particle inside a Paul Trap.

II. THE PAUL TRAP

The main idea of the ion traps is that ideally the best object for precision measurements is a particle floating in free space, and Paul Trap gives is the best approximation to this situation. The Paul Trap has two hyperbolic metal plates, or electrodes with their foci facing each other, and a third hyperbolic ring plate in between the other two electrodes. In order to keep the particle moving inside the trap, the electric field of the plates must be constantly varying between the two hyperbolic cap plates as well as the ring electrode. The charged particle inside the trap will be first pulled towards the upper and lower cap plates, while at the same time is pushed away from the ring plate. Then, as the electric field constantly changes between the plates, the particle will be pushed away from the cap plates, and pulled towards the ring electrode. If the frequency of the electric field change is high enough, this modification of the movement avoids collision with the plate, and thus traps the particle inside. The particle trapped has a complex movement due to the varying electric field.

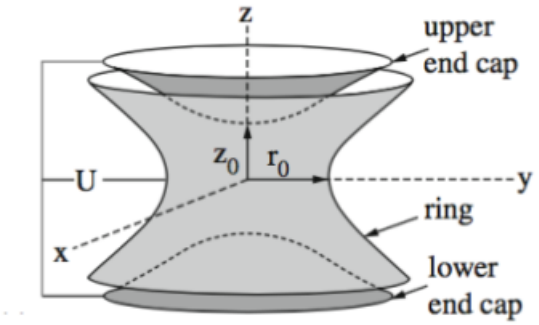

FIG. 1. Structure of a Paul Trap
[a]

[a] https://aquadrupauliontrap.wordpress.com/types-of-ion-traps/

A. Equations of motion

The ions inside the trap experience forces that pull them back towards the center of the trap. The forces come from the electric fields generated by the three metallic plates, and the movement of the particles can be described by the following equations of the movement:

$$\begin{aligned} a[t] &= \frac{q}{m}E[t] \\ v[t+1] &= v[t] + a[t]\Delta t \\ r[t+1] &= r[t] + v[t]\Delta t + \frac{a[t]}{2}t^2 \end{aligned} \tag{1}$$

Where E[t] is the time-varying electric field, q is the

charge, and m is the mass of the particle. In the simulation, time is discretized into short intervals, so that the acceleration can be assumed constant within them and only varies from one interval to the next, therefore it is correct to use the equations of a uniformly accelerated motion for the position and the velocity, changing the acceleration for every time step.

III. SIMULATION OF PAUL TRAP

A. Geometry

The first part of the simulation of the ion trap consists on creating the desired geometry. In this case, the geometries needed for the Paul Trap are two hyperbolic cap plates facing each other on the top and bottom of the structure, and a hyperbolic ring electrode halfway between the two plates. For the creation of the top and bottom plates, a mesh of points is created with a circular shape and later, it is given the hyperbolic shape desired, by modifying the height of the points with the following equation:

$$z = \frac{\sqrt{x^2 + y^2}}{2} + z_0^2 \tag{2}$$

For the case of the hyperbolic ring electrode in between the plates, the procedure is exactly the same, as the mesh of points is firstly created and then it is given the hyperbolic surrounding shape desired.

Once the mesh of the whole structure is obtained, the structure has to be triangularized so that later, a value of charge can be assigned to each of the triangles. In order to triangularize the structure, the function *delauanay* that returns the exact position of the three vertices of every triangle, and the center position as well.

Fig. 2 shows the structure of the Paul Trap used for this simulation after the triangularizaton process, in which all the triangles are approximately the same size, with few variations.

