How to trap an ion

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The goal of this white paper is to outline the basics of trapping an ion from a hardware perspective derived from first principles. The writing is informal and explained simply (at least I hope). At various points, I will provided ion trapping vocabulary given in parenthesis. At at other points, I hope I made you laugh. Mainly, I want to get some reps in with translating my explanation skills to writing.

Ion traps are a near-perfect platform for performing high-precision atomic measurements and suitable for conducting quantum informational studies due to stable trapping potentials and long quantum coherence times. [cit experimental issues here]. Ions have non-neutral charge, resulting in an imposed force due to the electric field, $\vec{F} = e\vec{E}$. Intuitively, we should be able to confine ions using electric fields alone as a result of this force. However, our intuition fails us, and we have to be clever in designing an apparatus that succeeds in stable confinement. It is my goal to walk you through how I would go about designing an apparatus that can faithfully confine an ion.

1 An amateur's attempt to trap an ion

I would like to begin by posing the question: What mathematical "signatures" embedded in our electric potential should we be looking for that would let us know that we have trapped an ion? In the ideal case, an electric potential that has a local minimum in all three spatial directions that is "smooth" and symmetric about this minimum.

To gain intuition, consider trapping an ion in two dimensions. How should we approach writing down the form of the electrical potential? In one direction, a harmonic (quadratic) potential has both a local minimum and is symmetric. A linear combination of harmonic potentials in x and y is a reasonable first guess:

$$\phi(x, y) = A(\alpha x^2 + \beta y^2). \tag{1}$$

To solve for the parameters α and β, we can use Laplace's equation, $\nabla^2\phi = 0$:

$$\nabla^2\phi = 0 = A(\alpha + \beta) \implies \alpha = -\beta. \tag{2}$$

The physical consequence of Laplace's equation here is that the set of parameters needed to achieve a potential whose summed curvature is zero confines in x ($\alpha > 0$) and anti-confines in y ($\beta < 0$). We can rewrite this potential as

$$\phi(x, y) = A(x^2 - y^2), \tag{3}$$

where $\alpha = 1$ and $\beta = -1$. This is the functional form of a generic quadrupole potential.

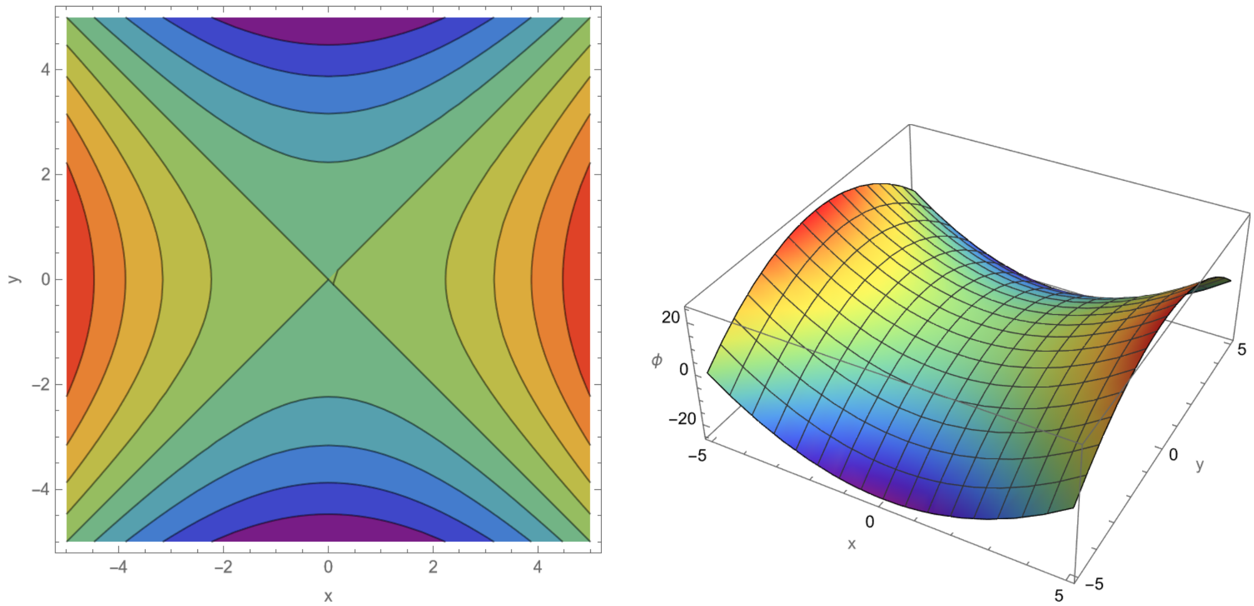

Figure 1: (a) A contour plot of (3). (b) A 3D plot of (3) ($A = 1$). Both figures here show that the potential confines in the x-direction and anti-confines in the y-direction. ($A = 1$)

