Simulation of a penning trap

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I. INTRODUCTION

II. METHODS

We model the particles being trapped inside the Penning trap with ordinary differential equations (ODEs) derived from foundational physics equations. Let us quickly go through them here, before using them to argue our model is valid. The first of these equations is Newton's second law (1), which we use to say something about how our particles' velocity is changed in relation to outside forces. Here m is the mass of the particle, while r is its position in Euclidean space. F_i is the ith force.

$$m\ddot{r} = \sum_i F_i \tag{1}$$

Next comes the equation for how strong an electric field is at a point r, when the field is set up by point charges (2). In this equation we introduce k_e as Couloumb's constant, q as charge, and say that q_j and r_j are the jth particles' charge and position respectively.

$$E = k_e \sum_{j=1}^{n} q_j \frac{r - r_j}{|r - r_j|^3} \tag{2}$$

Electric fields (E) and potential (V) are related through (3).

$$E = -\nabla V \tag{3}$$

Lastly, the Lorentz force (4) is the force acting on a charged particle moving through an electrical and magnetic field, where the magnetic field is represented by B.

$$F = qE + qv \times B \tag{4}$$

In addition to these fundamental equations, we have two equations describing how an idealized Penning trap work, that we need to use for our model as well. The electric potential inside the trap is defined by (5), where V_0 is the potential applied at the terminals, d is the characteristic distance, a dimensionless size, and x, y and z together make up a position.

$$V(x, y, z) = \frac{V_0}{2d^2}(2z^2 - x^2 - y^2) \tag{5}$$

The magnetic field in the trap is defined as in (6). Here, B_0 is the field strength.

$$B = B_0\hat{e}_z = (0, 0, B_0) \tag{6}$$

With these equations, we can start to model how particles would behave in proximity of or inside the trap. Using (1) and (4), and then inserting the properties of our electrical (5) and magnetic (6) fields, we get

$$\begin{aligned}
m\ddot{r} &= qE + q\dot{r} \times B \\
0 &= -m\ddot{r} + q(-\nabla V) + q\dot{r} \times B_0\hat{e}_z \\
0 &= -m\ddot{r} + q\frac{V_0}{2d^2}\begin{pmatrix} -2x \\ -2y \\ 4z \end{pmatrix} + q\begin{pmatrix} \dot{y}B_0 \\ -\dot{x}B_0 \\ 0 \end{pmatrix} \\
0 &= \frac{1}{m}\begin{pmatrix} \ddot{x} - qV_0x/d^2 - q\dot{y}B_0 \\ \ddot{y} - qV_0y/d^2 + q\dot{x}B_0 \\ \ddot{z} + qV_0 2z/d^2 \end{pmatrix}
\end{aligned}$$

If we now introduce $\omega_0 = \frac{qB_0}{m}$ and $\omega_z^2 = \frac{2qV_0}{md^2}$, and split the vector equations into separate equations, we have that

$$\ddot{x} - \omega_z^2 x/2 - \omega_0\dot{y} = 0 \tag{7}$$

$$\ddot{y} - \omega_z^2 y/2 + \omega_0\dot{x} = 0 \tag{8}$$

$$\ddot{z} + \omega_z^2 z = 0 \tag{9}$$

This is a set of three ODEs, where the two first of them are coupled. To solve them more easily, we introduce the complex function $f = x + iy$. Differentiating this twice with regards to time gives us two other equations that we can use to rewrite (7) and (8) into one complex equation.

$$\dot{f} = \dot{x} + i\dot{y}, \text{ and } \ddot{f} = \ddot{x} + i\ddot{y}.$$

We begin with (7), and insert expressions for $\ddot{x}$, $\dot{y}$ and x derived from our expression for f.

$$\begin{aligned}
\ddot{x} - \omega_0\dot{y} + \frac{1}{2}\omega_z^2 x &= 0 \\
\left(\ddot{f} - i\ddot{y}\right) - \omega_0\left(\frac{\dot{f}\dot{x}}{i}\right) + \frac{1}{2}\omega_z^2(f - iy) &= 0
\end{aligned}$$

