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# Ion dynamics in a Paul trap driven by various radio frequency waveforms

Hüsnü Aksakal [a,b,*]

[a] Nigde University, Department of Physics, 51240 Nigde, Turkey
[b] Kahramanmaraş Sütçü Imam University, Vocational School of Health Services, Department of Medical Imaging Techniques, 46100 Kahramanmaraş, Turkey

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ABSTRACT

In this study we explore single ion dynamics in a Paul trap (three-dimensional radio frequency (RF) quadrupole ion trap – 3D QIT), driven by Sinusoidal, Rectangular, Sawtooth and Triangular RF waveforms. A molecular dynamic simulation code in Python has been written to explore ion dynamics in the trap. It is shown that various radio frequency waveforms produce various shift in ion oscillation in the trap. Furthermore phase space plots and the magnitude of the potential well depth for these various waveforms are given. Possible influences of these various RF waveforms have been summarized.



## 1. Introduction

Trapping of ions has commenced from 1950s and is being used extensively in a wide range of scientific investigation, from mass spectrometer to the quantum computer [1]. One of interesting aspect is cold trapped ions were used to carry out quantum information process of ions at low temperature with coherent manipulation by laser of the quantum state of individual ions [2]. In the quantum world, the basic information carrier encoded by two-level system can be in any super-position of the ground and the excited state is called a quantum bit (qubit) which can be studied by trapped ions. Moreover, trapped and laser-cooled atoms or ions, due to having long coherence times and individual addressing, allow for the experimental implementation of quantum gates [3]. In addition to quantum process, chaos and order are also investigated using trapped atoms [4]. When cooling the ions to explore quantum effect, RF heating is one of source of ion instability in the trap. Various RF waveforms could arise different ion temperature. Therefore cooling could be needed different requirements in each RF waveform. However, investigation of a trap driven by various RF waveforms has not been studied in detail yet. In principle, an ion trap can be operated with any periodic RF wave-forms. Digital circuit can be used to obtain these periodic waveforms. The Paul trap, with a rectangular driving field, is known as digital ion trap (DIT) [5]. Ion motion in a DIT was described early in 1970s which can be seen in Ref. [6] and references therein. DIT is explored experimentally in Ref. [6]. Mass selective resonance method is described in 2000 under digital operation condition [5]. Rectangular, Sine and Triangular RF waveforms have been examined by experimentally in Ref. [7] and it has been emphasized that rectangular and triangular waveforms make the frequency scan in mass spectroscopy easier than conventional sine wave.

In the present study we assess collision-free single ion oscillation in the trap using Rectangular (Rect), Sinusoidal (Sine), Triangular (Tri) and Sawtooth (Saw) RF waveforms. To our knowledge, this study represents the first demonstration that the ion oscillation in a trap driven with these various RF waveforms compared with the case conventional sine based waveform. In addition we summarize possible influence of these operations on the ion motion. Macro and micro-motion characteristics are presented in the framework of Mathieu equation. Furthermore duty cycle effect for DIT is also investigated. For the investigation a molecular dynamic (MD) simulation code has been written in Python. The code Python for Digital ion trap (PyDIT) details are given in Appendix A.1 where comparison of our code with literature is presented. In Section 2 effect of RF waveforms and in Section 3 results are presented. Moreover potential well depth for these waveforms is presented in Section 3.

* Correspondence to: Nigde University, Department of Physics, 51240 Nigde, Turkey. Tel.: +90 5353058972.
*E-mail address:* haksakal@nigde.edu.tr

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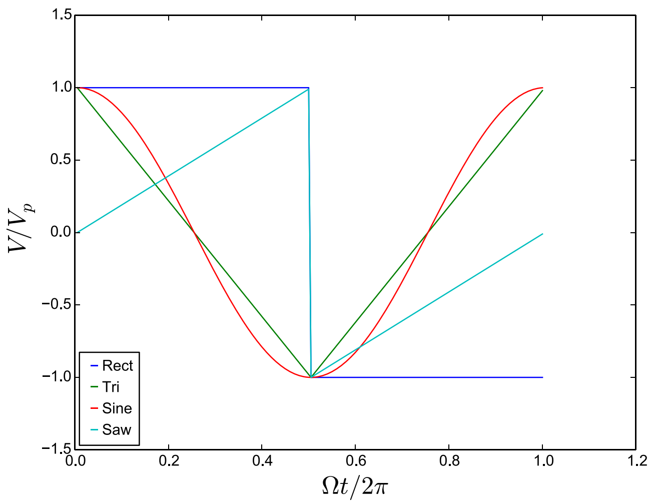


**Fig. 1.** One RF period of applied AC voltage ($V = V_pF(\xi)$) for various RF waveforms.

## 2. Theory of single ion dynamics in various RF waveform

### 2.1. Applied potential

In principle, AC component of trapping voltage can be replaced by any periodic signal to trap ions. The applied potential for a three-dimensional quadrupole ion trap (3D-QIT) is given as in Eq. (1).