B. Charge distribution

In order for the electric field to be time-varying, the charge distribution of the trap has to keep changing in time. This is mainly obtained with the use of the Green function for a electrostatic interaction in three dimensions. That convoluted with the function of the charge at every point in space will give us the potential.

$$V = q(r) * G = \int_S \frac{q(r')}{4\pi\epsilon|r - r'|} dr' \tag{3}$$

To compute the charge of the plates the integral is only calculated at the surface of them. In order to do that the Method of Moments will be used. It will be assumed

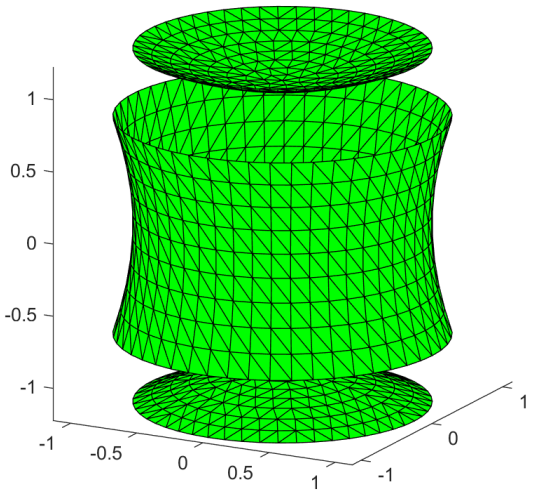

FIG. 2. Triangularized simulated structure of the Paul Trap electrodes

that for each triangle the charge is constant, so it can be taken outside the integral. This leads to the calculation of the linear coefficients that will relate the charge with the potential at the surface.

$$Z(r_m, T_n) = \int_{STn} \frac{1}{|r_m - r'|} dr' \tag{4}$$

Where the limit of integration STn represents the surface of the triangle. Once computed for every triangle and every point in space this function yields a matrix. Considering the vector of values of the initial potential V0, which is determined to be half $-V_0$ and the other half V_0, the charge can be obtained simply by using the Matlab *backslash* to solve for the equation:

$$[Z] * [q] = [b] \tag{5}$$

Where b is the vector of the initial potential values of each triangle and q the charge. Once the charge is computed, it can be plotted with the *fill3* function, so that the time-variation of the charge distribution on the whole surface can be seen. The following image represents the initial charge distribution where the red colour represents the maximum value while the blue one corresponds to the minimum:

During the simulation, the charge distribution changes from this initial condition to the distribution where the hyperbolic ring has a positive charge distribution (red), while the top and bottom plates have negative charge distributions (blue), and then back to the initial condition again.

