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# Truncated series solution of the equation of motion of ions trapped in a radiofrequency quadrupole trap with superimposed octopolar potential

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**Abstract**

The power series method is used to solve numerically the equation of motion of ions in a radiofrequency quadrupole ion trap when a small octopolar potential is present. Every time step, the coordinates of the ion are represented by a truncated series of degree 15. The stability diagram of the trap is obtained by using the method to simulate the behavior of hundreds of ions up to a relatively large time. The nonlinear resonance lines are observed. The ion's oscillation frequencies are then studied. Their theoretical expression is derived and compared to the results of the truncated series solution.


*Keywords:* Radiofrequency quadrupole ion trap; Series solution of the equation of motion; Stability diagram; Octopolar potential; Nonlinear resonances; Ion's oscillation frequencies

## 1. Introduction

The radiofrequency quadrupole ion trap is a small and versatile device which allows to maintain ions in a small volume of space by the application of a DC and a radiofrequency voltage. Since its invention in the 1950s by W. Paul and H. Steinwedel, it found multiple applications in physics, chemistry, biology, pharmacology and environmental sciences [1]. It is made of a ring having the radius $r_0$ closed by two end-caps located at the distance $z_0$ from the trap's center [2]. Usually $r_0^2 = 2z_0^2$. The three electrodes have hyperboloidal shape. The end-caps are connected together and a voltage $U_{DC} + V_{AC}\cos\Omega t$ is applied between them and the ring.

Ideally, the potential generated in the volume of the trap is quadrupolar but for real traps it is more complicated. Its general expression in the spherical coordinates $(\rho, \theta, \varphi)$ is given by [3]

$$\Phi(\rho, \theta) = (U_{DC} + V_{AC}\cos\Omega t)\sum_{n=0}^{\infty} b_n \rho^n P_n(\cos\theta) \quad (1)$$

$b_n$ are constants and $P_n$ the Legendre polynomial of order $n$. If in addition, the trap has a symmetry about the $z = 0$ plane ($z$ is the trap's axis), only the even terms have to be

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considered [4]. By taking only the terms of order 2 and 4, the potential (1) can be written in Cartesian coordinates as [5]

$$\Phi(r, z) = \frac{A_2}{r_0^2}(U_{DC} + V_{AC}\cos\Omega t) \times \left[\frac{r^2}{2} - z^2 - \frac{f}{r_0^2}\left(z^4 - 3r^2z^2 + \frac{3}{8}r^4\right)\right] \quad (2)$$

$A_2$ is equal to 1 for ideal traps and $f$ is a constant related to the strength of the octopolar contribution.

The equation of motion for an ion of mass $m$ and charge $q$ under the action of the potential (2) is

$$\frac{d^2u}{d\tau^2} + (a_u - 2q_u\cos(2\tau))ug_u(r, z) = 0 \quad (3)$$

where $u = x$, $y$ or $z$, $r^2 = x^2 + y^2$, $\tau = \frac{\Omega t}{2}$ and

$$g_{x,y}(r, z) = 1 - \frac{f}{r_0^2}\left(\frac{3}{2}r^2 - 6z^2\right)$$
$$g_z(r, z) = 1 - \frac{f}{r_0^2}(3r^2 - 2z^2) \quad (4)$$

$a_u$ and $q_u$ are the Mathieu parameters which have the expressions

$$a_z = -\frac{8A_2qU_{DC}}{mr_0^2\Omega^2} = -2a_x = -2a_y$$
$$q_z = \frac{4A_2qV_{AC}}{mr_0^2\Omega^2} = -2q_x = -2q_y \quad (5)$$

A trapped ion performs oscillations with the fundamental frequencies $\omega_u = \beta_u\frac{\Omega}{2}$ [5]. $\beta_u$ is function of the Mathieu parameters.

The trapping is possible only for $q_z$ and $a_z$ chosen in some regions of the ($q_z$, $a_z$) plane. The usual region is called the lowest stability domain and corresponds to $\beta_z$ and $\beta_x = \beta_y$ (noted $\beta_r$) having the values between 0 and 1 [6].

Simulations of the trapped ions dynamics in radiofrequency quadrupole ion traps have been realized since decades now [7,8]. The positions and velocities of every ion are calculated by solving numerically the equation of motion or using its analytical solution. The power series method has also been used to solve numerically the ion's equation of motion [9,10]. It allows to get accurate results with a relatively small calculation time. The trajectories of hundreds of ions up to several milliseconds can be calculated very quickly. This is useful when some parameters such as the Mathieu parameters are scanned with small steps. Several thousands of cases can be studied in few hours.

## 2. Resolution of the trapped ion equation of motion using the power series method

The use of the power series method for the resolution of the trapped ion equation of motion is explained in details in Refs. [9,10]. The variable $\xi = \Omega t$ (RF phase) is considered. To calculate the velocity and the position of an ion from $t = 0$ to $t_{max}$, the time step $\Delta t$ is taken equal to 19% of the RF period $T = \frac{2\pi}{\Omega}$. For the $N$th step the coordinates $x$, $y$ and $z$ are represented by the truncated series

$$x = \sum_{n=0}^{15} A_n(\xi - N\Delta\xi)^n$$
$$y = \sum_{n=0}^{15} B_n(\xi - N\Delta\xi)^n \quad (6)$$
$$z = \sum_{n=0}^{15} C_n(\xi - N\Delta\xi)^n$$

with $\Delta\xi = \Omega\Delta t = 0.38\pi$. The coefficients $A_0$, $A_1$, $B_0$, $B_1$, $C_0$ and $C_1$ are obtained from the initial conditions for $N = 0$, then by imposing the continuity of the position and the velocity for the other steps. The other coefficients are given by recursion relations.

## 3. Simulation of the trap's stability diagram

The truncated series solution of the ion's equation of motion can be used to simulate the first stability domain for a radiofrequency quadrupole trap. For that we considered the evolution of the position of 200 ions of mass 1 amu up to 10,000 periods of the RF field ($\xi_{max} = 2\times10^4\pi$) in a trap having $r_0 = 7$ mm and $z_0 = 5$ mm. The ions were first generated inside the trap volume with uniform random positions and Maxwellian velocities with the temperature 1000 K. They were considered individually and the trajectory of each one of them was calculated before considering the next one. To be trapped, the coordinates $x$, $y$ and $z$ must inside the volume of the trap which has hyperboloidal electrodes. The trapping conditions are then

$$r^2 - 2z^2 < r_0^2 \quad \text{and} \quad 2z^2 - r^2 < 2z_0^2 \quad (7)$$

This is tested every time step. If the test is negative, the ion is considered as lost and the calculations stopped for it. At $\xi = \xi_{max}$ the number of ions remaining trapped for a working point ($q_z$, $a_z$) is counted.

The number of ions trapped up to $\xi_{max}$ as function of the Mathieu parameters is shown in Fig. 1 in grayscale map. $q_z$ was scanned from 0 to 1.5 with a step of 0.0111 and $a_z$ taken from -0.5 to 0.2 with a step of 0.0044.