A keen eye can immediately spot the issue in Figure 1. If we were to place an ion at the center of the saddle, it would be confined only in the x-direction and fall down the saddle along the y-direction. Formally, (3) satisfies Laplace's equation, however, it is not symmetric about a local minimum. Therefore, we cannot trap an ion in 2D using electrostatic potentials.

Extending this idea to three dimensions results in the same conclusion– the only way Laplace's equation can be satisfied using static potentials is if the parameters that define the potential are a combination of positive and negative values:

$$\phi(x, y, z) = A(\alpha x^2 + \beta y^2 + \gamma z^2) \tag{4}$$

$$\nabla^2 \phi = 0 = A(\alpha + \beta + \gamma) \implies \alpha = -(\beta + \gamma) \tag{5}$$

A valid solution can be found by letting $\alpha = 2$ and $\beta = \gamma = -1$, giving

$$\phi(x, y, z) = A(2z^2 - x^2 - y^2). \tag{6}$$

The key takeaway here is that electrostatic potentials cannot contain local minimums. Meaning, charged particles cannot be trapped using static electric potentials. This is known as Earnshaw's Theorem.

This exercise is not for nothing. Can we use what we've learned so for to come up with an approach that allows us to achieve our dreams of trapping an ion? Equations (3) and

(4) say that we can confine in a singular direction while anti-confining in the remaining directions. If we could superimpose the two equations and vary the confinement between the two directions in (3) while maintaining the single-direction confinement in (4) and ensuring that this "varying" confinement is larger than the anti-confinement provided by (4), this should, in theory, confine an ion in three dimensions. Mathematically, our potential would have the form

$$\phi(x, y, z) = A(x^2 - y^2)f(\vec{k}) + B(2z^2 - x^2 - y^2). \tag{7}$$

Where $A > B$ and $f(\vec{k})$ is some function that depends on a set of parameters, $\vec{k}$. These parameters could have spatial and/or temporal dependence.

Note: Eearnshaw's Theorem also holds in one dimension. Additionally, if we lived in a N-dimensional universe, where $N > 3$, Earnshaw's theorem is still valid! Sorry to disappoint the $N > 3$-dimensional aliens out there.

2 A professional's attempt to trap an ion

How do we approach constructing an apparatus in the lab that applies the correct electric potential? I would like to discuss the process of going from equations to hardware.

Equation (3) corresponds to a generic electric quadrupole potential. Although not realistic in a lab setting, we know that having four charges with alternating signs at the corners of a square produces this potential. However, it does provide a stepping stone to an apparatus that can be constructed in the lab– situating four conducting rods at the corners of a square with alternating voltages (Figure 2) with boundary conditions

$$\phi(R, 0) = -V_o/2, \quad \phi(-R, 0) = -V_o/2 \tag{8}$$
$$\phi(0, R) = V_o/2, \quad \phi(0, -R) = V_o/2. \tag{9}$$

In general, going from an explicit electrode geometry to solving Laplace's equation can be difficult, especially for more involved electrode geometries and boundary conditions. Instead, we can make a qualitative guess on what the potential should look like, solve for parameters using our boundary conditions, and then use the Uniqueness Theorem to guarantee that our solution is the correct one.

We can begin by noticing the symmetry of the electrode geometry. The potential will be constant along the z direction, making this a 2D problem (independent of z). We know from the previous section that the potential must be symmetric. This puts a restriction on the form of the potential– only even powers are allowed, making (3) a valid ansatz.

