Project 3 - FYS4150

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We provide an overview of how to structure a scientific report. For concreteness, we consider the example of writing a report about an implementation of the midpoint rule of integration. For each section of the report we briefly discuss what the purpose of the given section is. We also provide examples of how to properly include equations, tables, algorithms, figures and references.

I. INTRODUCTION

Suggested introduction outline:

1. Introduce Penning Trap
2. Mention Lorentz force from potential and magnetic field of trap.
3. Single particle and multiple particles
4. Interactions
5. FE vs. RK4
6. Others (Trapped, ressonance, error, etc.)
7. Project outline

Say we were to contain one or more charged particles in motion inside some closed volume. A natural starting point would be to create a potential whose minimum is three-dimensional. Such a quadrupole potential would take the form $V(\mathbf{r}) = Ax^2 + By^2 + Cy^2$, however, Laplace's equation demands $\nabla^2 V = A + B + C = 0$. What this means, is that a three-dimensional static field will not do. One way around this is to use a strong homogeneous axial magnetic field together with a quadrupole electric field. The former incarcerate the particle(s) radially, whereas the latter limits their axial motion. A device of such a structure is called a "Penning trap" and was first built by Hans Georg Dehmelt under the influence of Frans Michel Penning's work. (((smooth transition)))

A particle with charge q in an electric field $\mathbf{E}$ and a magnetic field $\mathbf{B}$ undergoes the Lorentz force $\mathbf{F}$ given by

$$\mathbf{F} = q\mathbf{E} + q\mathbf{v} \times \mathbf{B}, \tag{1}$$

where $\mathbf{v}$ is the particle's velocity. Suppose the particle has mass m, then Newton's second law gives us the equation of motion for the particle:

$$\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \frac{\mathbf{F}}{m} \Rightarrow \frac{\mathrm{d}^2\mathbf{r}}{\mathrm{d}t^2} = \frac{q}{m}(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \tag{2}$$

The external electric field is related to the potential through $\mathbf{E} = -\nabla V$. We now have simple equations for predicting a single particle's motion inside of a Penning trap, and we will later discuss what is required of the initial conditions in order for it to stay put. If we were to accompany the single particle with another charged particle, however, we would need to consider the contribution to the electric field from the Coulomb interactions between the two of them. Adding more charged particles complicates the system even more in such a way that we generally will struggle to solve it analytically (IS THIS CORRECT?); we need to use numerical integration methods.

We consider two different numerical schemes for solving ordinary differential equations (ODEs)[1], forward Euler (FE) and fourth order Runge-Kutta (RK4). The former is a numerical procedure of first order, whereas the latter is of fourth order, resulting in global errors proportional to the step size and the step size to the power of four, respectively. That is, say we have a step size $h \sim 0.1$, the error arising from FE is $h^{1-4} \sim 1000$ times larger than that of RK4 (WAIT, WHAT?). However, one should keep in mind that the RK4 algorithm demands many more floating points operations (FLOPs) from our computer than what the FE algorithm does.

Now being able to solve the system of several interacting charged particles in the Penning trap in question, we should ponder the effect the Coulomb interactions have on the trap's ability to contain the particles. FILL WITH PONDERING

In addition, we will investigate the effect of adding an oscillating time-dependent perturbation to the external electric potential V. This is indeed similar to another approach for particle storage, named the Paul trap, in which the oscillating field is used instead of the magnetic field. The combined ion trap, the combination of these two structures, allows for storage of oppositely charged particles, but is vulnerable to some ranges of oscillation frequencies and amplitudes (CHECK THIS).

OUTLINE

II. METHODS

A. (appropriate title) -schematics or whatever

Consider an ideal Penning trap with characteristic dimension d, a length scale given by $d = \sqrt{z_0^2 + \frac{1}{2}r_0^2}$, where z_0 is the distinance between the endcaps and r_0 the radius

[1] We shall have to split the eq. (2) in two first order ODEs.

of of the ring REF TO SOME SCHEMATIC FIGURE. These electrodes create an external electric field $\mathbf{E}_{\rm ext}$ resulting from the potential

$$V(\mathbf{r}) = V(x,y,z) = \frac{V_0}{2d^2}(2z^2 - x^2 - y^2), \tag{3}$$

where V_0 is the potential applied to the electrodes. The external electric field is then

$$\mathbf{E}_{\rm ext} = -\nabla V = \frac{V_0}{d^2}(x,\, y,\, -2z). \tag{4}$$

A constant homogeneous magnetic field $\mathbf{B}_{\rm ext}$ is imposed in the z-direction,

$$\mathbf{B}_{\rm ext} = (0, 0, B_0). \tag{5}$$

B. (appropriate title) -math/analytical work

We restrict ourselves to dealing with only positively charged particles, $q > 0$. Consider the single-particle case, i.e. the situation with only one particle present in the trap or when we look at one of several particles that do not interact[2]. Now, the only contributions to the fields are external, hence $\mathbf{E} = \mathbf{E}_{\rm ext}$ and $\mathbf{B} = \mathbf{B}_{\rm ext}$. We use eq. (1) to find the Lorentz force,