We then insert an expression for $\ddot{y}$ derived from f, and get

$$\begin{aligned}
\ddot{f} - i\left(-\omega_0\dot{x} + \frac{1}{2}\omega_z^2 y\right) + i\omega_0\dot{f}\dot{x} + \frac{1}{2}\omega_z^2(f - iy) &= 0 \\
\ddot{f} + i\omega_0\dot{x} - \omega_0\dot{x} + \frac{1}{2}\omega_z^2 iy - \frac{1}{2}\omega_z^2 iy + i\omega_0\dot{f} - \frac{1}{2}\omega_z^2 f &= 0 \\
\ddot{f} + i\omega_0\dot{f} - \frac{1}{2}\omega_z^2 f &= 0
\end{aligned}$$

We now have two ODEs that together describe how particles behave in and around our trap. $\ddot{f} + i\omega_0\dot{f} - 1/2\omega_z^2 f = 0$ gives us information about the x-axis ($\mathrm{Re}(f)$) and y-axis ($\mathrm{Im}(f)$), and $\ddot{z} + \omega_z^2 z = 0$ describes the movement along the z-axis.

Let us now analyse how our model predicts the particles will behave in the xy-plane. The analytical solution of our complex ODE is

$$f(t) = A_+ e^{-\omega_+ t} + A_- e^{-\omega_- t}, \tag{10}$$

where

$$\omega_\pm = \frac{\omega_0 \pm \sqrt{\omega_0^2 - 2\omega_z^2}}{2},$$

and $A_\pm$ are constants set after inserting initial conditions. If we want to trap the particles, we want $|f(t)| < \infty$ even when $t \to \infty$. This means the real component of the exponent must be non-positive, in other words $\mathrm{Re}(-i\omega_\pm) \leq 0$. It could also be that only one of our two terms have non-positive exponents, and A associated with the other term is 0, but this is highly dependent on initial conditions, and thus very unstable. To understand the relationship between our trap's parameters (B_0, V_0 and d) and the particle's properties (q and m), let us expand our $\omega_\pm$-expression and solve the resulting equation.

$$\begin{aligned} 0 \geq &\ \mathrm{Re}\left(-i\omega_\pm\right) \\ &= \mathrm{Im}\left(-\omega_\pm\right) \\ &= \frac{1}{2}\mathrm{Im}\left(-\omega_0 \mp \sqrt{\omega_0^2 - 2\omega_z^2}\right) \\ &= \mathrm{Im}\left(-\omega_0\right) + \mathrm{Im}\left(\mp\sqrt{\omega_0^2 - 2\omega_z^2}\right) \\ &= \mp\mathrm{Im}\left(\sqrt{\omega_0^2 - 2\omega_z^2}\right). \end{aligned}$$

This means the imaginary component of the square root must have a strict equality with 0, which only happens if $\omega_0^2 - 2\omega_z^2 > 0$, meaning that we get

$$\frac{4V_0}{d^2 B_0^2} < \frac{q}{m},$$

if we insert our expressions for ω_0 and ω_z^2. This last equation gives us some opportunity to interpret how the particle should behave. The key insight it provides is perhaps that we have to balance the electrical field with that keeps the particles centered in the z-axis with the magnetic field that centers it in the xy-plane, because the electrical field also exerts an outwards-pushing force on the particle in the xy-plane. It also means that the higher the charge of the particle, and lower mass it has, the higher the potential applied to the terminals can be without it pushing the particle out of the trap in the xy-plane.

The fact that the real component of the exponents has to be 0 also lets us know something about the upper and lower bounds for the distance the particles can have from the origin in the xy-plane.

for $k \in \mathcal{Z}$

$$\mathrm{Im}(-i\omega_\pm \Delta t) = 2\pi k$$

THE ALGORITHM

In this project we will be using Runge-Kutta 4 to solve our ODE's on the time-interval $[0, T]$, for n intervals of length h. Runge-Kutta 4 is a fourth order Runge-Kutta method with an error of $\epsilon = \mathcal{O}(h^4)$. It is a general method for solving ODE's, but here we will adapt the algorithm to solve the equations of motion when an expression $a(r, t)$ for the acceleration is known from 1. Assuming that you know the initial position r_0 and initial velocity $\dot{r}_0 = v_0$ of a particle, we can approximate and discretise the differential equation with Runge-Kutta 4. To numerically solve the equations such that $r_i \approx r(ih)$ and $v_i \approx v(ih)$ for $i \in \{0, 1, 2, \ldots, n\}$, we use algorithm(ref TODO).

