Chapter 2

System Design

Before making an operational experimental apparatus, a thorough design phase is necessary to get the required performance. Our current system is a functioning ion trap apparatus and this chapter describes the efforts that went into designing the setup. In the first section, we shall go through the design of the ion trap and in the second section, we will discuss the design of the vacuum system that houses the trap.

2.1 Trap design

The trap design closely follows the design in [40]. Here we have a designed a linear Paul trap to confine charged Yb^+ ions. figure 2.1 shows the geometry of the trap. In this section, we will cover the theory behind trapping charged particles using radiofrequency potentials. Once the adequate fundamentals have been discussed we shall discuss the simulations of the ion trajectory in the designed trap.

2.1.1 Trapping fundamentals

A static potential cannot be confining in all three directions. The solutions of the Laplace equation have the property that the potential at any given point can be obtained by

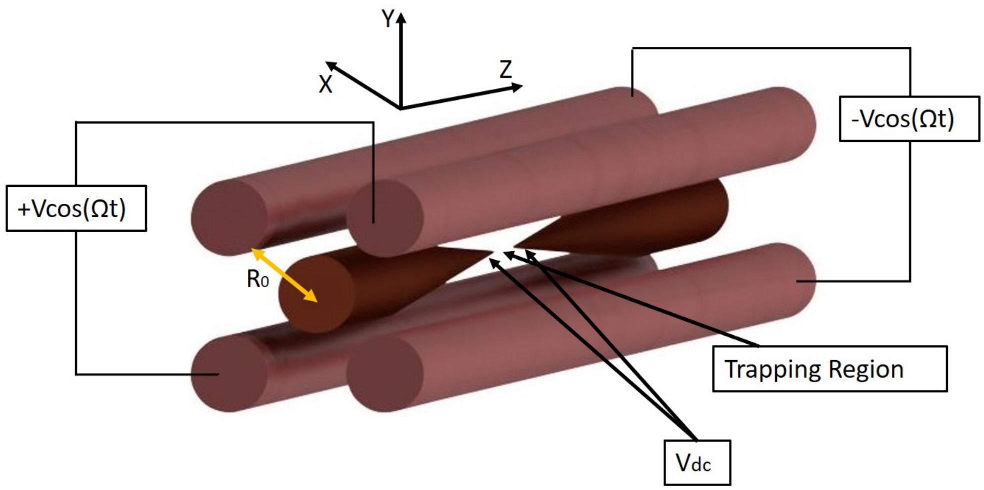

Figure 2.1: 4 rod trap schematic
The diameter of each rod is 0.5mm and the value of $R_o = 0.46$mm. The value of Ω for our design is $2\pi\times$ 22 MHz and typical values of RF amplitude V and V$_{dc}$ are 100-200V and 20-100V respectively.

averaging the potential on a sphere around it. This property makes it physically impossible to then have a potential minimum in all 3 directions. This is the famous theorem due to Earnshaw [12]. One way around this is using additional magnetic fields (Penning Traps). Another approach is to use a time-dependent potential (Paul traps). Wolfgang Paul and Hans Georg Dehmelt were both awarded the Nobel prize in 1989 for their contributions in the development of these devices. Though the penning trap achieves robust confinement of charged particles, these particles are under a constant $v \times B$ force due to the magnetic field. For this reason, the entire ion crystal rotates inside the trap at the cyclotron frequency. The RF paul trap does not have this drawback and hence most trapped ion quantum information experiments make use of time-dependent potentials for trapping charged particles. In our experimental setup we do have magnetic field coils but these are to define the quantization axis of the system and not for trapping.

The basic principle behind the working of the Paul trap is that even though a static potential minimum cannot be created, a static potential saddle can be. A particle which

