AN INVESTIGATION OF THE SPACE OF TRAJECTORIES IN A NOVEL OA-TOP GEOMETRY

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INTRODUCTION

Fourier Transform (FT) mass spectrometers have ultimate resolutions exceeding those of conventional Time-of-Flight (TOF) mass spectrometers. However, in order to achieve this, long acquisition times are required (of up to several seconds in some cases). In contrast, high-performance TOF mass spectrometers have typical flight times of ions of microseconds. This allows them, for example, to profile mobility separations lasting only a few milliseconds.

In this poster we present a theoretical treatment of a novel orthogonal acceleration (oa)-TOF geometry, utilizing the quadralogarithmic potential familiar from Orbitrap mass spectrometry, which could combine the high resolution of FT instruments with the speed of TOF analysis.

METHODS

The cylindrically symmetric quadro-logarithmic potential takes the form:

\[ V(r, \phi, z) = \frac{k}{r} \ln^2 \left( \frac{z}{R} \right) \]

This potential produces independent motion in the radial (trapping) and axial (chain) directions. The axial potential is characterized by a frequency that is n/a, a parameter that can be tuned to achieve the required performance.

In the Orbitrap mass spectrometer, the shape of the electrodes fixes the ratio between the logarithmic (log) and quadratic (q) parts of the potential. We propose instead to use a segmented construction allowing freedom of choice in this ratio. The method of construction (Figures 1 and 2) consists of two concentric sets of rings to which a set of voltages \( V_{1,2} \) are applied. A typical device geometry is shown in Figure 3, with an outer radius of 10cm and an inner radius of 0.1cm.

RESULTS

The sequence of events for a single ion injection is as follows:

1. Axial (2) beam expansion prior to injection to reduce turn-around time in low extraction fields.
2. Ion injection into stable circular orbits with \( V_{1} > V_{2} \) and \( V_{0} = 0 \).
3. Orthogonal and radial acceleration (\( v_{z} > v_{r} > 0 \)) increases the radial component of motion and provides a stabilizing potential for those ions.
4. Stable circular motion with period \( \tau \) in the 3D space.
5. Ions strike the detector on the final pass.

In order to produce this behavior, it is important to control the overlap between axial and orbital motion. The equations of motion are derived below starting from the Lagrangian written in cylindrical polar coordinates:

\[ L = T - V \]

The three Euler-Lagrange equations are

\[ \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{\phi}} \right) - \frac{\partial L}{\partial \phi} = 0 \]

\[ \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{z}} \right) - \frac{\partial L}{\partial z} = 0 \]

\[ \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{r}} \right) - \frac{\partial L}{\partial r} = 0 \]

The second equation allows expression of the \( \phi \)-component of angular momentum \( L_{\phi} \) and the first equation, remembering the sign of \( \phi \) in the form of an expression for effective potential containing a "centrifugal" term:

\[ V_{eff} = V + \frac{k}{r} \ln^2 \left( \frac{z}{R} \right) - \frac{1}{2} \frac{m v^2}{R^2} \]

For ions injected into circular orbits radius \( R_{c} \) through a potential drop \( \Delta V = \frac{k}{r} \ln^2 \left( \frac{z}{R} \right) \), and a switched electric sector helps to accomplish stable circular trajectories.

DISCUSSION

In this poster we have briefly reviewed the theoretical properties of a novel mass time of flight mass spectrometer utilizing a quadralogarithmic potential as a solution to practical problems (both electrical and mechanical) would have to be overcome before such a device could be constructed. Each of the ring electrodes in the assembly must be carefully machined and positioned, to achieve orthogonal acceleration must be pulsed accurately and rapidly from their initial value to their final value, the detector must be placed within a vacuum system, and a sufficient number of masers that can be utilized is limited by the initial radial spread of the ions. Nevertheless, with appropriate beam conditioning, it is anticipated that mass resolutions of several hundred thousand should be achievable in a relatively compact geometry.

CONCLUSION

Following axial beam expansion, the quadralogarithmic potential can be utilized for multi pass oa-TOP mass analysis.

The parameter space is clearly minimized for a chosen geometry, and a solution with a TOF path length of over 10cm has been identified.

Many technical challenges remain to be addressed before such a device could be constructed.