Aug 3rd, 9:00 AM - 12:00 PM

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Repository Citation

Alexander, Andrew; Kwong, Victor; Clarke, Brad; and Benavente, James, "Experimental determination of the stable boundary for a cylindrical ion trap" (2010). Undergraduate Research Opportunities Program (UROP). 6.  
https://digitalscholarship.unlv.edu/cs_urop/2010/aug3/6

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Experimental Determination of the Stable Boundary for a Cylindrical Ion Trap

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Introduction
The first radio frequency (rf) quadrupole ion traps were designed with hyperbolic trapping electrodes and had the advantage of a working theoretical model with an analytical solution for the equation of motion for an ion. This came at the cost of a difficult fabrication process by the nature of the hyperbolic design. Cylindrical designs were found to be an easily constructed and functional alternative for ion trapping, but a sound theoretical model for this geometry has yet to emerge. While the hyperbolic theory yields approximate parameters for stable ion trapping, experiments conducted near the stable/unstable boundary require an experimental determination of this boundary.

Objective
Experimentally determine a strategic section of the stable boundary for a cylindrical RF quadrupole ion trap and compare findings to theoretical and simulated results.

Methods
Two experiments were conducted with the same basic process to determine the boundary. For each scan line V₀ is held constant while U₀ is increased by a small amount (0.2 Volts) for each data point until we no longer see a signal intensity for our target ion, nitrogen singly charged (N⁺).

Experiment 1
- Trapping parameter values being investigated are held constant near the boundary
- Experimental boundary determined for ion "storage" times 345 ms and 690 ms

Experiment 2 (Delta U₀)
- Ions created and cooled within ideal trapping parameters for 700 ms
- Parameters are then abruptly changed to values under investigation
- Ions ejected after 2 ms exposure to near boundary parameters

Simulation and Theory

Mathieu Stability Diagram

For cylindrical and hyperbolic traps the two end cap electrodes are held at ground during the trapping sequence while the ring electrode carries an AC potential (V₀) with a DC offset (U₀). The simulation program allows us to numerically determine if an ion is trapped by calculating forces on an ion and it’s motion in time-steps. This becomes a valuable tool in the absence of a theoretical model for cylindrical geometry.

For hyperbolic geometry, these boundary conditions result in the ion’s equation of motion to be in the form of the Mathieu differential equation

\[ \frac{d^2x}{dt^2} + (Q - 2q_0 \cos(2\omega t))x = 0 \]

Where \( Q \) and \( q_0 \) are defined to be linearly related to \( V_0 \) and \( U_0 \), respectively. The solutions to these equations are known to have well defined regions defined by and \( q_0 \) that result in bounded stable motion.

The boundary conditions in the cylindrical case do not yield a simple analytical solution, however the potential surfaces near the center of the trap approximates those produced by the hyperbolic electrode geometry. We then assume similar bounded trapping conditions for cylindrical geometry and compare results to the hyperbolic case using the same definitions of \( q_0 \) and \( d_q \).

Results
- First experiment resulted in a disagreement for the determined boundary for separate ion storage times
- Noticed a difference of 0.5 Volts between boundary estimates
- The Delta U₀ approach agrees well with simulated boundary
- Experimental boundary on average within .6 Volts of simulated boundary

Conclusion
- Creation or storage of ions near the stable boundary adversely affect resolution and ion population
- Trap design appear to “leak” ions near boundary over time rather than conforms to stable/unstable characteristic as in theory
- Delta U₀ approach minimizes these complications with small exposure time

Acknowledgements
Thanks to my mentor, Dr. Victor Kwong, for the opportunity to perform this research, Brad Clarke for his help and guidance during this process, and James Benavente for his collaborative work on the project. Support from the REU program of the National Science Foundation under grant DMR-1005247 is gratefully acknowledged.