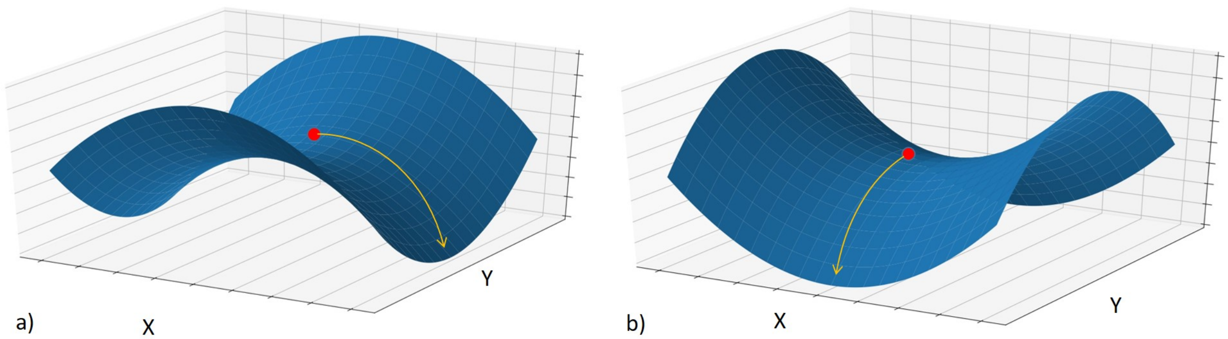

Figure 2.2: Trapping with an oscillating saddle
a)Trapping in X and anti-trapping in Y b) Trapping in Y and anti-trapping X.

is near the saddle point of this potential would experience a confining force in one of the direction and an anti-confining force in the perpendicular direction. Given some initial kinetic energy, the particle would start to 'roll off' from the saddle point along the anti-confining direction. At this moment if the potential is changed such that the confining and anti-confining directions are swapped the particle tends to 'roll off' again but in a different direction. Also, it is confined in the direction it was initially trying to roll off. This swapping of the directions of confinement can lead to the trapping of the particle near the saddle point of the potential. In practical traps, the swapping of the potential is not ON/OFF as described in the above discussion. Rather switching comes from multiplying the static potential with a sinusoidal function of time. The frequency of this is called the drive frequency Figure 2.1 shows a graphical description of an oscillating saddle.

From the crude model discussed above it can be said that the potential seen by the particle is 'on an average' a trapping potential. The average trapping potential here is called the **pseudopotential**. The particle executes simple harmonic motion about the minima of the pseudopotential. The motion/oscillation of the particle subject to the pseudopotential is called the **secular motion**. Also evident from the discussion above is the fact that the motion of the trapped particle would also have a component at the drive frequency. This motion is the fast oscillations of the particle about the secular motion. It is known as the **micromotion**. Figure 2.3 shows a simulated trajectory for a paul trap. One can see the

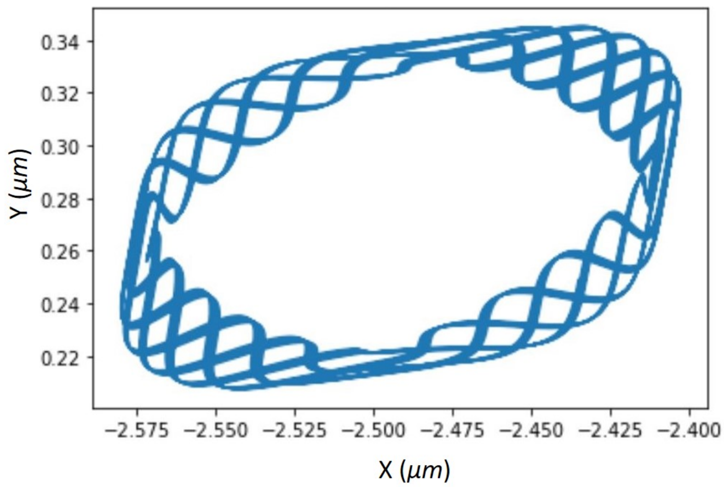

Figure 2.3: Simulated trajectory for a trapped Yb^+ particle in a RF paul trap.

secular motion with added micromotion on top of it. These are just for illustration, more on the simulation in the coming sections.

An obvious question that arises at this moment is what electrode geometry can create a saddle potential? if one can create the static potential in the shape of a saddle then adding the time dependence is just a matter of applying time-dependent voltages to the electrodes. We shall stick to creating a saddle potential along the XY plane and using a static potential for confining in the Z direction[1]. This best describes the mode of operation of the linear Paul trap.

The equation depicting a saddle potential in the XY plane is

$$\phi(x, y) = \alpha(x^2 - y^2) \tag{2.1}$$

From this, it is easy to guess that the ideal electrode cross-section in the XY plane should be hyperbolic. Though it is doable in principle, it is difficult to fabricate electrodes with a hyperbolic cross-section. A very good approximation is a circular cross-section. This is because the potential near the center of the trap is still approximately hyperbolic. Figure 2.1 shows the design of the 4-rod trap used in this work. On each pair of the diagonal

[1]This does not violate the Earnshaw's theorem.