We can solve for the coefficient A by plugging in the boundary conditions into our ansatz:

$$(a) \quad \phi(R, 0) = -\frac{V_o}{2} = AR^2 \tag{10}$$
$$(b) \quad \phi(0, R) = \frac{V_o}{2} = -AR^2. \tag{11}$$

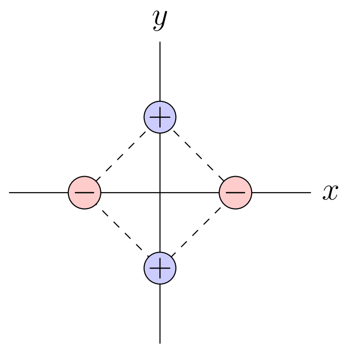

Figure 2: A cross-section of four rods situation at $(R, 0), (0, R), (-R, 0), (0, -R)$.

Subtracting (a) and (b) gives

$$A = \frac{V_o}{2R^2}. \tag{12}$$

Plugging A back into (3) results in

$$\phi(x, y) = \frac{V_o}{2R^2}(x^2 - y^2). \tag{13}$$

By the Uniqueness Theorem, since (13) satisfies Laplace's equation and matches our boundary conditions, then it is a valid solution!

Now, we need to modify our potential slightly so that it confines in both x and y. What would be nice is if we could switch the confinement between spatial directions in such a way so that on average the potential appears to have a local minimum. How (13) is currently written, it assumes that some DC voltage is applied to the rods. Instead, let's apply an AC voltage to our rods driven at a frequency of Ω_{rf}:

$$\phi_{rf}(x, y) = \frac{V_o \cos(\Omega_{rf} t)}{2R^2}(x^2 - y^2). \tag{14}$$

Figure 3 shows a single period, $2\pi/\Omega_{rf}$, of cosine driven at a frequency of 25 MHz. During the first half period, the overall sign is positive, resulting in $x^2 - y^2$ in (14). During the second half period, the overall sign is negative, giving $-x^2 + y^2$. Physically, this means that the potential is oscillating between confinement and anti-confinement at a frequency of Ω_{rf}. It should be noted that drive frequency, ω_{rf}, depends on the ion. For reference, in our lab we trap Yb171 and apply a drive frequency of around 25 MHz.

If you are anything like me, the statement "switch the confinement between spatial directions in such a way so that on average the potential appears to have a local minimum" comes across as vague when looking at (14). Against my better judgment, this will be addressed in the next section, and I will hopefully convince you that on average this potential appears to have a local minimum. Shown in Figure 4 is a cross-section of (14) at $t = 0$ and $t = T/2$. This shows the potential switching its maximal confinement every half-period, π/Ω_{rf}.

Okay great, we have found that applying alternating voltage to four parallel rods results in (suspected until next section) two dimensions of confinement for an ion. If we were to

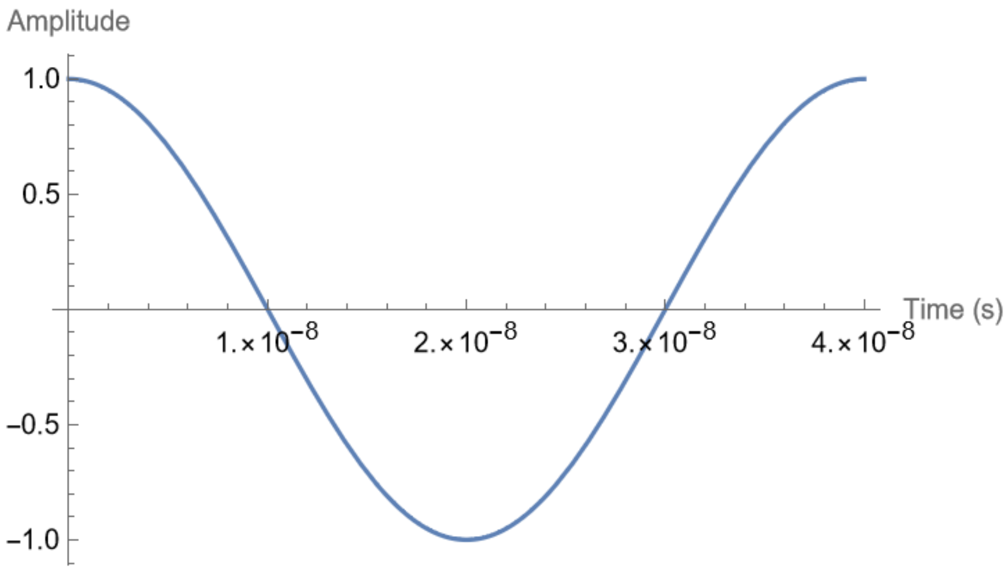

Figure 3: The ion dynamics in the radial plane with an RF potential driven at 25 MHz and 300 Volts. The amplitude of oscillation has been set to unity with geometric parameters, R, z_o being set to 460 and 335 μm respectively. DC needles (U_o) are set to 1 Volt.

