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STUDY OF FRACTIONAL RESOLUTION IN THE CYLINDRICAL ION TRAP WITH A PERIODIC IMPULSIONAL POTENTIAL FORM

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Abstract: In this article a cylindrical ion trap with $r_1 = z_1$ excited with a periodic impulsional potential form $f(t) = V_0 cos\Omega t/(1 - kcos2\Omega t)$ with $0 \leq k < 1$ is studied. Numerical computations allowed the determination of the stability diagrams in (U,V) plan using a fifth order Runge-Kutta derivative approximations and compared with basic case $k = 0$. The fractional mass resolutions $m/\Delta m$ of the confined ions in two first and second stability regions of both ion traps was analyzed for $\beta_z = 0.1$ and $\beta_z = 0.9$.

AMS Subject Classification: 35Qxx, 81V35, 81V45
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1. Introduction

An ion trap mass spectrometer may incorporate a Penning trap [1], Paul trap

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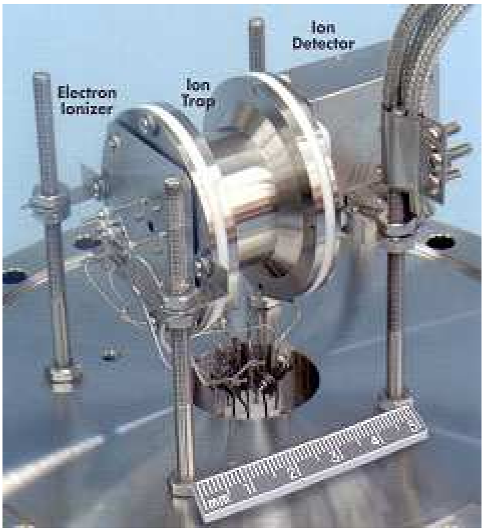


Figure 1: Schematic view of a cylindrical ion trap (CIT)

[2] or the Kingdon trap [4]. The Orbitrap, introduced in 2005, is based on the Kingdon trap [3]. The two most common types of ion traps are the Penning trap and the Paul trap (quadrupole ion trap) [9, 10, 11, 12]. 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 [5].

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 [7]. 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 [13] and Oak Ridge National Laboratory [6] have researched on the applications of the CIT to a miniaturized mass spectrometry.

2. Ion Movement in a Cylindrical Ion Trap with $r_1 = z_1$

Figure (1) show the electronics configuration of rectangular CIT with $r_1 = z_1$, 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 $0 \le k < 1$ is the modulation "index" parameter for the ring and end-caps electrodes,

$$\Psi_0 = \pm(U_{dc} - V_{ac}\cos\Omega t/(1 - k\cos 2\Omega t)) \quad \text{with} \quad 0 \le k < 1, \tag{1}$$

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:

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

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 $r_1^2 = z_1^2$, then the electric field in a cylindrical coordinates (r, z, θ) inside the CIT with $r_1 = z_1$ can be written:

$$(E_r, E_\theta, E_z) = E = - \bigtriangledown \Psi(r,z). \tag{3}$$

Here $\bigtriangledown$ is gradient and from Eq. (3) we have,

$$\begin{aligned} E_r &= \sum_i \frac{2\Psi_0}{r_1}.\frac{J_1(m_i r)}{J_1(m_i r_1)}.\frac{ch(m_i z)}{ch(m_i z_1)}, \\ E_\theta &= 0, \\ E_z &= -\sum_i \frac{2\Psi_0}{r_1}.\frac{J_0(m_i r)}{J_1(m_i r_1)}.\frac{sh(m_i z)}{ch(m_i z_1)}, \end{aligned} \tag{4}$$

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:

$$\begin{aligned} \frac{d^2u}{d\xi^2} - (\alpha - 2\chi\cos 2\xi/(1 - k\cos 4\xi)).\sum_i \frac{J_1(\lambda_i u)}{J_1(\lambda_i)}.\frac{ch(\lambda_i v)}{ch(\lambda_i \frac{z_1}{r_1})} &= 0, \\ \frac{d^2v}{d\xi^2} + (\alpha - 2\chi\cos 2\xi/(1 - k\cos 4\xi)).\sum_i \frac{J_0(\lambda_i u)}{J_1(\lambda_i)}.\frac{sh(\lambda_i v)}{ch(\lambda_i \frac{z_1}{r_1})} &= 0, \end{aligned}$$

with the following substitutions:

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

where α and χ are the trapping parameters, $\lambda_i = m_i r_1$ is roots of equation $J_0(m_i r_1) = 0$.

