

Study of Cylindrical Ion Trap with New Periodic Impulsional Potential Form

^{1,2}S. Seddighi Chaharborj, ¹I. Fudziah, ^{1,3}Z.A. Majid and ⁴Y. Gheisari

¹Department of Mathematics, Faculty of Science,
 Universiti Putra Malaysia, 43400 UPM, Malaysia

²Department of Mathematics, Science and Research Branch,
 Islamic Azad University, Bushehr Branch, Bushehr, Iran

³Institute of Mathematical Research Universiti Putra Malaysia,
 43400 UPM Serdang Selangor Darul Ehsan, Malaysia

⁴Department of Mathematics, Islamic Azad University, Bushehr Branch, Bushehr, Iran

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Abstract: The paper reports on some theoretical studies carried out on a cylindrical ion trap (CIT) supplied with a new periodic radio frequency impulsional potential of the form $V_{af}(t) = \frac{\cos \Omega t [1 + k \cos 2\Omega t]}{1-k}$ with $0 \leq k < 1$ ($\lfloor \cdot \rfloor$ means floor function). The performance characteristics of the cylindrical ion trap impulsional mode, for the two stability regions, were computed using fifth order Runge-Kutta method and compared to the classical sinusoidal mode $k = 0$. The physical properties of the confined ions in the r and z axes are illustrated.

Key words: Cylindrical ion trap • Impulsional potential • Fifth order Runge-Kutta method • Stability regions • Ion trajectory

INTRODUCTION

Ion trap mass spectrometry has developed through several stages to their current stage of relatively high performance and increasing popularity [1]. Quadrupole ion trap (QIT) invented by Paul and Steinwedel [2] has been widely applied to mass spectrometry [3-6], ion cooling and spectroscopy [7], frequency standards [8], quantum computing [9] and so on. To apply to various objectives, various geometries of ion trap for the mass spectrometer has been suggested [10]. 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 [11]. 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 [12] and Oak Ridge National Laboratory [13] have researched on the applications of the CIT to a miniaturized mass spectrometer.

In this article, the physical properties of the confined ions of the rectangular CIT supplied with a new periodic impulsional potential form is studied and compared.

Study the Motions of Ion Voltage Inside CIT: Figure (1) shows the electronics configuration of CIT, that is to say a combinations of d.c. voltage, U_{dc} and an alternative voltage $V_{af}(t)$ with $f(t) = \frac{\cos \Omega t [1 + k \cos 2\Omega t]}{1-k}$ with $0 \leq k < 1$ is the modulation “index” parameter for the ring and end-caps electrodes, $\Psi_0 = \pm(U_{dc} - V_{ac} \frac{\cos \Omega t [1 + k \cos 2\Omega t]}{1-k})$ with $0 \leq k < 1$, then the potential distribution inside the CIT at any point of a circle of radius r can be written as, $\Psi(r, z) = \sum_i \frac{2\Psi_0}{m_i r_i} \frac{J_0(m_i r)}{J_1(m_i r_i)} \frac{ch(m_i z)}{ch(m_i z_i)}$. 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, θ) inside the CIT can be written: $(E_r, E_\theta, E_z) = E = -\nabla \Psi(r, z)$ Here ∇ 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:

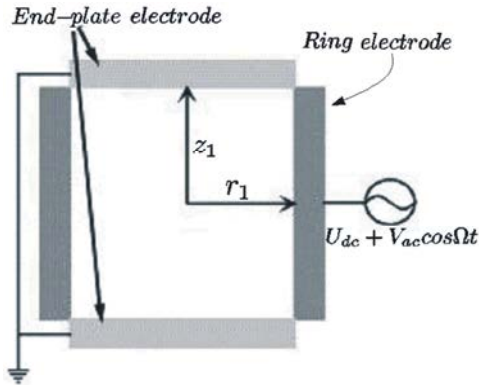


Fig. 1: Schematic view of a square cylindrical ion trap (CIT)