build this in a lab and try to trap an ion, we would observe that the ion would be trapped in the xy plane (radial/RF plane). However, the ion would be able to move freely along the z-direction (axial direction). We can "plug" this direction with two additional rods separated at some distance, $2z_o$. This will act like a capacitor, where voltage goes like $V \propto \text{Area}^{-1}$. Since we want as much voltage as possible from our rods, we can taper the ends and turn them into needles, making its area smaller, resulting in a larger voltage between the two electrodes. Without going through the details, since the approach of plugging in boundary conditions is similar to the one above, the potential will be of the form

$$\phi_{DC} = \frac{\kappa U_o}{2z_o^2}(2z^2 - x^2 - y^2). \tag{15}$$

Where U_o is the DC voltage applied to the electrodes, κ is a geometric constant of order unity, and z_o is the distance from the needle's tip to the center of the needle spacing (where the ion will ideally reside). Figure 5 shows the apparatus. This gives us three dimensions of confinement with a total potential of

$$\phi(x, y, z) = \frac{V_o \cos(\Omega_{rf} t)}{2R^2}(x^2 - y^2) + \frac{\kappa U_o}{2z_o^2}(2z^2 - x^2 - y^2). \tag{16}$$

The apparatus that produces these potentials is known as a Linear Paul Trap. It provides stable trapping by applying oscillating and static electric fields to electrodes. It is worth noting that the rod and needle (rod trap) approach is not unique. Typically, labs use more sophisticated electrode geometries for daily drivers, such as the traps used in our lab: segmented wafer electrodes or segmented blade electrodes. Rod traps are an intuitive use case for learning the basics of how to trap ions. However, they have been phased out for electrode structures that can be machined with higher machining tolerances. This allows

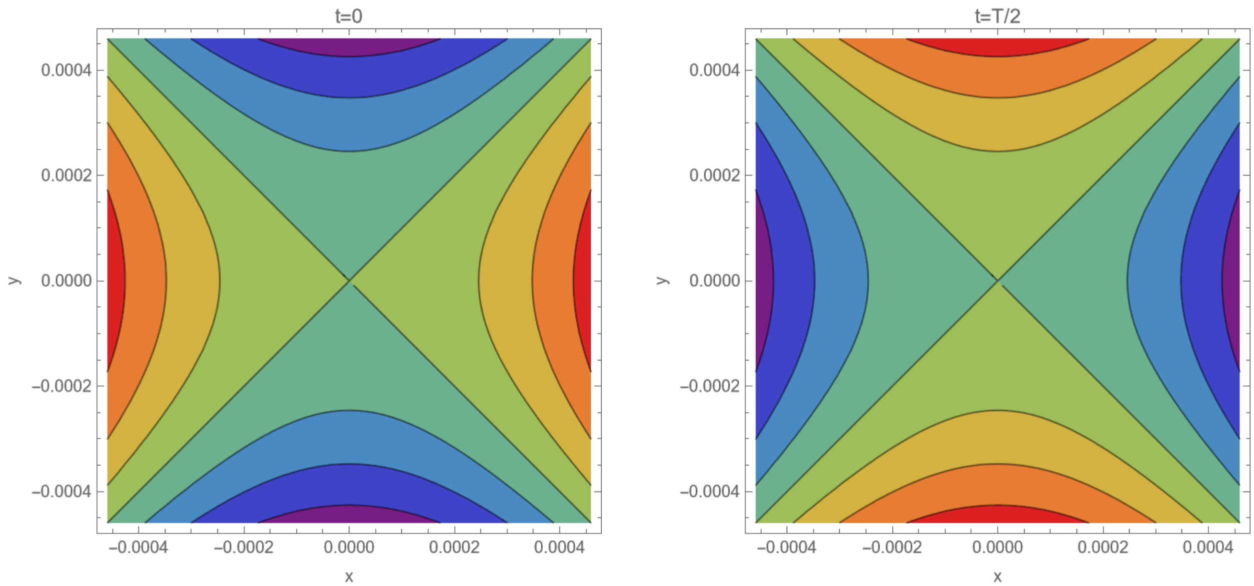

Figure 4: Contour plots of (14). (a) $t = 0$ (b) $t = T/2$. Parameters here include $\kappa = 1$, $R = 460\mu$m, $z_o = 350\mu$m, $V_o = 300$V, $U_o = 1$V, and $\Omega_{rf} = 25$MHz.