3. Numerical Results

3.1. Fractional Resolution

The resolution of a square cylindrical ion trap mass spectrometry in general, is a function of the mechanical accuracy of the cylindrical of the CIT with $r_1 = z_1$ Δr_1, and the stability performances of the electronics device such as, variations in voltage amplitude ΔV, the rf frequency $\Delta\Omega$ and Δk $(0 \le k < 1)$, which tell us, how accurate is the form of the voltage signal. The factor Δk plays an important role in building the stability diagrams for the purpose of the mass resolution. $\Delta k = 0$ is an ideal case for higher resolution value. To derive a useful theoretical formula for the fractional resolution, one has to recall the stability parameters of the impulsional excitation for the CIT with $r_1 = z_1$

$$\chi = 4\frac{e}{m} \times \frac{(V_{ac})_k(1-k)}{r_1^2\Omega^2} \tag{5}$$

By taking the partial derivatives with respect to the variables of the stability parameter χ for Eq. (5), then the expression of the resolution Δm of the CIT with $r_1 = z_1$ are as follows,

$$\Delta m = (\frac{8e(V_{ac})_k(1-k)}{r_1^3\Omega^2\chi})\,|\Delta r_1| + (\frac{4e(1-k)}{r_1^2\Omega^2\chi})\,|\Delta V_{ac}| + (\frac{8e(V_{ac})_k(1-k)}{r_1^2\Omega^3\chi})\,|\Delta\Omega| + (\frac{4e(V_{ac})_k}{r_1^2\Omega^2\chi})\,|\Delta k|\,. \tag{6}$$

Now to find the fractional resolution we have,

$$\frac{m}{\Delta m} = \{\left|\frac{\Delta V_{ac}}{V_{ac}}\right| + 2\left|\frac{\Delta\Omega}{\Omega}\right| + 2\left|\frac{\Delta r_1}{r_1}\right| + \left|\frac{\Delta k}{1-k}\right|\}^{-1}, \tag{7}$$

here Eq. (7) are the fractional resolutions for CIT with $r_1 = z_1$.

m	k	CIT with $r_1 = z_1$			
		U		V_{ac}	
		LT	UT	LT	UT
1	0.0	-5.696	1.213	0.000	15.442
1	0.95	-5.696	1.213	0.000	306.546
2	0.0	-11.378	2.515	0.000	30.743
2	0.95	-11.378	2.515	0.000	610.327

Table 1: The values of (U, V) at the lower and upper tips of the first stability regions of a CIT with $r_1 = z_1$ computed in this article for $m = 1, 2$ and $k = 0, 0.95$. Here "LT" is Lower tip and "UT" is Upper tip.

We have used the stability parameters az and q_z to establish the first stability diagrams in the (U, V_{ac}) plane. The following parameters are used: $r_0 = 10$ mm, $\Omega = 2\pi f = 2\pi \times 650 \times 10^3$ rad/s, $k = 0$ and 0.95 and for the mass range of $m = 1$, and 2 a.m.u. (hydrogen and hydrogen like isotopes). The computed stability diagrams in (U, V_{ac}) plane for CIT with $r_1 = z_1$ are depicted in Fig.(3) and their lower and upper limits are displayed in Table (1). From Fig. (3), it can be seen that, the size of stability diagrams for the same masses are much larger for the $k = 0.95$ than the sinusoidal classical mode $k = 0$ in CIT with $r_1 = z_1$. This means that, more confining voltage needed for $k = 0.95$ than $k = 0$ for the same ion mass-to-charge ration.

As for $m = 2$ a.m.u., $k = 0.95$ and $U = 0$, the limited confining voltage for a CIT with $r_1 = z_1$ is 610.327 (V). One can see that, the limits of confining voltage ratio are the same in CIT with $r_1 = z_1$. The same ratio also can be found for CIT with $r_1 = z_1$ when $k = 0$. As far as the fractional resolution is concerned, we have considered Eq. (7) for the cases of $k = 0$ and $k = 0.95$. For the fractional mass resolution we have used the following uncertainties for the voltage, rf frequency and the geometry; $\Delta V_{ac}/V_{ac} = \Delta V/V = 10^{-5}$, $\Delta\Omega/\Omega = 10^{-7}$, $\Delta r_1/r_1 = \Delta r_0/r_0 = 310^{-4}$ for $k = 0$ and for $k = 0.95$ we have taken arbitrary the modulation "index" parameter $\Delta k = 10^{-6}$. The fractional resolutions obtained for CIT with $r_1 = z_1$ with $\beta_z = 0.1$ are $m/\Delta m = 1345.4505$ for $k = 0$ and $m/\Delta m = 1311.9134$ for $k = 0.95$, with $\beta_z = 0.9$ are $m/\Delta m = 1603.8325$ for $k = 0$ and $m/\Delta m = 1555.7953$ for $k = 0.95$.