$$\begin{aligned}\mathbf{F} &= \frac{qV_0}{d^2}(x,\, y,\, -2z) + qB_0(\dot{y},\, -\dot{x},\, 0)\\ &= \frac{m}{2}\omega_z^2(x,\, y,\, -2z) + m\omega_0(\dot{y},\, -\dot{x},\, 0),\end{aligned} \tag{6}$$

where we defined $\omega_0 \equiv \frac{qB_0}{m}$ and $\omega_z^2 \equiv \frac{2qV_0}{md^2}$. The equation of motion in eq. (2) are three differential equations in each spatial component,

$$\ddot{x} - \omega_0\dot{y} - \frac{1}{2}\omega_z^2 x = 0, \tag{7}$$

$$\ddot{y} + \omega_0\dot{x} - \frac{1}{2}\omega_z^2 y = 0, \tag{8}$$

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

The general solution of eq. (9) is

$$z(t) = c_1\cos(\omega_z t) + c_2\sin(\omega_z t). \tag{10}$$

The other two, eqs. (7) and (8), are coupled. We introduce a complex function $f(t) = x(t) + iy(t)$ for which we have the time derivatives $\dot{f} = \dot{x} + i\dot{y}$ and $\ddot{f} = \ddot{x} + i\ddot{y}$. Multiply equation (8) with i and add to equation (7) to obtain the following:

[2] This is not physical.

$$\begin{aligned}\ddot{x} + i\ddot{y} + \omega_0(i\dot{x} - \dot{y}) - \frac{1}{2}\omega_z^2(x+iy) &= 0\\ (\ddot{x} + i\ddot{y}) + i\omega_0(\dot{x} + i\dot{y}) - \frac{1}{2}\omega_z^2(x+iy) &= 0.\end{aligned} \tag{11}$$

The single differential equation in terms of the complex function $f(t)$ is therefore

$$\ddot{f} + i\omega_0\dot{f} - \frac{1}{2}\omega_z^2 f = 0. \tag{12}$$

The general solution to equation (12) is

$$f(t) = A_+e^{-i(\omega_+t+\phi_+)} + A_-e^{-i(\omega_-t+\phi_-)}, \tag{13}$$

where ϕ_+ and ϕ_- are constant phases, A_+ and A_- are positive amplitudes and

$$\omega_\pm = \frac{\omega_0 \pm \sqrt{\omega_0^2 - 2\omega_z^2}}{2}. \tag{14}$$

The ω_+ is the modified cyclotron frequency and the ω_- is the magnetron frequency that composes the two modes in the orbital motion we will discuss later.

Stopped here (19.10.22), going to bed

We see from equation (13) that if $\omega_\pm$ is real, then $|f(t)| < \infty$ for $t \to \infty$ and we have a bounded solution in the xy-plane. For $\omega_\pm$ to be real we see from equation (14) that the following must hold:

$$\omega_0^2 \geq 2\omega_z^2 \tag{15}$$

$$\implies \frac{q}{m} \geq \frac{4V_0}{(B_0 d)^2}. \tag{16}$$

We may regard equation (13) as a sum of vectors $\mathbf{r}_\pm$ with amplitudes $r_\pm = A_\pm$ and directions given by the angles $\alpha_\pm = \omega_\pm t + \phi_\pm$ in the complex plane (representing the xy-plane). The magnitude $|f(t)| = |f|$ for this sum of vectors is then given by:

$$|f| = \sqrt{|\mathbf{r}_+|^2 + |\mathbf{r}_-|^2 + 2|\mathbf{r}_+||\mathbf{r}_-|\cos\left(|\alpha_+ - \alpha_-|\right)}. \tag{17}$$

The maximum distance from the origin, R_+, occurs when the two vectors are pointing in the same direction, i.e. $|\alpha_+ - \alpha_-| = 0 \implies \cos 0 = 1$, which yields:

$$\begin{aligned}R_+ &= \sqrt{A_+^2 + A_-^2 + 2A_+A_-} = \sqrt{(A_+ + A_-)^2}\\ &= A_+ + A_-\end{aligned} \tag{18}$$