Figure 5: Four conducting rods that confine an ion in the radial plane and two needles that confine the ion in the axial direction. Typically constructed from stainless steel, the machining tolerance of the needle's taper and relative placement will heavily influence the symmetry of the axial potential.

for more symmetric trapping potentials which can minimize negative side effects such as ion heating. In some cases, more sophisticated electrode geometries can increase the control of the axial potential's shape, which directly affects the ion spacing.

3 What does the ion feel?

From first principles, we have designed an apparatus that can be implemented in the lab that can trap ions. We are now suited to ask the question: How will an ion behave in a trap? First, we will solve the ion's equation of motion in full glory. This will motivate an approximation known as the "Pondermotive Approximation" that can be used in gaining an intuitive picture of the physics. Hopefully by the end of this section, you will be convinced that we have successfully trapped an ion at a local minimum, circumventing Earnshaw's Theorem.

We know that an ion in the presence of an electric field will feel a force:

$$\vec{F} = m\ddot{\vec{r}} = e\vec{E}(\vec{r},t) = -e\vec{\nabla}\phi(\vec{r},t). \tag{17}$$

Taking the gradient of our potential gives

$$\vec{\nabla}\phi(\vec{r},t) = \frac{V_o cos(\Omega_{rf}t)}{R^2}(x\hat{x} - y\hat{y}) + \frac{\kappa U_o}{z_o^2}(-x\hat{x} - y\hat{y} + 2z\hat{z}). \tag{18}$$

This gives us the following equations of motion:

$$\frac{d^2z(t)}{dt^2} + \frac{2e\kappa U_o}{mz_o^2}z(t) = 0 \tag{19}$$

$$\frac{d^2x(t)}{dt^2} + \frac{eV_o\cos(\Omega_{rf}t)}{mR^2}x(t) - \frac{e\kappa U_o}{mz_o^2}x(t) = 0 \tag{20}$$

$$\frac{d^2y(t)}{dt^2} - \frac{eV_o\cos(\Omega_{rf}t)}{mR^2}y(t) - \frac{e\kappa U_o}{mz_o^2}y(t) = 0. \tag{21}$$

If you're anything like me and you see the equations above, you immediately put your notebook away and begin checking engineering job postings online. Then you remember you chose physics as your career and at second glance you realize that the equations are not coupled and the radial EOM are the same up to a sign. This allows us to solve one of the radial EOM and axial EOM. Not bad!

Equation (19) looks like the ordinary differential equation (ODE) of a harmonic oscillator. We know how to do this by heart, so let's start here. We can rewrite (19) to match the form of a simple harmonic oscillator ODE:

$$\frac{d^2z(t)}{dt^2} = -\omega_z^2 z(t), \tag{22}$$

Where $\omega_z^2 = 2q\kappa U_o/mz_o^2$. This leads to the solution

$$z(t) = A_z\cos(\omega_z t); \quad \omega_z = \sqrt{\frac{2q\kappa U_o}{mz_o^2}}. \tag{23}$$

What this means is that the ion's position in the z-direction has the same behavior as a harmonic oscillator! This allows us rewrite the potential along z as an "effective" harmonic potential (what the ion effectively sees based on its dynamics)

$$\phi(z) = \frac{1}{2}m\omega_z^2 z^2. \tag{24}$$

Unfortunately, (20) and (21) cannot be solved in this manner. As I mentioned earlier, because these two equation's only differ by a sign, we can treat this as a one-dimensional problem and can later be modified to account for the sign difference. At first glance, (20) is a second-order differential equation that has a time-varying term and a static term. You realize that you have never seen an ODE of this form so you begin to panic. You seek comfort in the trapped-ion literature and find that (20) is a special case of the Mathieu equations which has the form

$$\frac{d^2y}{dx^2} + [a + 2q\cos(2x)]\, y = 0. \tag{25}$$

Where q is not to be confused with charge. With the properties of the solution are completely dictated by the dimensionless parameters a and q.

