Stability Regions in Quadrupole Ion Trap

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Abstract
In this article we used the fifth order of the Runge-Kutta method to compute the twelve stability regions of the quadrupole ion trap using a periodic potential of the form \( V_0 \cos \Omega t/(1 - k \cos 2 \Omega t) \) with \( 0 \leq k < 1 \) for \( k = 0, k = 0.1, k = 0.2, k = 0.3, k = 0.4, k = 0.5, k = 0.6, k = 0.7, k = 0.8, k = 0.9 \). We compare the first until five stability regions computed in this article with the first until five stability regions of article reported by H. Noshad and A. Droudi in 2009.

Keywords: Twelve stability regions; Higher order Runge-Kutta method; Quadrupole ion trap; Paul trap; Ion trajectories

1 Introduction
Ion trap mass spectrometry has developed though several stages to their current stage of relatively high performance and increasing popularity [4]. Quadrupole ion trap invented by Paul and Steinwedel [6] has been widely applied to mass spectrometry [4], ion cooling and spectroscopy [2], frequency standards [7], quantum computing [3], and so on. To apply to various objectives, various geometries of ion trap for the mass spectrometer has been suggested [1, 10]. An ion trap is a combination of electric or magnetic fields that captures ions in a region of a vacuum system or tube. Ion traps have a number of scientific uses such as trapping ions while the ion’s quantum state is manipulated and mass spectrometry. When using ion traps for scientific studies of quantum
state manipulation, the Paul trap is most often used. This work may lead to a trapped ion quantum computer and has already been used to create the worlds most accurate atomic clocks [8].

The purpose of this article is to accurately compute twelve stability regions for a quadrupole ion trap in the $a-q$ plane using the Runge–Kutta methods with higher order derivative approximations [9] for different $k$’s. We compare the first until five stability regions computed in this article with the first until five stability regions of article reported by H. Noshad and A. Droudi in 2009 [5].

2 Theory

Fig. (1) shows a schematic view of a quadrupole ion trap (QIT). The QIT is the ion trap with quadrupole geometry. The QIT is composed of a ring and two end cap electrodes facing each other in the $z$–axis. $z_0$ is the distance from the center of the QIT to the end cap and $r_0$ is the distance from the center of the QIT to the nearest ring surface. To obtain the equation of motion in the QIT, the electric potential applied to the end cap electrodes is as follows

$$
\phi_0 = U - V \cos \Omega t / (1 - k \cos 2\Omega t), \tag{1}
$$

where $U$ and $V$ are dc and ac potentials, respectively. $\Omega$ is the angular frequency in rad/s of the rf voltage. Considering that $r_0^2 = 2z_0^2$ is the square of ring electrode radius. The electric field components into the trap become

$$
E_z = \frac{(U - V \cos \Omega t / (1 - k \cos 2\Omega t))}{z_0^2} z, \tag{2}
$$

$$
E_r = \frac{(U - V \cos \Omega t / (1 - k \cos 2\Omega t))}{r_0^2} r. \tag{3}
$$

The equation of motion for a singly charged positive ion is given

$$
\frac{d^2 z}{d\tau^2} + (a_z - 2q_z \cos 2\tau / (1 - k \cos 4\tau))z = 0, \tag{4}
$$

$$
\frac{d^2 r}{d\tau^2} + (a_r - 2q_r \cos 2\tau / (1 - k \cos 4\tau))r = 0. \tag{5}
$$

The $a$ and $q$ parameters for $z$ and $r$ components as well as the dimensionless parameter $\tau$ are defined as follows $\tau = \frac{\Omega t}{2}$, $a_z = -2a_r = \frac{4eU}{mz_0^2\Omega^2}$, $q_z = -2q_r = \frac{2eV}{mz_0^2\Omega^2}$, where $m$ is the ion mass and $e$ is the electronic charge.
3 Results

3.1 Stability regions

Fig. (2) up to Fig. (6) present the stability regions of Paul 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 0.9.

Figure 2: The first stability region for a Paul trap. (a): The first stability region for $k = 0$, (b): The first stability region, for $k = 0, k = 0.1, k = 0.2, k = 0.3, k = 0.4, k = 0.5, k = 0.6, k = 0.7, k = 0.8, k = 0.9.
Figure 3: The second stability region for a Paul trap. (a): The second stability region for $k = 0$, (b): The second stability region, for $k = 0, k = 0.1, k = 0.2, k = 0.3, k = 0.4, k = 0.5, k = 0.6, k = 0.7, k = 0.8, k = 0.9$. 
Figure 4: The third stability region for a Paul trap. (a): The third stability region for \( k = 0 \), (b): The third stability region, for \( k = 0, k = 0.1, k = 0.2, k = 0.3, k = 0.4, k = 0.5, k = 0.6, k = 0.7, k = 0.8, k = 0.9 \).
Figure 5: The fourth stability region for a Paul trap.  

(a): The fourth stability region for $k = 0$, 

(b): The forth stability region, for $k = 0, k = 0.1, k = 0.2, k = 0.3, k = 0.4, k = 0.5, k = 0.6, k = 0.7, k = 0.8, k = 0.9$. 

Figure 6: The fifth stability region for a Paul trap. (a): The fifth stability region for $k = 0$, (b): The fifth stability region, for $k = 0, k = 0.1, k = 0.2, k = 0.3, k = 0.4, k = 0.5, k = 0.6, k = 0.7, k = 0.8, k = 0.9$. 
4 Discussion and conclusion

The results of the numerical integration of the Mathieu equation with the help of the fifth-order Runge-Kutta method using 0.001 steps increment showed that, the apex of the stability parameters \( a_z \) stayed the same but the higher limit of \( q \) decrease substantially when \( k \) increase form 0 to 0.9. It has been demonstrated that, higher confinement voltages are needed for QIT when the modulated "index" parameter \( k = 0.9 \) is applied.

References


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