Quadrupole Ion Trap

Contents

1 Introduction

Ion traps are devices used to confine ions in free space through the use of electric and/or magnetic fields. In this experiment, we are going to explore a simple quadrupole ion trap, also known as a Paul trap in honor of Wolfgang Paul, who invented the device and was awarded the Nobel prize in Physics in 1989 for this work. Nowadays, quadrupole ion traps have a number of important applications such as mass spectrometry, high precision measurement and notably quantum computing.

The aim of this experiment is to understand the operation of a Paul trap and apply this knowledge to determine the charge of lycopodium spores in combination with other basic experimental techniques.

2 Theory

2.1 Ion Trapping

A quadrupole ion trap is designed to confine ions in free space exclusively through the use of electric fields. This cannot be done using electrostatic fields alone as this would violate the Gauss law. One solution is to use a combination of a static electric field and an oscillating electric field at frequency Ω: if the particle motion is slow compared to the frequency scale of the oscillating field, the average effect will effectively trap the particle at a potential minimum. The total potential Φ of such a field at a given point $\mathbf{r}$ reads

$$\Phi(\mathbf{r}, t) = \Phi_{DC}(\mathbf{r}) - \Phi_{AC}(\mathbf{r}) \cos \Omega t, \tag{1}$$

where Φ_{DC} and Φ_{AC} are the static and oscillating components of the potential, respectively. Let's consider only the contribution from Φ_{AC} to the motion of a trapped particle in a 2D plane, with $\mathbf{r} = (x, y)$. Expanding Φ_{AC} around the minimum $\mathbf{r} = 0$ we have

$$\Phi_{AC}(\mathbf{r}) = c_0 + \frac{1}{2}\left(c_{2,x}x^2 + c_{2,y}y^2 + c_{2,xy}xy\right) + \mathcal{O}(|r|^3). \tag{2}$$

Here, c_0 is constant offset and can be set to 0. With an appropriate choice of the coordinate system, the cross term $c_{2,xy}$ can be set to zero. Along the x or y

direction, the potential takes the form of a modulated harmonic potential. The motion of the ion in such a potential can be separated along x and y independently, which are now the directions of the normal modes of motion. In the following we consider the motion along the x direction, but the same holds for y.

The equation of motion for an ion of charge q and mass m is given by

$$\frac{\partial^2 x}{\partial t^2} = -\frac{q}{m}\frac{\partial \Phi}{\partial x} = \frac{q}{m}(c_{2,x} x \cos \Omega t). \tag{3}$$

Using the coordinate transformation $\tau = \frac{\Omega t}{2}$ and $q_x = \frac{2qc_{2,x}}{m\Omega^2}$ simplifies this equation to

$$\frac{\partial^2 x}{\partial \tau^2} - 2q_x x \cos 2\tau = 0. \tag{4}$$

This is a **Mathieu differential equation**, and its solutions are **Mathieu functions**. Depending on the value of q_x the solution can be stable, i.e. the particle is trapped around the zero field point, or not.

For $q_x \ll 1$, the particle takes a stable solution. Its orbit can be written as

$$x(t) = C_i \cos(\beta\tau)[1 - \frac{q_x}{2}\cos(2\tau)], \tag{5}$$

where $\beta = |q_x|/\sqrt{2}$. Since $|q_x| \ll 1$, the motion of the particle is dominated by a slow oscillation at frequency $\omega_s = \beta\Omega/2 \ll \Omega$. It is modulated by a small amplitude, fast oscillation at the driving AC voltage frequency Ω. These are known as the **secular motion** and **micromotion** respectively.

The secular oscillation can be interpreted as the average effect of the fast oscillating electric force on the particle $\langle F_x \rangle_\tau$. In this case, it is equivalent to a restoring force pushing the particle back to the zero field point as if there is a harmonic pseudo-potential Φ_{PS}, such that $\langle F_x \rangle_\tau = -\partial \Phi_{PS}/\partial x$.