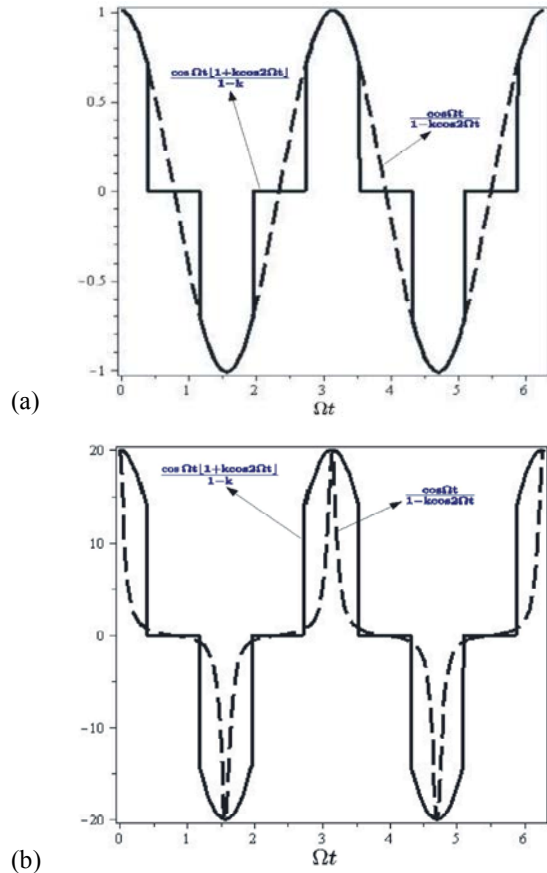


Fig. 2: Shape of potential function for impulsive potentials, dash line: periodic impulsive potential of the form $V \frac{\cos \Omega t}{1-k \cos 2\Omega t}$, solid line: periodic impulsive potential of the form $V \frac{\cos \Omega t [1+k \cos 2\Omega t]}{1-k}$, (a): $k=0.1$ and (b): $k=0.95$

$$\frac{d^2 u}{d\tau^2} - (\alpha - 2\chi \frac{\cos 2\tau [1+k \cos 2\Omega t]}{1-k}) \sum_i \frac{J_1(\lambda_i u)}{J_1(\lambda_i)} \frac{ch(\lambda_i v)}{ch(\lambda_i \frac{z_1}{r_1})} = 0,$$

$$\frac{d^2 v}{d\tau^2} + (\alpha - 2\chi \frac{\cos 2\tau [1+k \cos 2\Omega t]}{1-k}) \sum_i \frac{J_0(\lambda_i u)}{J_1(\lambda_i)} \frac{sh(\lambda_i v)}{ch(\lambda_i \frac{z_1}{r_1})} = 0,$$

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

α and χ are the trapping parameters and $\lambda_i = m_i r_1$ is roots of equation $J_0(m_i r_1) = 0$. Figure (2).(a) and (b) show the comparison of periodic impulsive potential of the form $V \frac{\cos \Omega t [1+k \cos 2\Omega t]}{1-k}$, presented in this paper and periodic impulsive potential of the form $V \frac{\cos \Omega t}{1-k \cos 2\Omega t}$, reported by S. M. Sadat Kiai in 1991 [sadat2], when $k = 0.1$ and $k = 0.9$.

RESULTS

Stability Regions: There are two stability parameters which control ion motion for each dimension u ; α , χ in the case of quadrupole ion trap. In the plane (α, χ) for the axis z , the ion stable and unstable motions are determine by comparing the amplitude of the movement to one for various values of α , χ . To compute the accurate elements of the motion equations for the stability diagrams, a fifth order Runge-Kutta method is employed. Figure (3).(a) and Figure (4).(a) and Figure (3).(b) and Figure (4).(b) present the calculated first and second stability regions for the cylindrical ion trap, when $k = 0.0$ and $k = 9.9$, dash line: CIT with periodic impulsive potential of the form $V \frac{\cos \Omega t}{1-k \cos 2\Omega t}$, solid line: CIT with periodic impulsive potential of the form $V \frac{\cos \Omega t [1+k \cos 2\Omega t]}{1-k}$.

