Problem 4: Mass Spectrometry

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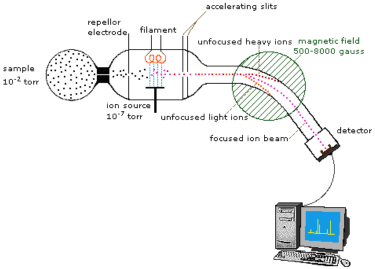
Mass Spectrometry



- Mass spectrometry is a technique used to determine the chemical composition of an unknown substance.
- A typical device separates charged atoms and molecules based on their charge to mass ratio.
- Many different techniques and devices are used to do this; the one presented to us was the quadrupole method.

The Quadrupole Mass Spectrometer

- A mass filter that uses a combination of AC and DC voltages to create an electric field with a narrow range of mass passing through to reach the detector.
- By controlling both the AC and DC voltage, particles with a specific mass pass through the device.
- AC gets rid of particles with smaller mass, DC gets rid of particles with larger mass.

The Problem

- Want to measure multiple masses all at once with an area detector.
- Don't want to lose any ions.
- Can we achieve higher mass resolution using only an electric field?
- Don't want to use a magnetic field.

Initial Ideas

- Binary separation system.
- Ion trapping.

Binary System

- Use electric fields to constantly separate groups of particles until they can no longer be separated.
- Solves the problem of finding all the masses all at once, only uses an electric field, and we don't lose any ions.
- Downfall is that it would be impossible to model and manufacture.

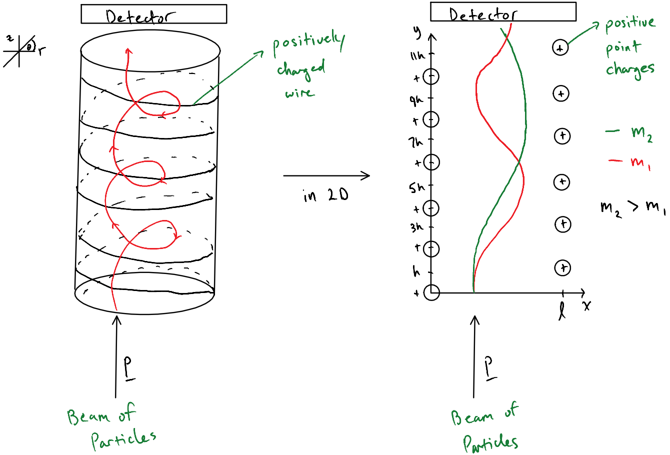
Ion Trapping

- Send the particles into a quadrupole like device where there would be an electric field opposing the particles motion.
- Carefully place special curvature traps where the particles would then be separated by mass.
- The opposing electric field acts like a potential barrier for the particles, this allows the particles with not enough energy to get trapped.
- Then can measure (possibly through the magnetic field) the charged particles in each trap.

The Final Idea

- Send particles into a positively charged solenoid.
- The frequency of oscillation for the particles trajectory differ due to the particles mass.
- Akin to how a prism can separate the different colours of light, the solenoid will create a dispersion pattern of the particles being studied ($\vec{E}$-prism).

3D to 2D


Detector
z
θ
r
positively charged wire
P
Beam of Particles
in 2D
Detector
y
11h
9h
7h
5h
3h
h
x
l
positive point charges
m2
m1
m2 > m1
P
Beam of Particles

Electrostatics

Using Coulombs law,

$$V(x,y) = \frac{Ze}{4\pi\epsilon_0}\sum_{j=0}^{N} \underbrace{\frac{1}{\sqrt{(x-l)^2+(y-2nh)^2}}}_{r_j} + \underbrace{\frac{1}{\sqrt{(x-l)^2+(y-(2n-1)h)^2}}}_{\rho_j}$$

and the equations of motion come from

$$\langle \ddot{x}, \ddot{y} \rangle = -\beta \nabla V(x,y).$$

where

$$\beta = \frac{Ze^2}{4\pi\epsilon_0 m W U_0^2},$$ and U_0 is the initial speed.