3 Experiment

3.1 Quadrupole Ion Trap

3.1.1 Electric field configuration

In this experiment, we are going to investigate a linear ion trap consisting of four parallel cylindrical copper rods, see Figure 1. The distance between the rods was chosen such that the potential inside the trap best approximates a quadrupole potential [1]. The choice of cylindrical geometry eases the trap fabrication and allows for large access to the trap center.

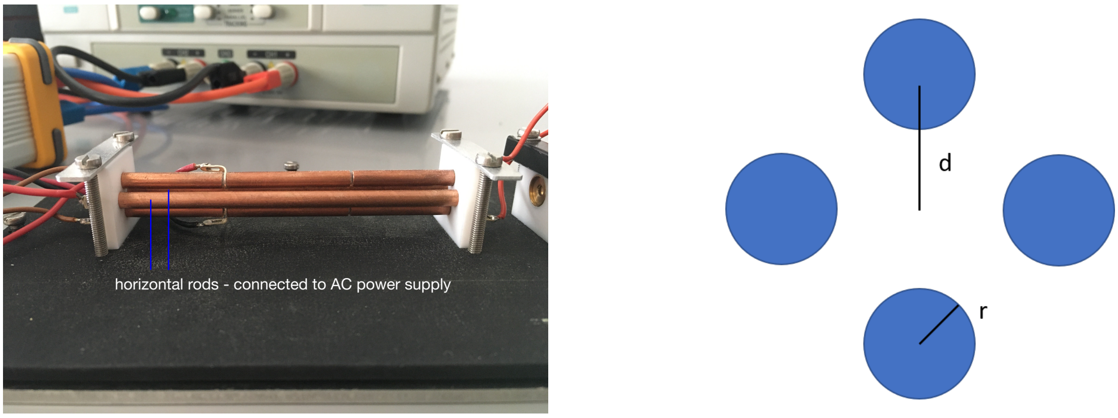

Figure 1: Picture of the ion trap setup, and a sketch of the trap geometry in the transverse plane.

The four rod configuration allows for trapping of charged particles in the transverse plane perpendicular to the electrodes along the zero field line, which is the symmetry axis. The top and bottom electrodes are divided in three segments. The center segments, called *bias*, can be used to adjust the vertical position of the trapped particles. The outer segments, called *endcaps*, can be used to push the particles to the trap center and trap them along the axial direction.

Later on, you will need to calculate the electric field in the trap center due to the applied voltages on the bias electrodes. This amounts to solve a Laplace problem for the electrostatic potential in free space with boundary conditions given by the voltages on the rods. There is no analytical solution for our trap geometry, so solving the problem requires the use of numerical methods such as the finite element method. However, There are simpler geometries with analytical solutions that you can solve to get an understanding of the relevant parameters.

Task 1.

- Calculate the electric field at the origin $\mathbf{r} = (0, 0)$ for two planar electrodes, where the bottom one is located at $y = -d$ and held at a potential V_0 and where the top one is located at $y = d$ and held at a potential $-V_0$ (Fig. 2a). What's the order of magnitude of the electric field?
- Calculate the electric field at the origin for one single rod electrode of radius r, located at $y = -d$ and held at a potential V_0. You can set the electric potential at the origin $V(\mathbf{r} = 0) = 0$ (Fig. 2b). How does the electric field depend on the geometry of the problem? What is the correct "scaling factor"?
- Measure the relevant quantities for our trap geometry and use them to determine the electric field at the trap center when setting the bottom electrode at $V_0 = 1\,\mathrm{V}$ and the top electrode at $-V_0$. See Appendix A.1. Use this result to calculate the electric field at the trap center for an arbitrary set of DC voltages on the four electrodes.

Bonus: The Poisson or Laplace equation with boundary conditions is the typical problem that can be tackled by FEM. Try to set up a FEM simulation of the electric fields in the quadrupole trap. You can find both specific software (COMSOL) and numerical packages for many different programming languages (Pyhton, Matlab, Mathematica) designed to solve this kind of problems.