Ion Trajectories: Figure (5) and Figure (6) show the ion displacements both in real time and in the phase space for some characteristic equivalent operating points within two stability diagrams, $k = 0$ and 0.95 when $\beta_z = 0.4$, respectively. Figure (5), (6). (a): ion trajectories in real time for $\beta_z = 0.4$ when $k = 0; 0.95$, respectively, P: CIT with periodic impulsive potentials of the form $V \frac{\cos \Omega t}{1-k \cos 2\Omega t}$,

N: CIT with periodic impulsive potentials of the form $V \frac{\cos \Omega t [1+k \cos 2\Omega t]}{1-k}$ and Figure (5), (6). (b): evolution of the phase space ion trajectory for different values of the phase τ_0 for $\beta_z = 0.4$ when $k = 0; 0.95$, respectively, line: QIT with periodic impulsive potentials of the form $V \frac{\cos \Omega t}{1-k \cos 2\Omega t}$, dot line: QIT with periodic impulsive potentials of the form $V \frac{\cos \Omega t [1+k \cos 2\Omega t]}{1-k}$. Table (1) shows

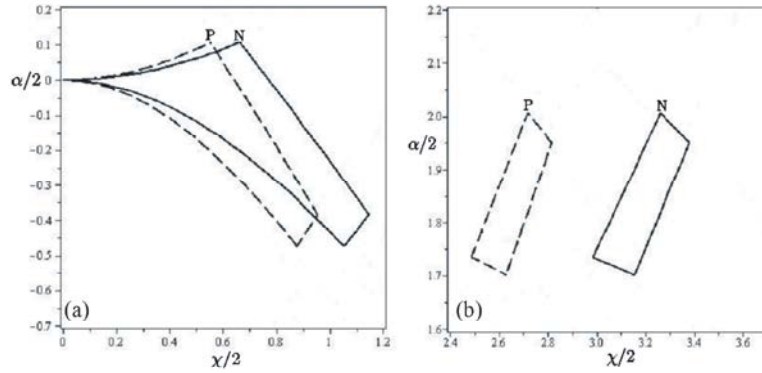


Fig. 3: The first and second stability regions for the CIT when $k=0.0$, (a): first stability region and (b): second stability region, dash line: CIT with periodic impulsional potential of the form $V \frac{\cos \Omega t}{1-k \cos 2\Omega t}$, solid line: CIT with periodic impulsional potential of the form $V \frac{\cos \Omega t [1+k \cos 2\Omega t]}{1-k}$.

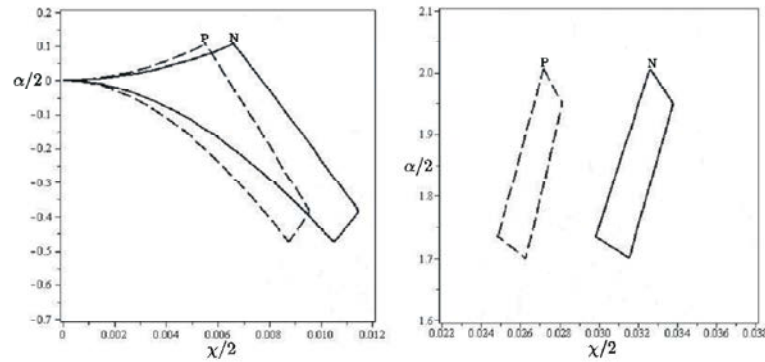


Fig. 4: The first and second stability regions for the CIT when $k=0.99$, (a): first stability region and (b): second stability region, dash line: CIT with periodic impulsional potential of the form $V \frac{\cos \Omega t}{1-k \cos 2\Omega t}$, solid line: CIT with periodic impulsional potential of the form $V \frac{\cos \Omega t [1+k \cos 2\Omega t]}{1-k}$.

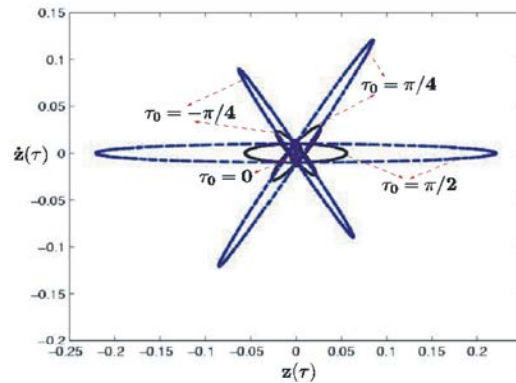


Fig. 5: Ion trajectories in real time for $\beta_z = 0.4$ when $k=0.0$, black color: CIT with periodic impulsional potentials of the form $V \frac{\cos \Omega t}{1-k \cos 2\Omega t}$, blue color: CIT with periodic impulsional potentials of the form $V \frac{\cos \Omega t [1+k \cos 2\Omega t]}{1-k}$ and (b): evolution of the phase space ion trajectory for different values of the phase τ_0 for $\beta_z = 0.4$ when $k=0.0$, black color: CIT with periodic impulsional potentials of the form $V \frac{\cos \Omega t}{1-k \cos 2\Omega t}$, blue color: CIT with periodic impulsional potentials of the form $V \frac{\cos \Omega t [1+k \cos 2\Omega t]}{1-k}$.