$r_0 \leftarrow r(0)$
$v_0 \leftarrow v(0)$
$n \leftarrow \frac{T}{h}$
for $i \in \{1, 2, \ldots, n\}$ **do**
  $K_{1,v} \leftarrow a(r_i, t_i)$
  $K_{1,r} \leftarrow v_i$
  $K_{2,v} \leftarrow a(r_i + \frac{h}{2}K_{1,v}, t_i + \frac{h}{2})$
  $K_{2,r} \leftarrow v_i + \frac{h}{2}K_{1,r}$
  $K_{3,v} \leftarrow a(r_i + \frac{h}{2}K_{2,v}, t_i + \frac{h}{2})$
  $K_{3,r} \leftarrow v_i + \frac{h}{2}K_{2,v}$
  $K_{4,v} \leftarrow a(r_i + hK_{3,v}, t_i + h)$
  $K_{4,r} \leftarrow v_i + hK_{3,r}$
  $v_i = \frac{h}{6}(K_{1,v} + 2K_{2,v} + 2K_{3,v} + K_{4,v})$
  $r_i = \frac{h}{6}(K_{1,r} + 2K_{2,r} + 2K_{3,r} + K_{4,r})$
return v, r

In reality, the code may be slightly more complex than what is found in the (REF) as multiple particles are able to interact with each other.

III. RESULTS AND DISCUSSION

For a time-dependent electric field we repeated simulations of 100 Ca^{2+}-ions with amplitudes $f = 0.1, 0.4, 0.7$. We did the simulations for evenly spaced frequencies ω_V in the interval $(0.2, 2.5)$MHz, and counted the number of particles left in the penning trap after $500\mu s$. Figure (TODO) shows that for $f = 0.1$ there is a significant lowering of the number of particles left in the trap when the frequency $\omega_V = 0.62$. For an amplitude of $f = 0.4$, the figure shows that the number of particles left is 0 for the tested frequencies between 0.56 and 0.66, and that there is a lowering of particles left for $\omega_V = 0.3$. Similarly for $f = 0.7$, the number of particles left is zero for ω_V between 0.52 and 0.7, between 0.28 and 0.3, and there is a lowering in the number of particles left for $\omega_V = 0.2$.

The behavior of the simulated particles in the time-dependent electric field can be explained with resonance. As the external electric force is a periodic, time-dependent force, it is natural to explain the behavior of the particles with resonance. If a calcium ion had a resonance frequency equal to the frequency ω_V of the electric field, the oscillation of the particle would be amplified. This is seemingly what is happening in our simulations. As the frequency of the electric field approaches the resonance frequency of calcium ions,

We can also see that the breadth of the interval of frequencies where the particles all leave the trap increases as the magnitude of the electric field oscillation increases. As the magnitude increases, the oscillations become bigger.

The largest interval where the particles all leave the penning trap corresponds to a resonance frequency of about 0.6. Assuming that 0.6 is a resonance frequency, half of that would also be a resonance frequency. For $\omega_V = 0.4, 0.7$ we see that particles also are lost out of the trap at a frequency of about $0.3 = \dfrac{0.6}{2}$. We would also expect to see that a third of the frequency is another resonance frequency, and in fact we do see a reduction in particles as $0.2 = 0.6/3$ for $f = 0.7$. The behavior of the paricles is in other words consistent with what we would expect from a system with a resonance frequency of about 0.6.

Further work can be done on resonance within penning trap simulations. It could be interesting to check if there are any resonance frequencies outside of the interval we have investigated. A natural place to start would be in the frequencies below 0.2. Given that 0.30 is a resonance frequency, 0.15, 0.075, and so on should also be resonance frequencies. It could also be quite useful to study the specific resonance frequency of approximately 0.6 to better pinpoint the value of the frequency. More simulations of particles, in a smaller interval around $f = 0.6$ could give us a better insight. It could also be informative to investigate the resonance frequencies of calcium ions in a real, non-idealized Penning Trap.

IV. CONCLUSION

V. APPENDIX I

To test our implementation, we want to find a specific analytical solution given some initial conditions, and compare this with what our numerical approach gives us. Let us therefore assume we have a single charges particle in our Penning trap, with

$$x(0) = x_0, \quad \dot{x}(0) = 0, \quad y(0) = 0, \quad \dot{y}(0) = v_0,$$
$$z(0) = z_0, \text{ and } \quad \dot{z}(0) = 0.$$

Next, we find the general analytical solution for the z-axis by rewriting (9) as two first order differential equations

$$\dot{z}_0 = z_1, \text{ and } \dot{z}_1 = -\omega_z^2 z_0 \tag{11}$$

where $z_0 = z$, and $z_1 = \dot{z}$.