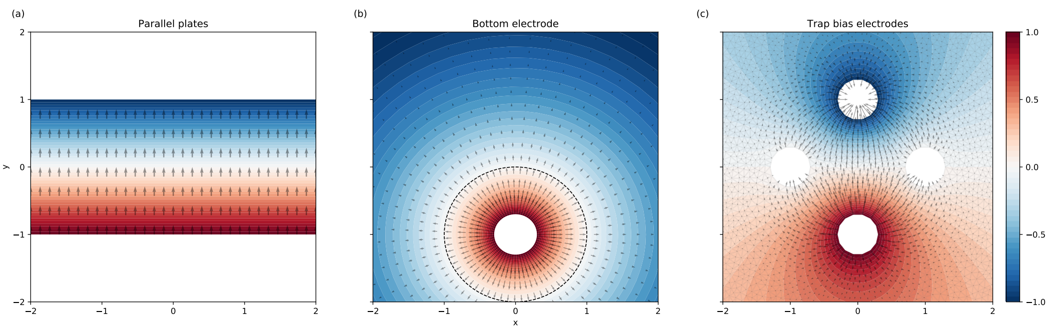

Figure 2: DC Electric field in the xy plane for three electrode configurations.

3.1.2 Setup

Task 2. Remind yourselves the basic safety rules when working with electricity.

A variable transformer (variac) and a DC power supply are used to provide the necessary 50 Hz AC and DC voltages. For safety reason, we limit the current below 1 µA by adding a safety box containing high resistance resistors between the trap electrodes and the power supplies.

Task 3. Connect the trap. You will find the safety box already connected to the AC/DC power supply, please leave it connected as it is. The task here is to understand and explain what are the meaningful connections to the trap electrodes that will generate the required potential.

> Connect the AC electrodes first, and draw a sketch of quadrupole electric field. Then connect the bias electrodes and justify the choice of voltages required to compensate gravity according to the sign of the charge of the particle. Finally, connect the endcap electrodes such that the particles will be confined inside the trap along the trap axis.
>
> Prepare all the electrical connections without switching on the power supply, and check them with the TA before continuing the experiment. Read Section 3.4.2 now, it will give details about the safety box circuit and its proper use, and define other safety-related tasks that will be required for the final report.

The experiment is powered by a Raspberry Pi (RPi), that you will use to control a laser to illuminate the trapped particles and a camera to image them.

Task 4. Setup the experiment control. Read Section 3.3 now, where you will find instructions and tasks for using the RPi for this experiment. Connect the laser to the driver circuit and the RPi, and write a Python script to control it in continuous and pulsed mode.

Task 5. Remind yourselves the safety rules when working with laser. Do we need laser goggles for this experiment?

Align the laser through the trap center, using the opening holes on the trap mounts as a guideline.

A transparent wind shield is used to cover the trap, to protect the setup from air currents which could disturb the particle motion. Place the wind shield over the trap. Then focus the camera to the trap center.

3.1.3 Trapping of charged lycopodium spores

We are now ready to trap charged lycopodium spores. Set the AC voltage to 220 V, and the DC voltage to 30 V. For further safety, do not remove the wind shied while the trap is in operation.

Task 6. Load the trap

Charge the teflon stick by rubbing it on e.g. clothes, and lightly dip it into the container with the lycopodium spores. Insert the stick into the trap through the hole on the windshield, and gently shake the teflon to release the lycopodia into the trap. We can observed bright spot(s) inside the trap by bare eye if lycopodium spores are successfully trapped. Now, focus the camera on the trapped particle.

Task 7. Observation of the particle in the trap

> Keep the laser continuously on and observe the image of the particle on the camera. Explain the shape of the trace of the moving particle.
>
> Pulse the laser on for 1 ms at 49 Hz, 50 Hz and 51 Hz. How do the images look now? Draw conclusions about the nature of the particle motion.