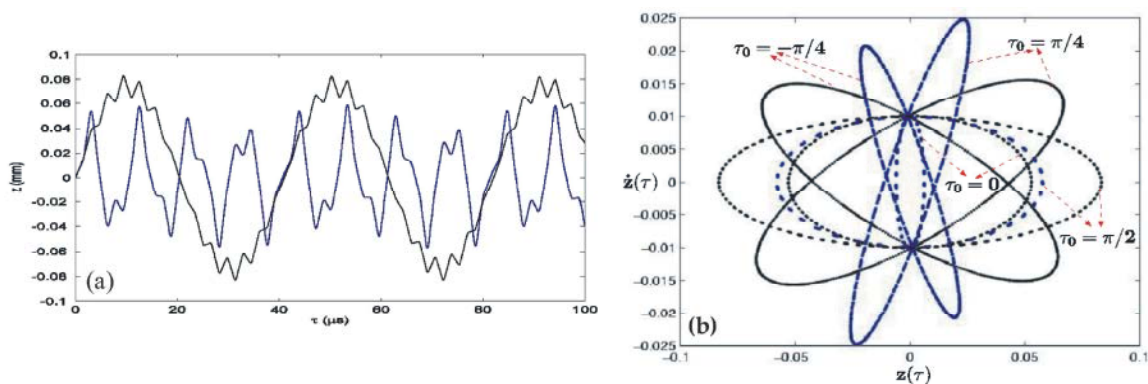


Fig. 6: Ion trajectories in real time for $\beta_z = 0.4$ when $k=0.95$, black color: CIT with periodic impulsive potentials of the form $V \frac{\cos \Omega t}{1-k \cos 2\Omega t}$, blue color: CIT with periodic impulsive potentials of the form $V \frac{\cos \Omega t [1+k \cos 2\Omega t]}{1-k}$ and (b): evolution of the phase space ion trajectory for different values of the phase τ_0 for $\beta_z = 0.4$ when $k=0.95$, black color: CIT with periodic impulsive potentials of the form $V \frac{\cos \Omega t}{1-k \cos 2\Omega t}$, blue color: CIT with periodic impulsive potentials of the form $V \frac{\cos \Omega t [1+k \cos 2\Omega t]}{1-k}$.

Table 1: The values of $x/2$ for the cylindrical ion trap with periodic impulsive potentials of the form $V \frac{\cos \Omega t}{1-k \cos 2\Omega t}$ and $V \frac{\cos \Omega t [1+k \cos 2\Omega t]}{1-k}$ when $\beta_z = 0.4; 0.8; 0.99$ and $k=0.0; 0.95$

β_z	k	$x/2$	$x/2$
		$V \frac{\cos \Omega t}{1-k \cos 2\Omega t}$	$V \frac{\cos \Omega t [1+k \cos 2\Omega t]}{1-k}$
0.4	0.00	0.3753	0.4503
0.4	0.95	0.0188	0.0225
0.8	0.00	0.6102	0.7322
0.8	0.95	0.0305	0.0366
0.99	0.00	0.6420	0.7704
0.99	0.95	0.0321	0.0385

the values of $x/2$ for the CIT with periodic impulsive potentials of the form $V \frac{\cos \Omega t}{1-k \cos 2\Omega t}$ and CIT with periodic impulsive potentials of the form $V \frac{\cos \Omega t [1+k \cos 2\Omega t]}{1-k}$ for $\beta_z = 0.4; 0.8; 0.99$ and $k = 0; 0.95$.

DISCUSSION AND CONCLUSION

In this article, we have studied some theoretical studies carried out on a quadrupole ion trap supplied with a new periodic radio frequency impulsive potential of the form $V \frac{\cos \Omega t [1+k \cos 2\Omega t]}{1-k}$ with $0 \leq k < 1$. The new impulsive potential form presents a better zero potential zone when compared with the latest impulsive potential

form. This characteristic of the new signal might have useful when dealing with ion cooling. As the zero potential zone is a suitable region for sending photons or other particles inside the ion trap.

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