$$\phi = \frac{U + V_pF(\xi)}{\sqrt{(r_0^2 + 2z_0^2)}}(x^2 + y^2 - 2z^2) \tag{1}$$

where $U$ is DC potential, $r_0$ is radius of ring electrode in the central horizontal plane, $2z_0$ is separation of two end-cap electrodes measured along axis of the ion trap, $V_p$ is zero to peak amplitude and $F(\xi)$ is periodicity of AC potential, where $\xi = \Omega t/2$ and $\Omega$ is frequency. The frequency dependence values of proposed AC potentials are given in Eqs. (2)–(5) and they have periodic waveform $F(\xi + \pi) = F(\xi)$ [7]. Proposed waveforms for one RF period are presented in Fig. 1.

$$F_{Sine}(\xi) = \cos(2\xi) \tag{2}$$

$$F_{Rect}(\xi) = \begin{cases} 1, & \text{if} \quad 0 \le \xi < \pi/2 \\ -1, & \text{if} \quad \pi/2 \le \xi < \pi \end{cases} \tag{3}$$

$$F_{Tri}(\xi) = \begin{cases} 1 - \dfrac{4\xi}{\pi}, & \text{if} \quad 0 \le \xi < \pi/2 \\ -3 + \dfrac{4\xi}{\pi}, & \text{if} \quad \pi/2 \le \xi < \pi \end{cases} \tag{4}$$

$$F_{Saw}(\xi) = \begin{cases} \dfrac{2\xi}{\pi}, & \text{if} \quad 0 \le \xi < \pi/2 \\ -2 + \dfrac{2\xi}{\pi}, & \text{if} \quad \pi/2 \le \xi < \pi \end{cases} \tag{5}$$

### 2.2. Equation of motion

The trap used in present study consists of hyperbolic trap which has a single point in coordinate space to trap particle, contrary to the linear trap which has a trap axis in coordinate space where the micro-motion vanishes. Using previously defined applied potential, the equation of motion of trapped ion is given as Mathieu equation [1,7–12]:

$$\frac{d^2u}{d\xi^2} = -(a_u - 2q_uF(\xi))u \tag{6}$$

**Table 1**
Trap and ion initial condition.

| Parameters | Value used in PyDIT |
|---|---|
| $r_0, z_0$ (mm) | 10.0, 7.071 |
| $m/z$ (Th) | 100 |
| $a_z, q_z$ | 0.0, 0.4 |
| x, y, z (mm) | 0.5, 0.5, 0.5 |
| $\dot{x},\dot{y},\dot{z}$ (m/s) | −150, −350, 694.57 |
| RF Frequency (MHz) | 1.1 |
| Time step (μs) | 0.01 |

where $u$ indicates ($x$, $y$ and $z$) coordinate, $a_u$, $q_u$ are dimensionless Mathieu parameters, in three-dimensions; they are given as in Eq. (7).

$$a_z = -2a_r = -\frac{16ZeU}{m\sqrt{(r_0^2 + 2z_0^2)}\Omega^2}$$
$$q_z = -2q_r = \frac{8ZeV}{m\sqrt{(r_0^2 + 2z_0^2)}\Omega^2} \tag{7}$$

where $r$ is $x$ or $y$, $m$ is mass of ion, $Z$ is the charge number, $e$ is the elemental charge [7,10–12]. By rearrangement of Eq. (6), substitution $\xi$ in Eqs. (2)–(5) time dependent form of equation of motion is obtained as Eq. (8).

$$\frac{d^2u}{dt^2} = -\frac{\Omega^2}{4}(a_u - 2q_uF(t))u \tag{8}$$

In the simulation we used RF waveforms given in Fig. 1. Eq. (8) is used to explore ion oscillation in the trap. Harmonic expansion of these waveforms is used to estimate potential depth of waveforms which is explained in the next section. Using these RF waveforms would help to understand impact of quadrupole potential phase relation on the ion motion [10]. In the present study ion dynamics in these RF waveforms have been investigated.

## 3. Results and discussion

Parameters, presented in Table 1 are used in the simulation. Proposed RF waveforms are chosen with same amplitude and frequency. Using these RF waveforms for same trap with same initial condition of ion (velocity, coordinate) given in Table 1, oscillations in $x$ and $z$ dimension can be seen from Fig. 2(a) and (c) respectively.

As it can be seen from figures, once trapped at various RF waveforms, ion will have different macro-oscillation periods than conventional sine based RF waveform. While sawtooth and rectangular ($Duty = 0.5$) waveforms represent bigger macro-motion amplitude than sinusoidal RF waveform, triangular has same macro-motion amplitude. Moreover rectangular waveform has less micro-motion than sine based RF waveform and for long trapping time a modulation in sawtooth RF waveform can be also seen from the same figure.

Using parameters in Table 1, three-dimensional trajectory of ion in the trap for various RF waveforms can be seen in Fig. 3. In the case of rectangular and sawtooth RF waveforms ion will have longer trajectory than Sinusoidal and Triangular RF waveforms can be seen from the figure.

Phase space plots are presented in $x$ and $z$ dimensions in Figs. 4 and 5 respectively. As it can be seen from the figures rectangular and sawtooth RF waveforms have different orientation than conventional sine based phase space plot. Another properties can be seen from each phase space plot that the ion has different turning points and different velocities inside the trap. Oscillation and phase space plots in $y$ dimension are not presented here because of symmetry properties with $x$ dimension.