In practice, the secular motion is quickly damped by the air friction. The ion motion is dominated by the micromotion whose amplitude depends on the average electric force acting on the ion. Intuitively, the further away from the trap center (zero field point), the larger the electric force. Gravity pulls the particles out of the zero field point. By applying a bias field compensating for the gravity, one can push the particles closer to the zero field point and thus obtain a minimal oscillation amplitude.

Now, adjust the DC voltage such that the micromotion is minimized.

Task 8. Trap stability

> Slowly lower the AC voltage. How does this modify the image? Adjust again the DC voltage to minimize the micromotion. Repeat this process until the ion escapes the trap, and record the last DC voltage value before reducing the AC voltage. Comment on the sensitivity of the micromotion compensation.

Reload another particle into the trap and compensate for gravity. Slowly increase the AC voltage. Observe the behaviour of the trapped particle. Explain what happens.

From the value of the bias DC voltage that best compensate for the gravity, we can calculate the charge to mass ratio q/m of the particle as $mg = qE_c$, where E_c is the bias electric field at the center of the trap. Note the sign of the voltages applied and deduce the sign of the charged particle.

Task 9. Measure E_c for at least 10 different particles. Comment on the distribution of the q/m values.

3.2 Mass and size measurements

Task 10. Guess the mass and size of a single lycopodium spore.

Measuring the mass of a single lycopodium spore directly with a scale is very challenging. Alternatively, we can measure the terminal velocity of the particle during a free fall in air.

The density of air at 1 atm pressure is $\rho = 1.2\,\mathrm{kg}^3\,\mathrm{m}^{-1}$, and its dynamic viscosity is around $\mu = 1.8 \times 10^{-5}\,\mathrm{kg\,m^{-1}\,s^{-1}}$. After a long enough falling time, the particle attains a final velocity at which the air friction is equal to its weight. While falling in a non-turbulent fluid, the damping force on the spores can be expressed by Stokes' law

$$F_d = -6\pi\mu R v, \tag{6}$$

with R being the spore radius. Once the terminal velocity v_T has been reached, the following equation holds:

$$mg = 6\pi\mu R v_T \quad . \tag{7}$$

Thus, measuring v_T allows to measure the ratio m/R.

3.2.1 Radius measurement

Since lycopodium spores are rather small, we can use optical methods to measure their size. Illuminating some spores dispersed on a surface with a laser beam, each spore behaves as circular obstacle diffracting light in an Airy disk pattern. Since the size of the fringes is much larger than the distance between the spores, almost identical patterns add up giving a strong enough signal that can be observed directly by naked eye.

In an Airy pattern, the angle θ at which the first minimum occurs, measured from the direction of incoming light, is given by

$$\sin\theta \simeq 1.22\frac{\lambda}{2R}. \tag{8}$$

Task 11. Laser diffraction on lycopodium spores

Sandwich lycopodium powder between two glass slides. Illuminate the powder with the laser and record the diffraction pattern on a millimeter paper placed about 50cm away. Slightly move the powder in the transverse direction to obtain the best contrast. Then use Eq. (8) to deduce the average radius of the spores.

Task 12. Measure the spore size with a Pi-microscope

Try to take an image of the spores using the Picamera. Adjust the lens to obtain a maximal magnification. Focus the image on a few spores at the center of the image. Without changing the focus, take an image of your phone screen. Compare the size of a spore with the size of a pixel, and from this deduce the radius of a single spore. The actual size of a pixel can be calculated from the PPI (pixels per inch) number of your phone screen.

Hint: If you screenshot the camera images, be sure that the full images are captured. To compare the lengths in different images, one can use an image processing programme such as ImageJ, or an image processing library such as scikit-image.

Task 13. Compare the results from the two methods.