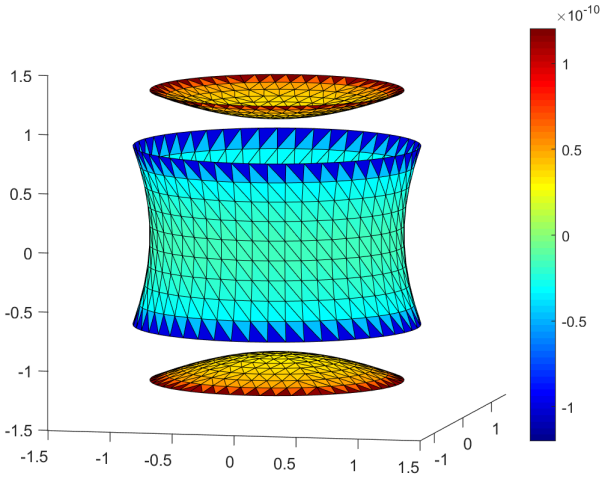

FIG. 3. Initial charge distribution of the simulation

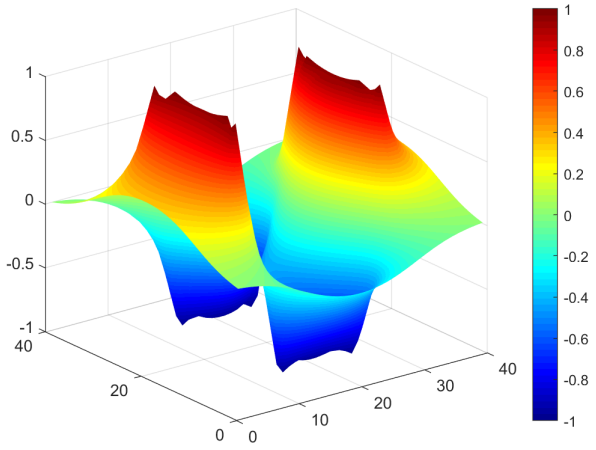

FIG. 4. Initial potential at a vertical section of the simulation

C. Potential

With the time-varying charge obtained, the next step of the simulation is to calculate the time-varying potential. The equation needed relates to the tmp function, as it is the usual equation of the Coulomb Potential (3).

The potential is computed at all the points of space, not only on the plates. First of all, a new mesh of points is defined containing all the points in space between -2 and 2 in all directions, and the potential is calculated using equation (5) in all points of space, with the help of the function *intSdivR*, for the calculation of the integral.

The potential is plotted using the Matlab function *surf*, of only a vertical section of the plates, taking advantage of the symmetry of the system, so that it is easier to see the time-variation of the potential. In this case, the red colour represents the positive potential, while blue corresponds to the negative one. The initial potential in the section is shown in Fig. 4. Initially, the two red peaks represent the top and bottom electrodes, while the blue peaks correspond to the hyperbolic ring plate, which has a negative charge distribution. With the evolution of time in the simulation, the charge distribution of the plates changes and so does the potential, so that when the hyperbolic ring plate has a positive charge distribution and the top and bottom plates have negative charge distributions, the potential corresponding to the top and bottom plates is represented in blue while the one corresponding to the hyperbolic ring is represented in red.

D. Ions and movement

Once a harmonic time varying potential is achieved the ions have to be modeled. A simulation of its trajectories is created using the aforementioned equations for the dynamics of the ions. This trajectories are started from different points and velocities, always starting near the equilibrium point found in the center of the trap. Since the stability of the system cannot be taken for granted, the frequency of the harmonic variation of the potential in the plates must be tuned for different types of ions.

Since the only parameter from the modeled ions that can change its trajectory is the ratio between the charge q and the mass m, as can be seen in the movement equations, only the mass has been modified, keeping the charge at $1.6 * 10^{-19}$.

IV. RESULTS

With a fixed time step, set at $3 * 10^{-6}$, and after simulating different frequencies of variation of the potential of the plates it can be seen that for lower frequencies the rate of change of the potential is not enough to keep the particle inside the trap. Nevertheless when the frequencies are increased we achieve stability, allowing the particle to stay inside.

Until this point only particles of the mass of a proton has been taken into account. If the mass is increased it is much harder for the electric field to move the particle, since the force exerted by the plates gets reduced by the relative value of m.

Running the simulation for different masses and frequencies, relative to the mass of the proton and the original frequency respectively, we can observe that as the mass increases, the range of stable frequencies decreases.

In the simulations of the trajectories it can also be seen that, for the chosen starting conditions, if the frequency is too small, the particle tends to go to the top or bottom plate, the collision is signaled in the Fig. 5 as a red dot. On the other hand if the frequency of the plates is too big the particle travels horizontally until it collides with the ring plate.

