CIT and QIT with a Periodic Impulsional Potential

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Abstract

The purpose of this article is the comparison of a cylindrical ion trap supplied by a periodic impulsional potential with quadrupole ion trap. To compute the five stability regions for the cylindrical ion trap (CIT) and quadrupole ion trap (QIT) in the $a - q$ plane we use the Runge-Kutta method with the fifth order derivative approximations. The first up to five stability regions obtained in this article for CIT compared with the first up to twelve stability regions of article reported by S. Seddighi Chaharborj and S. M. Sadat Kiai in 2010.

Keywords: Confinement, Ions, Cylindrical ion trap, Quadrupole ion trap, Impulsional potential, Fifth order Runge-Kutta method, Stability regions, Ion trajectory

1 Introduction

Ion trap mass spectrometry has developed though several stages to their current stage relatively high performance and increasing popularity. Quadrupole ion trap (QIT) invented by Paul and Steinwedel has been widely applied to mass spectrometry [2, 3, 6, 4], ion cooling and spectroscopy, frequency standards, quantum computing, and so on. To apply to various objectives, various geometries of ion trap for the mass spectrometer has been suggested. An ion trap mass spectrometer may incorporate a Penning trap, Paul trap or the Kingdon trap. The Orbitrap, introduced in 2005, is based on the Kingdon
trap. The two most common types of ion traps are the Penning trap and the Paul trap (quadrupole ion trap). Other types of mass spectrometers may also use a linear quadrupole ion trap as a selective mass filter. Computation of stability regions is of particular importance in order to design and assemble an ion trap. Analytical and matrix methods, on one hand, have been widely used to calculate the stability regions.

A quadrupole ion trap mass analyzer with simplified geometry, the cylindrical ion trap (CIT), was shown to be well-suited to use in miniature mass spectrometers and even mass spectrometer arrays. Experiments with a single miniature CIT showed acceptable resolution and sensitivity, limited by the ion trapping capacity of the miniature device.

The CIT has received much attention of a number of research groups because of several merits. The CIT is easier to fabricate than the Paul ion trap which has hyperbolic surfaces. And the relative simplicity and small size of the CIT make it an ideal candidate for miniaturization. With these interests, many groups in, such as Purdue University and Oak Ridge National Laboratory have researched on the applications of the CIT to a miniaturized mass spectrometer.

2 Study the motions of ion voltage inside CIT

Figure (1) show the electronics configuration of rectangular CIT, that is to say a combinations of d.c. voltage, \(U_{dc}\), and an alternative voltage \(V_{ac} f(t)\) with \(f(t) = V_0 \cos \Omega t / (1 - k \cos 2\Omega t)\) with \(0 \leq k < 1\) is the modulation “index” parameter for the ring and end-caps electrodes,

\[
\Psi_0 = \pm (U_{dc} - V_{ac} \cos \Omega t / (1 - k \cos 2\Omega t)) \quad \text{with} \quad 0 \leq k < 1
\] (1)

then the potential distribution inside the CIT with \(r_1 = z_1\) at any point of a circle of radius \(r\) can be written as:

\[
\Psi(r, z) = \sum_i \frac{2\Psi_0}{m_ir_1} \frac{J_0(m_i r)}{J_1(m_i r_1)} \frac{ch(m_i z)}{ch(m_i z_1)}.
\] (2)

Here \(J_0\) and \(J_1\) are the Bessel functions of first kind, of order 0 and order 1, respectively, \(ch\) is the hyperbolic cosine function, \(m_i r\) is roots of equation \(J_0(m_i r) = 0\), \(U_{dc}\) and \(V_{ac}\) are the amplitudes and the radio frequency (rf) drive frequency. Assuming that \(r_1^2 = 2z_1^2\), then the electric field in a cylindrical coordinates \((r, z, \theta)\) inside the CIT with \(r_1^2 = 2z_1^2\) can be written:

\[
(E_r, E_\theta, E_z) = E = -\nabla \Psi(r, z).
\] (3)

Here \(\nabla\) is gradient. The basic equation of the ion motions of mass \(m\) and electric charge \(e\) into the trap taking into account the effect of damping force
may be treated independently:

\[
\frac{d^2u}{d\xi^2} - (\alpha - 2\chi \cos 2\xi/(1 - k\cos 4\xi)) \sum_i \frac{J_1(\lambda_i u)}{J_1(\lambda_i)} \frac{ch(\lambda_i v)}{ch(\lambda_i r_1)} = 0,
\]

\[
\frac{d^2v}{d\xi^2} + (\alpha - 2\chi \cos 2\xi/(1 - k\cos 4\xi)) \sum_i \frac{J_0(\lambda_i u)}{J_1(\lambda_i)} \frac{sh(\lambda_i v)}{ch(\lambda_i r_1)} = 0,
\]

with the following substitutions:

\[
\xi = \frac{\Omega t}{2}, \quad m_ir_1 = \lambda_i, \quad \frac{r}{r_1} = u, \quad \frac{z}{r_1} = v, \quad \alpha = -8e m \times \frac{U_{dc}}{r_1^2 \Omega^2}, \quad \chi = 4e m \times \frac{V_{ac}}{r_1^2 \Omega^2},
\]

where \(\alpha\) and \(\chi\) are the trapping parameters, \(\lambda_i = m_ir_1\) is roots of equation \(J_0(m_ir_1) = 0\).

Figure 1: Schematic view of a cylindrical ion trap (CIT).

3 Results

3.1 Stability regions

Fig. (2) up to Fig. (7) present the stability regions of cylindrical ion trap (CIT) and quadrupolion trap the a-q plan for different \(k\)'s. We observe that the apex of the stability parameter \(a\) stayed constant, but the higher limit of \(q\) decrease substantially when \(k\) increase form 0 to 1.

4 Discussion and conclusion

In this article we used the higher order of Runge-Kutta method to compute the five stability regions for a cylindrical ion trap and quadrupole ion trap
Figure 2: (a): The stability regions I until XII for the cylindrical ion trap with $k = 0$. (b): The stability regions I until XII for the quadrupole ion trap with $k = 0$.

Figure 3: The first stability region for the CIT and QIT with $k = 0$, (a): The first stability region for CIT, (b): The first stability region for the CIT and QIT.
Figure 4: The second stability region for the CIT and QIT with $k = 0$, (a): The second stability region for CIT, (b): The second stability region for the CIT and QIT.

Figure 5: The third stability region for the CIT and QIT with $k = 0$, (a): The third stability region for CIT, (b): The third stability region for the CIT and QIT.
Figure 6: The forth stability region for the CIT and QIT with $k = 0$, (a): The forth stability region for CIT, (b): The forth stability region for the CIT and QIT.

Figure 7: The fifth stability region for the CIT and QIT with $k = 0$, (a): The fifth stability region for CIT, (b): The fifth stability region for the CIT and QIT.
with accuracy enough. In this computation, the size of the integration step was considered as 0.01. The first stability regions obtained in this article compared with the first stability regions of article reported by S. Seddighi Chaharborj and S. M. Sadat Kiai in 2010 [6]. The results of this paper showed that, the apex of the stability parameters \( a_z \) stayed the same and the apex of the stability parameters \( q_z \) decrease when \( k \) increase from 0 to 1.

### References


Received: September, 2011