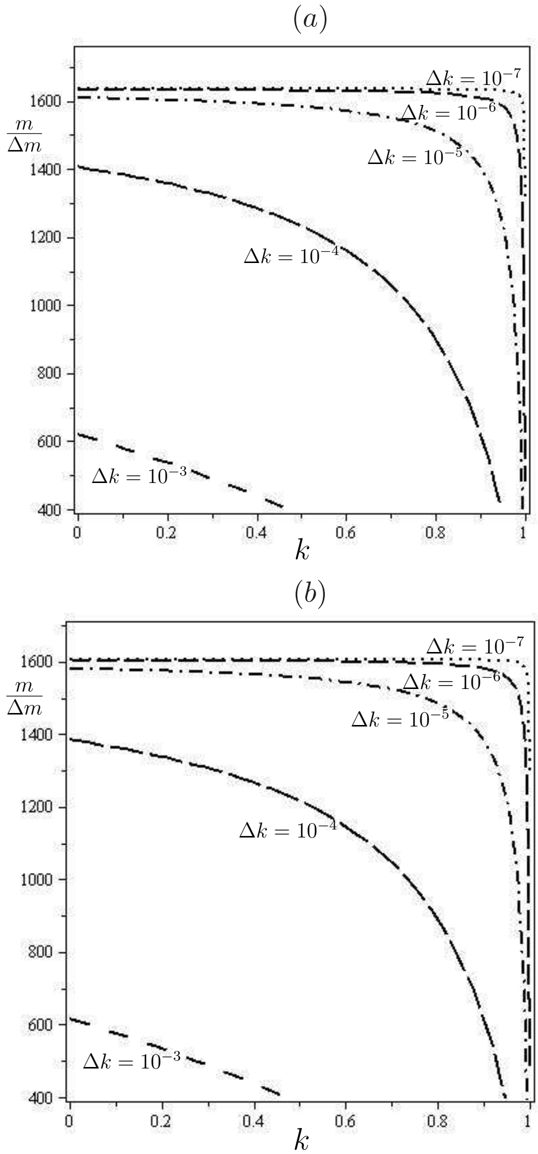
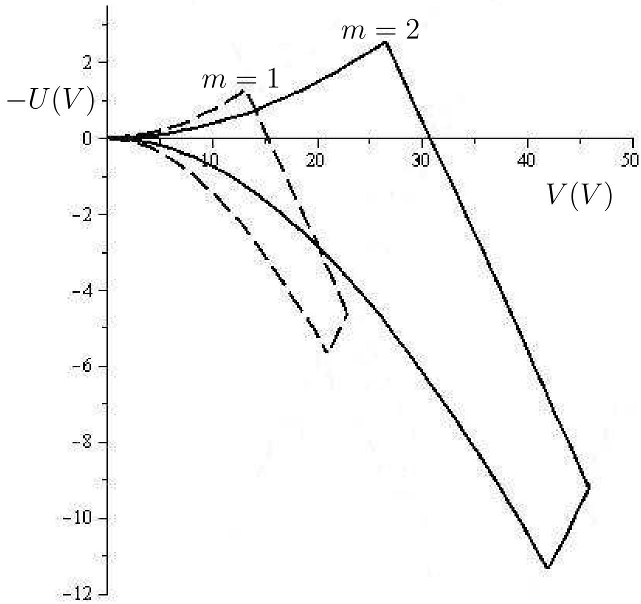


Figure 2: The fractional resolution as a function of the modulation "index" parameter k for a CIT with $r_1 = z_1$ when $\beta_z = 0.1$ and $\beta_z = 0.9$, (a) $\beta_z = 0.1$, (b) $\beta_z = 0.9$.

(a)



4. Conclusion

The behavior of a CIT with $r_1 = z_1$ has been demonstrated. It has been demonstrated that, higher confinement voltages are needed for CIT with $r_1 = z_1$ cases when the modulated "index" parameter $k = 0.95$. The ratio of confinement voltage is the same for $k = 0$ and $k = 0.95$. These types of functioning behavior of CIT with $r_1 = z_1$, preformed to have higher resolution in mass as far as theoretical study concerned.

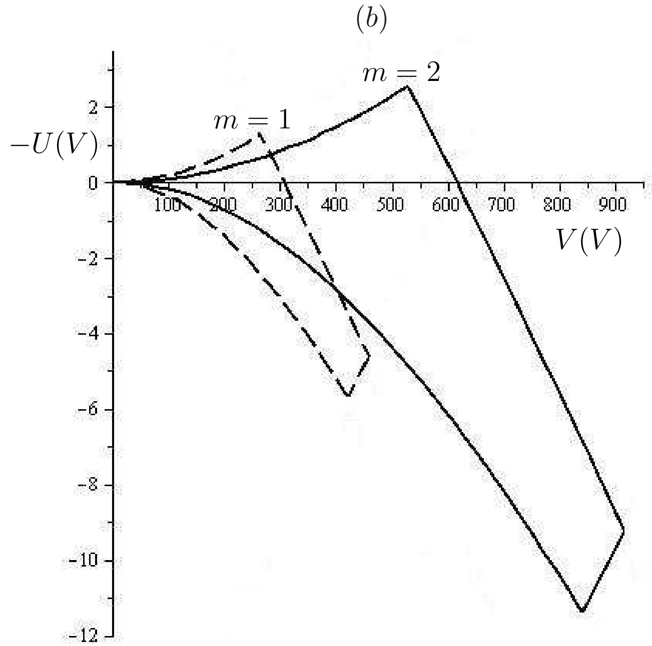


Figure 3: (a) and (b) The stability diagram in (U,V) plan in the CIT with $r_1 = z_1$ for $m = 1, 2$ and (a) $k = 0$, (b) $k = 0.95$.

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