Now we need to match (20) to (25) so we can simply write down the general solution in terms of a and q. To begin, let $2\xi = \Omega_{rf} t$

$$\frac{\Omega^2}{4}\frac{d^2x}{d\xi^2} + \left[-\frac{e\kappa U_o}{mz_o^2} + \frac{eV_o}{mR^2}\cos(2\xi)\right] x = 0. \tag{26}$$

Dividing by $4/\Omega_{rf}^2$ gives

$$\frac{d^2x}{d\xi^2} + \left[-\frac{4e\kappa U_o}{m\Omega_{rf}^2 z_o^2} + \frac{4eV_o}{m\Omega_{rf}^2 R^2}\cos(2\xi)\right] x = 0. \tag{27}$$

If we let $a = 4e\kappa U_o/m\Omega_{rf}^2 z_o^2$ and $q = 2eV_o/m\Omega_{rf}^2 R^2$, we arrive at our destination:

$$\frac{d^2x}{d\xi^2} + [a + 2q\cos(2\xi)]\, x = 0. \tag{28}$$

Recall, the EOM in the radial plane only differs by a sign in the time-varying term. Therefore, only q is affected, resulting in the dimensionless parameters

$$q_x = -q_y = \frac{2eV_o}{m\Omega_{rf}^2 R^2}, \quad a_x = a_y = -\frac{4e\kappa U_o}{m\Omega_{rf}^2 z_o^2}. \tag{29}$$

In the limit that the confinement provided by the static potential (a) is much smaller than the confinement provided by the time-varying potential (q), i.e. $a_i << q_i^2 << 1, i \in \{x, y\}$, we can write down the general solution to first order in a_i and second order in q_i

$$u_i(t) = A_i\left(\cos(\omega_i t + \phi_i)\left[1 + \frac{q_i}{2}\cos(\Omega_{rf} t) + \frac{q_i^2}{32}\cos(2\Omega_{rf} t)\right] + \beta_i\frac{q_i}{2}\sin(\omega_i t + \phi_i)\sin(\Omega_{rf} t)\right). \tag{30}$$

Where $u_i(t) = x(t), y(t)$ and the value of A_i depends on initial conditions. Additionally,

$$\omega_i = \beta_i\frac{\Omega_{rf}}{2}, \quad \beta_i \approx (a_i + q_i/2)^{1/2}. \tag{31}$$

Plugging in $a_{x,y}$ and $q_{x,y}$ into (31) gives the secular frequencies in the radial direction

$$\omega_x \approx \omega_y = \sqrt{\frac{e}{m}\left(\frac{qV_o}{4R^2} - \frac{\kappa U_o}{z_o^2}\right)}; \quad q = \frac{2eV_o}{mR^2\Omega_{rf}^2}. \tag{32}$$

The plot of (30) is shown in Figure 6. We can see that there are two relevant timescales at play. The ion experiences fast oscillations at Ω_{rf} due to micromotion that are small in amplitude. This motion is intrinsic to the experiment and is difficult to suppress. Additionally, the ion experiences a slower oscillation, typically called "secular" motion, that is driven at $\omega_{x,y}$.

If we only consider (30) to zeroth order in q, we see that the ion's dynamics has the same motion as a harmonic oscillator. Therefore, the ion is at rest in the time periods of the secular motion: $(T/2, T, 3T/2, 2T...)$. This can be seen explicitly by taking the time derivative of the ion's motion to zeroth order in q and plugging in the periods listed above. When at rest, the ion is maximally displaced from the origin (RF null), and therefore, the effects of micromotion are more noticeable, as shown in Figure 6.

The effects of micromotion have been studied in great detail [cite papers], some of which include ion heating and effects on atomic transition line shapes. There are two orientations of 2D ion crystals: radial and lateral. Radial crystals are completely defined in the radial $(x-y)$ plane. Lateral crystals are defined by one of the radial axes (x, y) and the axial direction (z). Therefore, it is important that the axial potential's minimum overlaps with the RF null so that experienced micromotion is symmetric across the crystal. 1D chains are typically located along the axial direction. Since the RF null and the axial potential's minimum are overlapped, 1D ion chains directed along the axial potential are less affected by micromotion than 2D crystals.