ODE's

Equations of Motion:

$$\ddot{x} = \beta \sum_{j=1}^{N} \left(\frac{x}{r_j^3} + \frac{x-1}{\rho_j^3} \right),$$

$$\ddot{y} = \beta \sum_{j=1}^{N} \left(\frac{y-2jh}{r_j^3} + \frac{y-(2j-1)h}{\rho_j^3} \right)$$

Initial Conditions:

$$x(0) = x_0, 0 < x_0 < \frac{1}{2}, \dot{x}(0) = 0,$$

$$y(0) = y_0, y < 0, \dot{y}(0) = u_0, u_0 > 0.$$

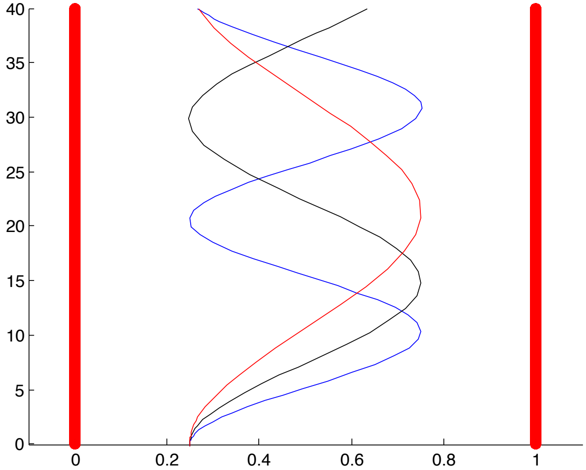
Initial Velocity

Want to select an initial velocity so the charged particles can overcome the potential barrier it sees from the charges and still have some velocity left over.

After using conservation of energy:

$$u_0 > \sqrt{\frac{Z\beta N}{\sqrt{[(x-\frac{1}{2})^2+(Nh)^2]}}} - \sqrt{\frac{Z\beta N}{\sqrt{[(x_0-\frac{1}{2})^2+(y_0-Nh)^2]}}}.$$

Numerical Trajectories



Sums are gross!

Since $N \gg 1$ approximate the potential sums as integrals but turning it into a Riemann sum:

$$\beta \sum_{j=1}^{N} \frac{x}{r_j^3} \approx -\frac{\beta N}{2M} \int_{y}^{y-2M} \frac{x}{(x^2+s^2)^{3/2}} ds$$

$$\beta \sum_{j=1}^{N} \frac{y-2jh}{r_j^3} \approx -\frac{\beta N}{2M} \int_{y}^{y-2M} \frac{t}{(x^2+t^2)^{3/2}} dt$$

New Trajectories

After integrating,

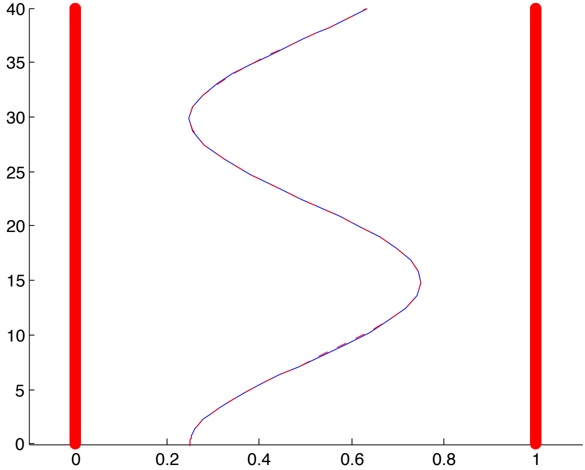
$$\ddot{x} = -\frac{\beta N}{2Mx}\left(\frac{y-2M}{\rho_{x,y-2M}} - \frac{y}{\rho_{x,y}}\right) - \frac{\beta N}{2M(x-1)}\left(\frac{y-2M}{\rho_{x-1,y-2M}} - \frac{y}{\rho_{x-1,y}}\right)$$

$$\ddot{y} = -\frac{\beta N}{2Mx}\left(\frac{1}{\rho_{x,y}} - \frac{1}{\rho_{x,y-2M}} + \frac{1}{\rho_{x-1,y}} - \frac{1}{\rho_{x-1,y-2m}}\right)$$