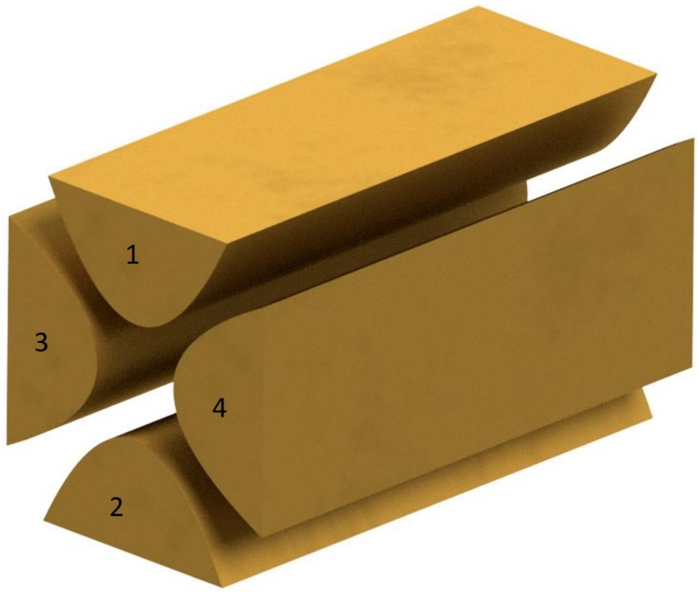

Figure 2.4: The ideal paul trap with hyperbolic electrodes

electrodes is applied a radio-frequency potential such that they oscillate out of phase with each other. This provides an oscillating saddle potential in the XY plane. The Z-axis confinement is provided by needle electrodes by applying a positive voltage V_{dc} to these.

Let us now derive the potential between the electrodes when the electrode cross-section is hyperbolic as shown in figure 2.4. Since the electrodes have a translational symmetry along the z-axis it would suffice to work in the z = 0 plane. The contours defining each of the electrodes is

$$\frac{x^2 - y^2}{R_o} = \pm 1 \tag{2.2}$$

where plus sign denotes the electrodes 1,2 and the minus sign denotes the electrodes 3,4. The boundary conditions for our solution are given by the potentials on these electrodes. We have +V/2 volts on the diagonal pair 1,2 and -V/2 volts on the diagonal pair 3,4. It is easy to check that the potential between the electrodes is given by

$$\phi(x, y) = \frac{V_o}{2R_o^2}(x^2 - y^2) \tag{2.3}$$

When we apply oscillating potentials to the diagonal pairs of electrodes the time dependent potential is given by

$$\phi_{hyp}(x, y, t) = \frac{V_o}{2R_o^2}(x^2 - y^2)cos(\Omega t) \tag{2.4}$$

We will make use of this in the following sections for the derivation of the pseudopotential seen by the ion and for finding the equation of the trajectory of the ion motion.

The Pseudopotential

There is a slick method for finding the secular motion of a particle in a high-frequency electric field. This method combines ideas from [28] and [15]. Let the field experienced by a particle be given as

$$E(r, t) = E_o(r)cos(\Omega t) \tag{2.5}$$

We can write the Taylor expansion of this up to the first order about a point r_o as follows.

$$E(r, t) = E_o(r_o)cos(\Omega t) + (r - r_o) \cdot \nabla E_o(r_o)cos(\Omega t) \tag{2.6}$$

The force experienced by a particle with charge q in such a field is given as

$$m\ddot{r} = qE(r, t) = q\Big(E_o(r_o)cos(\Omega t) + (r - r_o) \cdot \nabla E_o(r_o)cos(\Omega t)\Big) \tag{2.7}$$

defining r_o, r_1 such that $r = r_o + r_1$, we can split the above equation into two parts.

$$m\ddot{r}_1 = qE_o(r_o)cos(\Omega t) \tag{2.8}$$

and

$$m\ddot{r}_o = qr_1 \cdot \nabla E_o(r_o)cos(\Omega t) \tag{2.9}$$

r_1 can be thought of as being the excursion about the mean position r_0. Hence r_1 can be thought of as the micromotion component of the motion and r_o can be thought of as the secular motion. equation 2.8 just says that the micromotion is dependent on the electric field at that point. Integrating this we can solve for r_1