3.2.2 Terminal velocity measurement

The setup used for determining the lycopodium terminal velocity is shown in Figure 3. It consists of a transparent tube, with a laser mounted at the bottom to illuminate the particles dropped from the top. There are two caps which can be inserted at the top: one with a pendulum (cap A) and one with two small openings

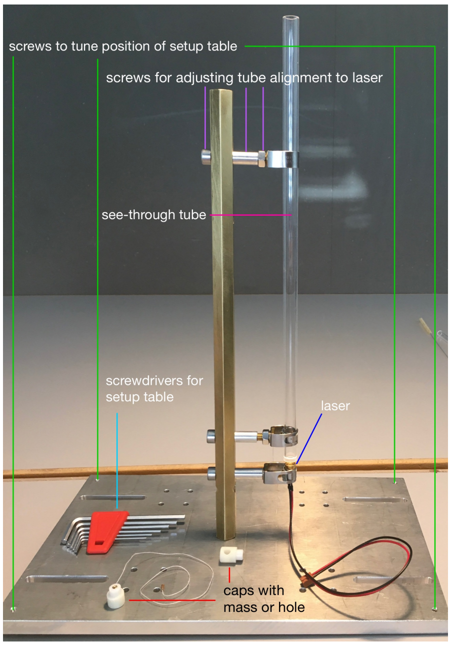

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Figure 3: The setup used for determining the lycopodium mass and a description of its components.

on top and one on the side (cap B). The scattered light from the falling particles is captured by the Pi camera.

The idea of this measurement is to take a picture of falling lycopodia illuminated by a pulsed laser. Since the camera is necessarily exposed for a certain duration of time (called exposure time) the illumiated falling lycopodia is seen as a trail in the picture. By pulsing the laser, one obtains a segmented instead of a straight line. From the pulse duration Δt and the length Δs of a segment, one can calculate the velocity v of the falling particle as $v = \Delta s/\Delta t$. If the tube is long enough, the particle reaches its terminal velocity before being recorded by the camera.

Task 14. Laser alignment

> It is crucial to assure that the spores are well illuminated. For this cap B is inserted into the tube. It has a small hole in the middle of its top. Adjust the laser and the orientation of the tube using the screws of the tube fixture (indicated in Figure 3) such that the laser shines exactly through the small hole of the cap. As one should avoid directly looking at the laser, the spot illuminated on the ceiling by the laser light can be used as reference. Tweak the screws in order to maximize the light that shines through the opening.

Task 15. Adjusting the setup such that the direction of gravity is along the laser beam.

In order to do this, cap A is inserted onto the tube. The string is aligned along the direction of gravity. Adjust the inclination of the pedestal by tweaking the screws at the corners (see Figure 3) until the weigh at the end of the string is right in front of the laser output.

Task 16. Setting up the Picamera and laser

Leave cap A in the tube, and focus the Picamera on the lower end of the string, such that part of the cylindrical weight is also visible in the frame. The diameter of the weight is 2 mm and is used as a reference length. Set the exposure time of the camera to 500 ms. You might need to change the frame rate to accept this long exposure time. Set the laser period and the duty cycle such that we can capture at least 2 bright segments in each image. The duty cycle is the percentage of one period T during which the laser is turned on. For example with $T = 1$s and 50 % duty cycle, the laser is on for 0.5 s and then off for the other 0.5 s. Take a picture of the pendulum for later reference.

Task 17. Measure terminal velocity

Replace cap A by cap B on top of the tube. Turn on the laser and the camera. Turn off the room light for better visibility. Drop the lycopodium spores through the side hole of cap A. Take screenshots of any camera pictures which feature trails. You might want to change the period T and the duty cycle for better images. *Hint*: It might be challenging to capture the right frames. You can use screen record software such as Game Bar on Windows to record the falling particles and afterwards select the appropriate frames for data processing.

Calculate the terminal velocity of the lycopodium spores. Calculate the Reynolds number

$$Re = \frac{2\rho v_T R}{\mu}, \tag{9}$$

that quantifies the balance between turbulent and viscous effects in the air flow around the falling spore, and comment on the validity of Eq. (6).

Task 18. Estimation of average charge

Calculate the average mass of a spore using Eq. (7). From Section 3.1, estimate the charges of the trapped lycopodium spores.