Similarily, the minimum distance, R_-, from the origin occurs when the vectors are pointing in opposite directions, i.e. $|\alpha_+ - \alpha_-| = \pi \implies \cos\pi = -1$, which yields:

$$\begin{aligned}R_- &= \sqrt{A_+^2 + A_-^2 - 2A_+A_-} = \sqrt{(A_+ - A_-)^2}\\ &= |A_+ - A_-|\end{aligned} \tag{19}$$

$$\ddot{x}_i - \omega_{0,i}\dot{y}_i - \frac{1}{2}\omega_{z,i}^2 x_i - k_e \frac{q_i}{m_i}\sum_{j\neq i} q_j \frac{x_i - x_j}{|\mathbf{r}_i - \mathbf{r}_j|^3} = 0, \quad (20)$$

$$\ddot{y}_i + \omega_{0,i}\dot{x}_i - \frac{1}{2}\omega_{z,i}^2 y_i - k_e \frac{q_i}{m_i}\sum_{j\neq i} q_j \frac{y_i - y_j}{|\mathbf{r}_i - \mathbf{r}_j|^3} = 0, \quad (21)$$

$$\ddot{z}_i + \omega_{z,i}^2 z_i - k_e \frac{q_i}{m_i}\sum_{j\neq i} q_j \frac{z_i - z_j}{|\mathbf{r}_i - \mathbf{r}_j|^3} = 0, \quad (22)$$

C. (appropriate title) -coding

We aim to create a program in C++ that simulates a set of N_p particles inside a Penning trap. An object-oriented code is befitting this task and we present in the following descriptions of the classes `Particle` and `PenningTrap`.

The purpose of `Particle` is to hold the parameters, such as the position, of a particle. We let an object of this class be initialised with a charge q, a mass m, a position $\mathbf{r} = (x, y, z)$ and a velocity $\mathbf{v} = (v_x, v_y, v_z)$. We add functions to update the latter two.

The `PenningTrap`-class imitates the physical system that is the Penning trap of magnetic field $\mathbf{B} = B_0\hat{e}_z$, electric potential $V = \frac{V_0}{2d^2}(2z^2 - x^2 - y^2)$ and characteristic dimension d. It is friend with the `Particle`-class and, in order to resemble the physical situation as much as possible, accepts only input particles of this type. When filled with $N_\mathrm{p} \geq 1$, an object of `PenningTrap` is ready to simulate the evolution of the `Particle` object(s) for a given period of time and time step with either a Forward-Euler or a 4th order Runge-Kutta numerical scheme.

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`PenningTrap` offers several additional functionalites. Amongst other things, the class:

- offers the choice between 4th order Runge-Kutta or Forward-Euler as integration method
- provides the option to include or exclude Coloumb interactions in the simulation, as they are computationally greedy
- includes a method for adding a time-dependent perturbation to the external electric potential, $V_0 \to V_0(1 + f(1 + \cos(\omega_V t)))$
- has the ability to count the number of particles still trapped, that is the number particles whose position $\mathbf{r}$ is such that $|\mathbf{r}| \leq d$
- can generate a set of identical particles with positions and velocities that are normally distrubuted within the trap's dimensions

D. Initial conditions

For simulations of one or two particles, we use the following initial conditions:

- Particle 1

$$(x_0, y_0, z_0) = (20, 0, 20)\mu\mathrm{m}.$$
$$(v_{x,0}, v_{y,0}, v_{z,0}) = (0, 25, 0)\mu\mathrm{m}/\mu\mathrm{s}.$$

- Particle 2

$$(x_0, y_0, z_0) = (25, 25, 0)\mu\mathrm{m}.$$
$$(v_{x,0}, v_{y,0}, v_{z,0}) = (0, 40, 5)\mu\mathrm{m}/\mu\mathrm{s}.$$

III. RESULTS

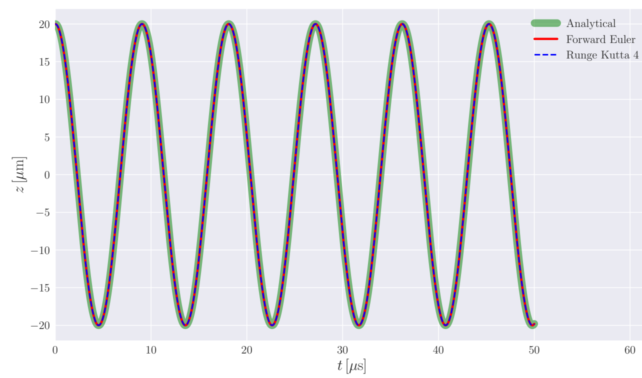

FIG. 1. Movement in the z for a single particle, simulation for 50 μs. The analytical solution from equation 10 is plotted in green, and the integrated solutions using the forward Euler and Runge-Kutta 4 scheme is shown in red and blue respectively. Initial conditions are those of particle 1, given in II D

FIG. 2. Movement of two particles in the xy-plane simulated for 50 μs. The left panel show their trajectories computed without particle interaction. In the right panel we have allowed for the particles to interact. We have used the Runge-Kutta 4 scheme to obtain these trajectories. Particle 1 is shown in blue, and particle 2 in green. Both panels use the same initial conditions as specified in rection II D. The staring points of their trajectories are indicated with a cross, their ending points with a star.

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IV. DISCUSSION

V. CONCLUSION

In this section we state three things in a concise manner: what we have done, what we have found, and what should or could be done in the future.

FIG. 3. Some caption

FIG. 4. Some caption

FIG. 5. Some caption