$$r_1 = -q\frac{E_o(r_o)cos(\Omega t)}{m\Omega^2} \tag{2.10}$$

Substituting this in equation 2.9 we get that

$$m\ddot{r_o} = -\frac{q^2 E_o(r_o) \cdot \nabla E_o(r_o)}{m\Omega^2}cos^2(\Omega t) \tag{2.11}$$

we can use the formula

$$E \cdot \nabla E = \frac{\nabla E^2}{2} - E \times (\nabla \times E)$$

in equation 2.11 to get

$$m\ddot{r_o} = -\frac{q^2 \nabla E_o^2}{2m\Omega^2}cos^2(\Omega t) \tag{2.12}$$

Here we have set the term $E \times (\nabla \times E) = 0$ in the quassistatic approximation. let us define $< r_o(t) >= \int_{t-\tau}^{t} dt' r(t')$[2], where τ is the time period corresponding to the drive frequency Ω. equation 2.12 then becomes

$$m < \ddot{r_o} >= -\frac{q^2 \nabla E_o^2}{4m\Omega^2} \tag{2.13}$$

Where we have replaced $cos^2(\Omega t)$ by it's average 1/2.
This tells us that averaged over the time period of the drive frequency Ω, the force felt by the ion is given by

$$F_{avg} = -\nabla\frac{q^2 E_o^2(r)}{4m\Omega^2} \tag{2.14}$$

[2]This basically amounts to averaging out the high frequency oscillations.

Hence Pseudopotential that describes the secular motion of the ion is given as

$$\boxed{\phi_{ps} = \frac{q^2 E_o^2(r)}{4m\Omega^2}} \tag{2.15}$$

Note that this is the **mechanical potential** seen by the particle and not the electrical potential. ϕ_{ps} has the dimensions of energy and not voltage.

Deriving the secular motion

Now that we have derived the formula for the pseudopotential we can use it do derive the secular motion in the trap. equation 2.4 gives the exact form of the potential for electrodes with a hyperbolic cross-section. We saw earlier that the circular electrodes approximate the hyperbolic potential quite well near the trap center. Hence we can write the potential for the 4-rod trap with circular electrodes as

$$\phi_{circ}(x, y, t) = \eta \frac{V_o}{2R_o^2}(x^2 - y^2)cos(\Omega t) \tag{2.16}$$

Here the fudge factor η accounts for the deviation from the hyperbolic geometry. The electric field generated by this potential is

$$\begin{aligned} E(x, y, t) &= -\nabla \phi_{circ} \\ &= \frac{-\eta V_o}{R_o^2}(x\hat{x} - y\hat{y})cos(\Omega t) \\ &= E_o(x, y)cos(\Omega t) \end{aligned} \tag{2.17}$$

Using the formula for the pseudopotential we can write the equations of motion as

$$m\ddot{x} = -\frac{q^2 \eta^2 V_o^2}{2m\Omega^2 R_o^4} x \tag{2.18}$$

A similar equation of motion is derived for y as well. It is clear from the form of the equation that this the equation of motion of a Harmonic Oscillator. The angular frequency is then given as

$$\omega_x = \omega_y = \frac{1}{\sqrt{2}}\frac{q\eta V_o}{m\Omega R_o^2} \tag{2.19}$$

This is known as the secular frequency.

Deriving the micromotion

From equation 2.17 we can write the actual equation for motion of the ions in the XY plane as:

$$\begin{aligned} \ddot{x} + \frac{q\eta V_o}{mR_0^2}cos(\Omega t)x = 0 \\ \ddot{y} - \frac{q\eta V_o}{mR_0^2}cos(\Omega t)y = 0 \end{aligned} \tag{2.20}$$

with substitutions $\Omega t = 2\tau$ and $q_{x/y} = \mp\frac{2q\eta V_o}{m\Omega^2 R_O^2}$ we can rewrite these as :

$$\frac{d^2x}{d\tau^2} - 2q_x cos(2\tau)x = 0 \tag{2.21}$$

$$\frac{d^2y}{d\tau^2} + 2q_y cos(2\tau)y = 0 \tag{2.22}$$

These are just the Mathieu equations with a = 0. The canonical form of the Mathieu equation is

$$\frac{d^2u}{d\tau^2} + \big(a_u - 2q_u cos(2\tau)\big)u = 0 \tag{2.23}$$

The general solution (stable) for the Mathieu equation can be written in terms of even and odd periodic functions as follows [16]

$$u(\tau) = \sum_{n=-\infty}^{n=\infty} \alpha_1 C_n cos\big((2n \pm \beta)\tau\big) + \alpha_2 C_n sin\big((2n \pm \beta)\tau\big) \tag{2.24}$$