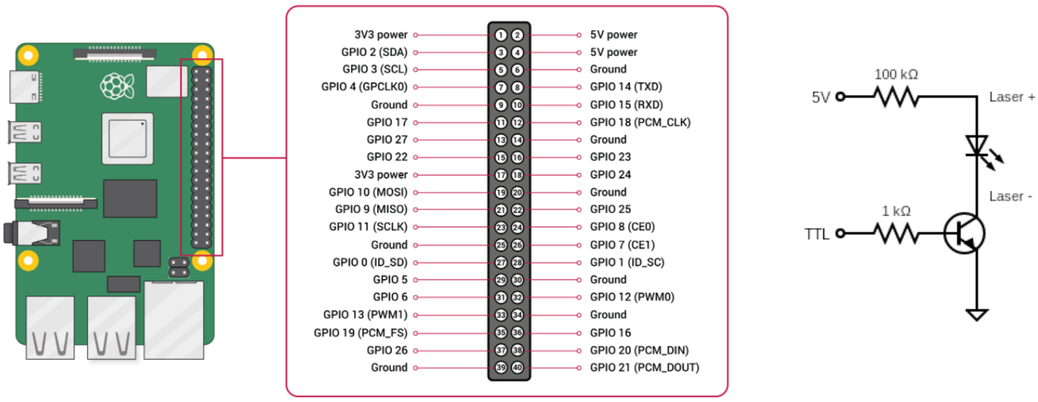


Figure 4: Raspberry Pi GPIO pinout and laser driver circuit.

Assume that the spore is a smooth sphere. Estimate the electric field at the spore surface. Compare with the breakdown electric field of air of about 3000 V/mm.

3.3 Raspberry Pi

A Raspberry Pi, in simple words, is a low cost linux PC with extended capability of executing different communication protocols. In this experiment, we used a RPi to control the laser and the Picamera.

The Pi operates as a headless system, i.e., without any interactive devices such as monitor, mouse and keyboard. It runs a Wi-Fi hotspot which allows for remote control via a SSH (secure shell) protocol from any machine (laptop, phone) in the same network. For more convenience, a SSH server can be accessed either from a SSH client or a web browser, and web-based file browse and text editor allows to easily transfer and edit files on the RPi.

Task 19. Contact the TA to obtain the necessary login credentials.

3.3.1 Laser control

The laser module is basically a light emitting diode powered by a 5 V pin from the RPi via a current limiting resistor. The driving circuit is a current-driver NPN transistor controlled by a TTL signal from the RPi, i.e., a two-level voltage signal corresponding to a logical high-low signal. For periodical signals, it is convenient to use the Pulse Width Modulation (PWM) function.

There are two ways to generate a PWM signal: a software based and a hardware based. The former uses a software library to time the pulses and can generate PWM on any GPIO (General Purpose Input/Output) pin. The latter can be done on a certain pins which are wired to a built-in oscillator as a reference to time keeping. WiringPi is a widely used GPIO interface library that provides both software and harware PWMs.

Task 20. Write a Python script to generate a 50 Hz pulse train at 50% duty cycle using software and hardware PWMs. Observe the generated signals on the oscilloscope and compare the two methods.

> *Hint*: A Python wrapped package of WiringPi has been installed on the RPi. Ask the TA if you have any problem importing the module.
>
> The main power line is a very stable 50 Hz source. You may want to trigger the oscilloscope on the AC line. Please refer to the `http://wiringpi.com` and `https://github.com/WiringPi/WiringPi-Python` for more information on the library as well as necessary commands.

Task 21. Correctly connect the laser to the driver circuit and to the RPi. Check the correct pins on the GPIO header. See Fig. 4 and the official RaspberryPi documentation for reference.

3.3.2 Camera control

A Picamera is a camera module designed to be easily connected and controlled by a RPi. Here we use it with a custom lens mount suited to image the small subjects of this experiment. By screwing the lens tube, one can change the focus and the magnification of the camera.

To simplify the task, a web interface has been set up where the laser and the camera can be controlled via any web browser running on a laptop or cell phone connected to the same network.