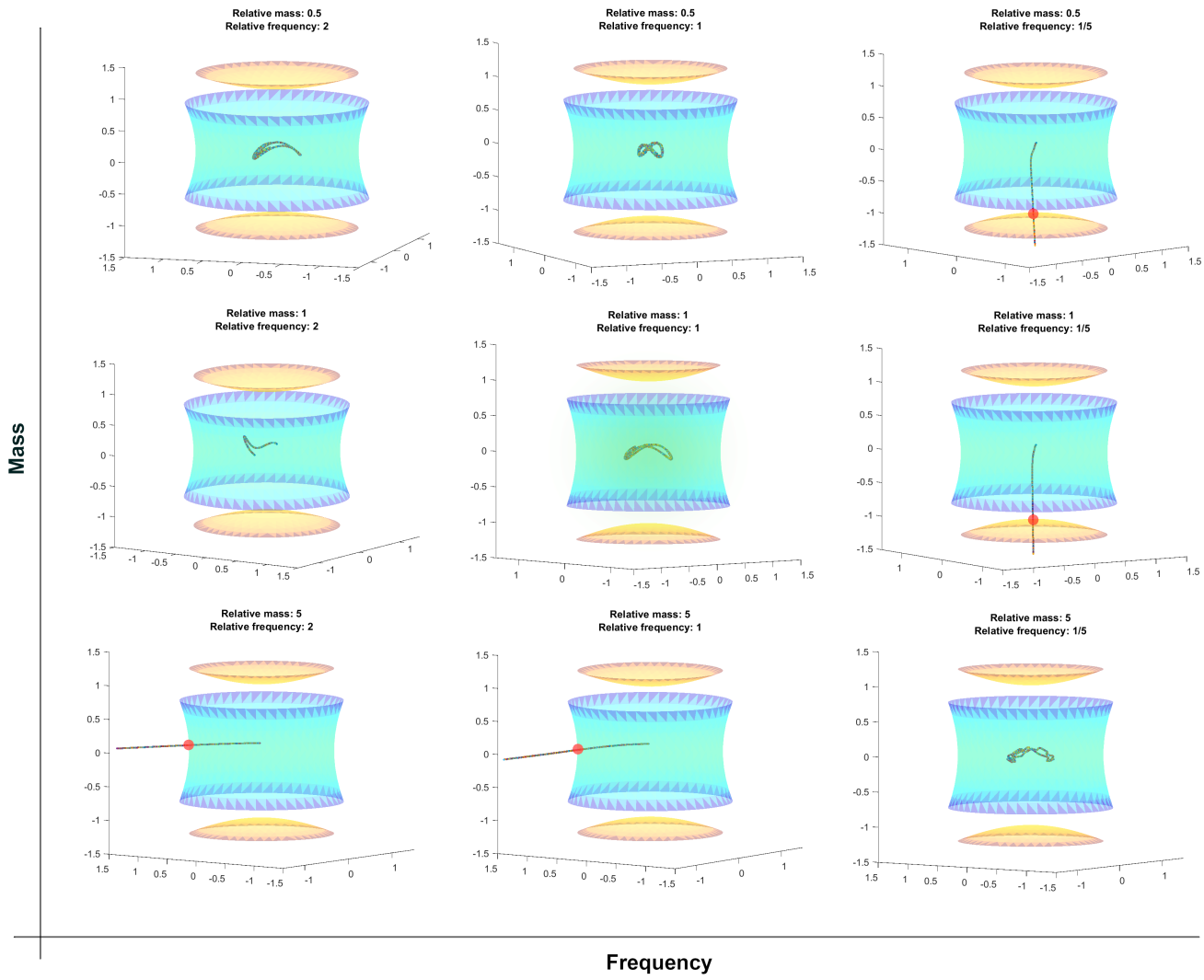

FIG. 5. Stability of the trajectories for different masses and frequencies

V. CONCLUSIONS

With the realization of this project we have managed to successfully simulate a Paul Trap using Matlab. We have built the geometry and defined the time-varying charge distribution and the potential in order for the trap to trap ions inside.

Finally we have also defined the equations of motion of the particles assuming the time to be discretized into short intervals, so that we could simulate the movement of the charged particles inside the trap.

We have found that the frequency used determines whether the charged particles are trapped inside or not. We changed the frequency and other variables such as the mass in order to find a relation between such variables for us to be able to choose a frequency for which particles are always trapped and it can be observed, at least for the range of frequencies studied that the stable frequencies are inversely proportional to the mass of the particle, which means that if we put a particle with two times the mass of the original one we must reduce the frequency by half.