We can see that the lowest frequency term (n = 0) in the solution is

$$\omega_0 = \beta\tau \tag{2.25}$$

the next order terms (n = 1) give the frequencies

$$\begin{aligned} \omega_{+1} &= (2 + \beta)\tau \\ \omega_{-1} &= (2 - \beta)\tau \end{aligned} \tag{2.26}$$

The lowest frequency term here corresponds to the secular motion of the ion and the higher-order terms give the micromotion. We shall limit ourselves to only the first order and look for an approximate solution for the equation 2.21 as follows:

$$x(\tau) = 2C_0 cos(\beta\tau) + C_1\big[cos((2 + \beta)\tau) + cos((2 - \beta)\tau)\big] \tag{2.27}$$

Note that this is an even solution and the odd solution can be done in the same way.

From our previous analysis, we already have an expression for the secular motion in equation 2.18. Comparing equation 2.18 and equation 2.24 and from the definition of q_x we have

$$\beta = \frac{q_x}{\sqrt{2}} \tag{2.28}$$

substituting equation 2.27 in equation 2.21 we get

$$\begin{aligned} -2C_o\beta^2 cos(\beta\tau) - C_1[(2+\beta)^2 cos((2+\beta)\tau) + (2-\beta)^2 cos((2-\beta)\tau)] = \\ 2C_o q_x[cos((2+\beta)\tau) + cos((2-\beta)\tau)] + 2C_1 q_x cos(\beta\tau) + \\ C_1 q_x[cos((4+\beta)\tau) + cos((4-\beta)\tau)] \end{aligned} \tag{2.29}$$

The most dominant term here is the term with $cos(\beta\tau)$. Hence comparing the coefficients on boh sides we get

$$\frac{-C_1}{C_0} = \frac{\beta^2}{q_x} = \frac{q_x}{2} \tag{2.30}$$

substituting this back in equation 2.27 we get the equation of motion in the X direction

$$x(\tau) = 2C_o cos(\beta\tau)[1 - \frac{q_x}{2} cos(2\tau)] \tag{2.31}$$

Similar equation can also be derived for the motion in the y direction. Substituting back the values of q_x, q_y, β, τ the equation of motion in the x and y direction can be written as

$$\begin{aligned} x(t) &= C_x cos(\omega_x t + \phi_x)[1 - \frac{q_x}{2} cos(\Omega t)] \\ y(t) &= C_y cos(\omega_y t + \phi_y)[1 + \frac{q_y}{2} cos(\Omega t)] \end{aligned} \tag{2.32}$$

Where C_x, C_y, ϕ_x, ϕ_y given by the initial conditions.

Based on the analysis above we can draw some important conclusions about the motion of the ions in the trap:

- The dominant frequency comprising the motion of the ion is the secular frequency $\omega_{x/y}$. The fast oscillations i.e. the micromotion is at the frequencies $\Omega - \omega_{x/y}$ and $\Omega + \omega_{x/y}$.
- The micromotion increases as the ion moves further from the center of the trap. This makes the ion's motion very susceptible to stray electric fields. Hence there is a provision to apply separate DC voltages on each RF electrode to compensate for the stray fields. The goal is to have the ion confined to the center of the pseudopotential(also known as the RF null)
- The pseudopotential is isotropic i.e. the secular frequency in the x and y direction is the same

2.1.2 Trap simulations

The discussion above is quite sufficient for the design of a 4-rod trap but the fudge factor η in equation 2.16 makes it difficult to predict the exact voltages for the operation of the trap. For this reason, it was decided to simulate the trajectory of a trapped ion in the exact geometry given by the trap.

It may seem like a daunting task to simulate the trajectory of the ions because of the time-dependent electric fields but it is not very complicated. This is because we can use the quasi-static approximation. The drive frequency for the trap is about 22 MHz. The wavelength that corresponds to this frequency is about 13.66m. This is much larger than the scale of the geometry to be simulated. This warrants the use of the quasi-static approximation. Ref[31] is a fantastic review for using the quasi-static approximation. For our purpose, it boils down to the fact that only the potentials at the ion's time step matter, the potentials from times before each time step of the ion do not matter.

To find the trajectories of the ions in the quasistatic approximation, one has to solve an electrostatic problem at each time step of the ion's motion. There are 6 electrodes in this