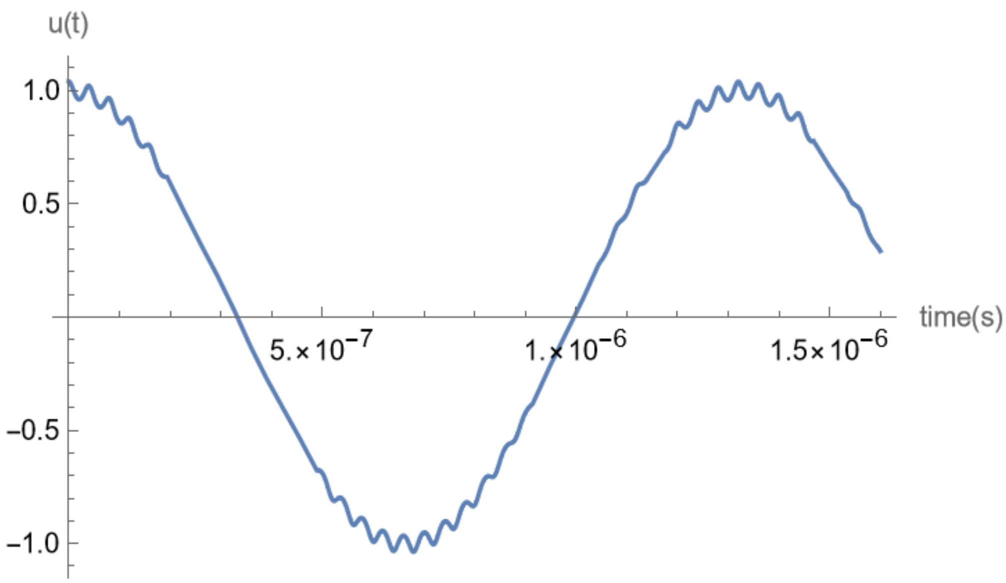

Figure 6: The ion dynamics in the radial plane with an RF potential driven at 25 MHz and 300 Volts. The amplitude of oscillation has been set to unity with geometric parameters, R, z_o being set to 460 and 335 μm respectively. DC needles (U_o) are set to 1 Volt.

As mentioned above, to zeroth order in q (neglecting micromotion), the ion's dynamics is that of a harmonic oscillator:

$$u_i(t) = A_i \cos(\omega_i t + \phi_i). \tag{33}$$

As in the axial direction, we can say that in the radial plane the ion has an effective potential of

$$\phi(x, y) = \frac{1}{2} m(\omega_x^2 x^2 + \omega_y^2 y^2). \tag{34}$$

Including the effective potential in the z-direction, we can say that the ion experiences a three-dimensional harmonic oscillator potential that is completely characterized by the secular frequencies:

$$\phi(x, y, z) = \frac{1}{2} m(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2). \tag{35}$$

Phew, we did it! This is great news– an ion in a Paul Trap will behave as if it were in a three-dimensional harmonic oscillator. As physicists, this is best-case scenario, as harmonic oscillators are our bread-and-butter.

4 Pondermotive Approximation (an intuitive snapshot of the physics)

I would like to give an alternative explanation that will hopefully paint a more intuitive picture of how the ion is being trapped. This is known as the "pondermotive approximation". To begin, let us forget about the form of our electric potentials and consider an inhomogenous electric field of the form

$$E(z, t) = \cos(\Omega t) E(z). \tag{36}$$

Where $E(z)$ is some function that is spatially dependent that we don't explicitly care about. In this derivation, we only care about the time-varying term. The ion will feel a force that depends on the electric field:

$$F(z, t) = m\ddot{z} = eE = e\cos(\Omega t) E(z). \tag{37}$$

The average force, $\langle F \rangle$, here is zero because $\langle \cos(\Omega t) \rangle = 0$. Meaning, the ion feels nothing. For any sort of confinement, the ion must feel a force! So ideally, we would like to produce something that when time-averaged results in a non-zero expression.