Task 22. Ask the TA for the IP address and play around with the web interface.

Note: Please shut down the RPi before removing the power after use. Use either `sudo poweroff` or the Shutdown button on the web interface to shut down the RPi. Wait a few seconds until the LEDs on the RPi stop blinking before you remove the power.

3.4 Safety

3.4.1 Laser

Since the laser light is in the visible range and its power at 1mW, it should not pose any serious danger. Still, it would be advised for the experimenters not to wear any jewellery or arm watches, since those could reflect the laser light. Also, it should be made sure that the end of the laser beam is blocked, so that the light cannot leave the table.

3.4.2 Electric Current

In order to reduce the current which would flow in case an experimentator touches the electrodes, a safety box is being used. A configuration of the safety box is schematically shown in Figure 5.

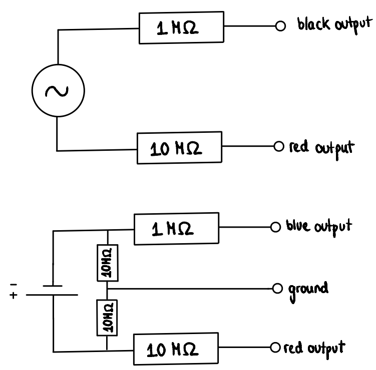


Figure 5: Sketch of safety box which is used to limit the current.

In Figure 6, different scenarios where the experimentator touches an electrode are shown.

Task 23. What is the maximum current which flows through the experimentator's body in Figure 6?

> For the calculation, assume that the human body has a resistance of 0 Ohm and that no current flows in direction of the open circuit elements. These assumptions are not true, but nonetheless yield an upper boundary for the current through the experimentators body, which is the quantity we are interested in. Furthermore, assume that the maximum AC (DC) voltage is 220V (90V). Is the current below the safe limit of 1mA?

We do **not** recommend that you test physically whether your calculation is correct.

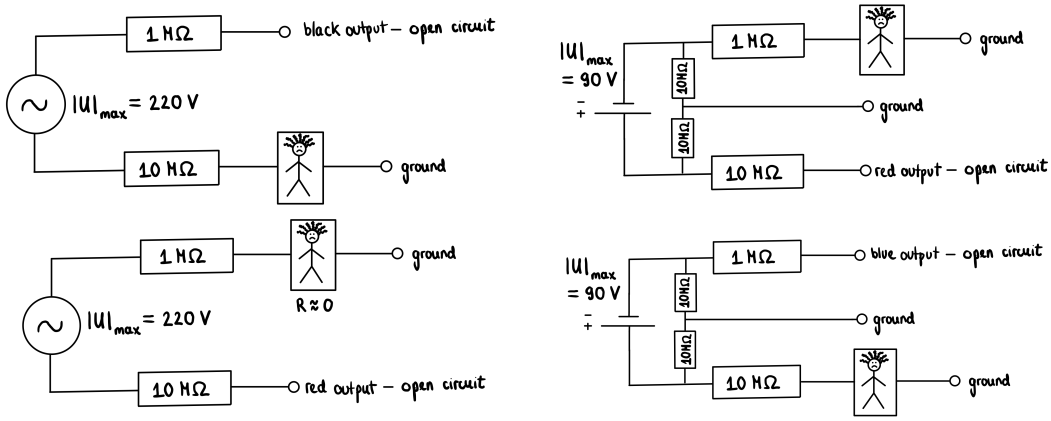


Figure 6: Sketches of four possible circuits resulting from an experimentator touching an electrode.

References

[1] D. R. Denison. "Operating Parameters of a Quadrupole in a Grounded Cylindrical Housing". In: *Journal of Vacuum Science and Technology* 8.1 (1971), pp. 266–269. DOI: 10.1116/1.1316304. eprint: https://doi.org/10.1116/1.1316304. URL: https://doi.org/10.1116/1.1316304.