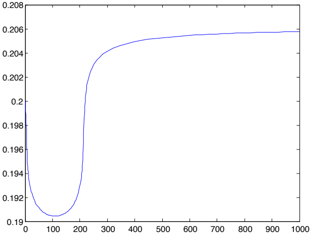
where

$$\rho_{a,b} = \sqrt{(x-a)^2 + (y-b)^2}.$$

Sums vs. Integrals



Vertial Acceleration



We notice that the y acceleration essentially vanishes. Averaging over the entire domain for integral formulation, $\ddot{y} \approx 0$ like we see in numerics. Likewise, averaging $\ddot{x}$ and letting $M \to \infty$,

$$\ddot{x} = \frac{\beta}{h}\left(\frac{1}{x} + \frac{1}{x-1}\right)$$

Period of Oscillation

Through conservation of energy, we can integrate explictly and obtain an equation for the velocity,

$$\dot{x} = \pm\sqrt{\frac{2\beta N}{M}\log\left(\frac{x(x-1)}{x_0(1-x_0)}\right)},$$

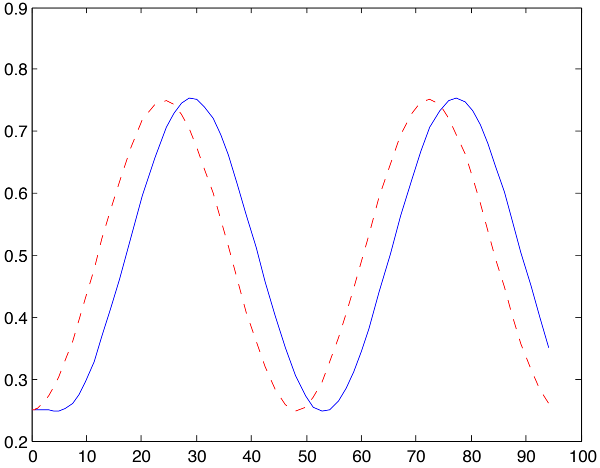
and after integrating once more, we obtain the half-period,

$$T_{1/2} = \sqrt{\frac{2M}{\beta N}} I(x_0),$$

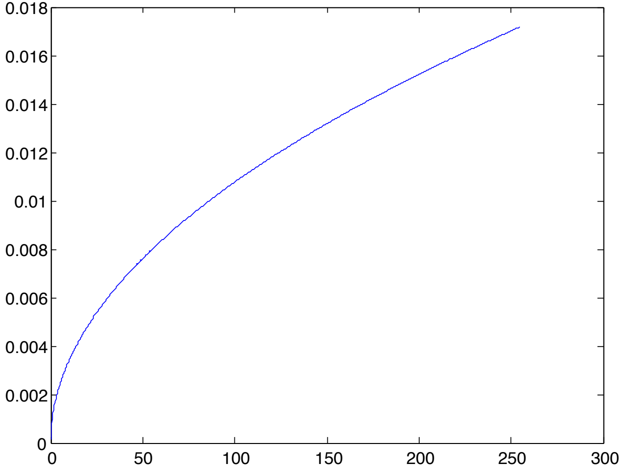
where

$$I(x_0) = \int_{1/2}^{1-x_0} \frac{dx}{\sqrt{log[x(1-x)] - c_0}}.$$

Period Matching



Dispersion Relation



Conclusion

- Designed a device that disperses ions based on mass
- Requirements were no trapping or magnetic field
- Simplifications are still quite accurate and produce simple $T \sim \frac{1}{\sqrt{m}}$ curve
- Measurements could come from an area detector at end of device after separation occurs or from a FT type analysis that measures the frequencies

Future Work

- Extend to 3D device
- Do the Fourier analysis