A quick and clean approach to this is recalling that our electric potential is inhomogenous, which allows us to Taylor expand about the ion's initial position:

$$E(z) \approx E(z_o) + \frac{\partial E(z)}{\partial z}\Big|_{z=z_o} (z(t) - z_o). \tag{38}$$

We can plug this into our expression for the electric field, $E(z, t)$, giving

$$E(z, t) = \cos(\Omega t) \left[E(z_o) + \frac{\partial E(z)}{\partial z}\Big|_{z=z_o} (z(t) - z_o) \right]. \tag{39}$$

We can integrate (37) twice to get the ion's equation of motion:

$$z(t) - z_o = -\frac{e}{m\Omega^2}\cos(\Omega t)E(z). \tag{40}$$

Plugging this back into our electric field gives

$$E(z,t) = \cos(\Omega t)\left[E(z_o) + \frac{\partial E(z)}{\partial z}\Big|_{z=z_o}\left(-\frac{e}{m\Omega^2}\cos(\Omega t)E(z)\right)\right]. \tag{41}$$

Let's clean this up by pulling out the constants and cosine in the last term and distributing the cosine out front:

$$E(z,t) = \cos(\Omega t)E(z_o) - \frac{e}{m\Omega^2}\cos^2(\Omega t)\frac{\partial E(z)}{\partial z}\Big|_{z=z_o}E(z). \tag{42}$$

We can use the reverse-chain rule trick to simplify the expression further:

$$E(z,t) = \cos(\Omega t)E(z_o) - \frac{e}{2m\Omega^2}\cos^2(\Omega t)\frac{\partial E^2(z)}{\partial z}\Big|_{z=z_o}. \tag{43}$$

We can make the assumption that the derivative of the electric field near the ion's initial position (trap center) is larger than its derivative far away from this point, which allows us to replace z with z_o in the last term. Although this assumption may seem obtuse and convenient, in the lab, the electric potential near the center is ideally a quadrupole However, due to mechanical imperfections, far away from its center can deviate from this idealization. Making this a valid assumption.

$$E(z,t) = \cos(\Omega t)E(z_o) - \frac{e}{2m\Omega^2}\cos^2(\Omega t)\frac{\partial E^2(z_o)}{\partial z_o}. \tag{44}$$

Great, we have Taylor expanded the electric field, and now we can ask what the average force the ion will experience:

$$\langle F\rangle = \frac{1}{T}\int_0^T dt\left[e\cos(\Omega t)E(z_o) - \frac{e^2}{2m\Omega^2}\cos^2(\Omega t)\frac{\partial E^2(z_o)}{\partial z_o}\right] \tag{45}$$

$$= -\frac{e^2}{4m\Omega^2}\frac{\partial E^2(z_o)}{\partial z_o} \tag{46}$$

$$= -e\frac{\partial}{\partial z_o}\underbrace{\frac{e}{4m\Omega^2}E^2(z_o))}_{\psi_p} \tag{47}$$

$$= -e\frac{\partial \psi_p}{\partial z_o}. \tag{48}$$

Where ψ_p is the effective potential the ion experiences. We can easily generalize this to dimensions larger than one:

$$\langle\vec{F}\rangle = -e\vec{\nabla}\psi_p,\ \text{where}\ \psi_p = \frac{e}{4m\Omega^2}|E_o(x,y,z)|^2. \tag{49}$$

Where ψ_p is known as the "pondermotive" potential. As we can see, the time-averaged force on the ion does not vanish. Moreover, the net force on the ion always points towards the region of weaker electric field, hence the negative sign. The physics here is similar to that of a restoring force. Instead of the force being proportional to the displacement about some equilibrium position, it is proportional to the gradient of the square of the electric field amplitude. Here, the nature of this restoring force comes from the ion wanting to minimize its energy when placed in the pondermotive potential. Therefore, when the change in the electric field squared becomes large, it wants to go back to where this change is small. This is the essence of how an inhomogeneous and oscillating electric potential is able to provide confinement to an ion! It is worth mentioning that if higher order terms in (38) were introduced, the motion of the ion would be different. These higher order terms are where micromotion shows up.

5 Bring it on home!

We have shown that static electric potentials cannot contain a local minimum and therefore cannot confine an ion. However, by going through this exercise we were able to come up with an approach to circumvent this limitation. By using a combination of static and oscillating electric potentials, the ion will, on average, see a restoring force that depends on the gradient of the electric field squared. By considering the total trapping potential, we were able to solve the equations of motion and found that the ion will behave as if it were in a three-dimensional harmonic oscillator whose properties are dictated by experimental trapping parameters such as voltages and electrode geometries.