A Appendix

A.1 Scaling with trap geometry

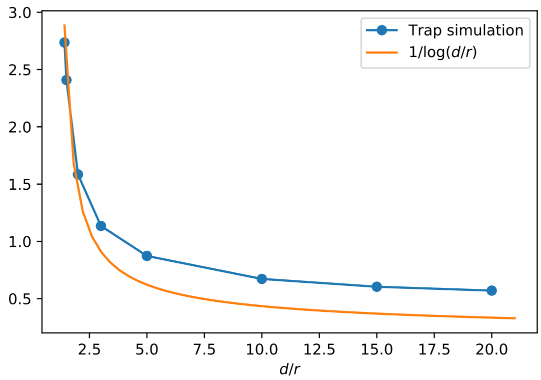
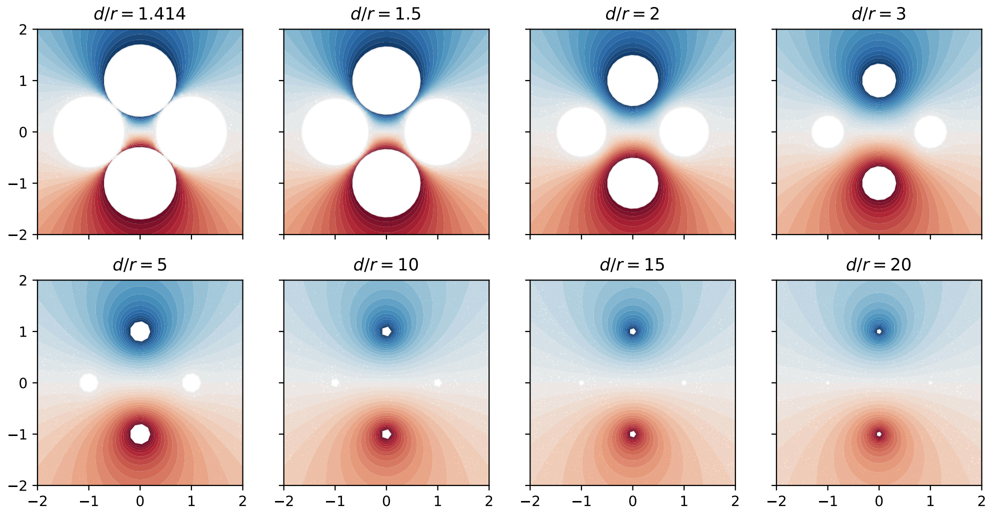
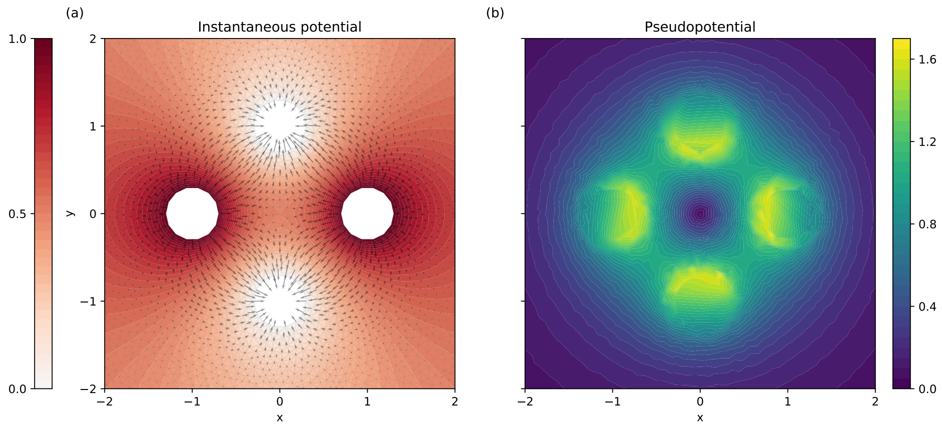


Figure 7: Scaling factor for our trap configuration (simulated data) and for the single rod electrode.

A.2 FEM simulations



(a) Gallery of trap FEM simulations



(b) Instantaneous potential given by the AC electrodes and pseudopotential.