International Journal of Mass Spectrometry 281 (2009) 79–81

Contents lists available at ScienceDirect

International Journal of Mass Spectrometry

journal homepage: www.elsevier.com/locate/ijms

Computation of five stability regions in a quadrupole ion trap using the fifth-order Runge–Kutta method

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ARTICLE INFO

Article history:
Received 21 October 2008
Received in revised form 15 December 2008
Accepted 19 December 2008
Available online 31 December 2008

Keywords:
Five stability regions
Fifth-order Runge–Kutta method
Quadrupole ion trap
Mathieu equation

ABSTRACT

An algorithm based on the fifth-order Runge–Kutta (RK5) method was used to compute the five stability regions in a quadrupole ion trap (Paul trap). Except for the first region, the calculations were made for the positive values of *a* in the *a*–*q* plane. Computation of these regions for a Paul trap has been carried out for the first time using the fifth-order Runge–Kutta method.

1. Introduction

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 [1–3]. The analytical method allows the analytical formulation of an ion trajectory over an unlimited number of cycles [1]. As a weakness of the analytical method in comparison with the matrix method, it should be noted that analytical method is limited to the cosine-shaped trapping waveforms [1], and cannot be directly used for solution of the more general Hill equation [1,4]. On the other hand, numerical methods are generally simple and convergent techniques using the Runge–Kutta methods. Among these methods, the fourth-order Runge–Kutta (RK4) method is most popular. It is accurate, stable and easy to program. Nevertheless, for some applications one might prefer to use the Runge–Kutta methods with higher order derivative approximations [5,6].

Some articles deal with two-dimensional quadrupole mass filters operating in higher regions of stability [7]. These regions are of interest because they obtain higher mass resolution in comparison with the mass filters operating in lower stability regions [3,8,9]. Moreover, they offer the ability to analyze the masses of ion beams with high kinetic energy or unit resolution with ions of 10 keV energy [3,7]. It is worth noting that with operation in higher stability regions, only a very small mass range of ions can be trapped simultaneously, which are determined by the sizes of the stability regions. Thus, operation in these regions may be limited to specialized applications. Computation of such regions is practically a time-consuming and tedious work to do, and it needs high accuracy and precision due to the narrowness of the regions. As an example, one can see the inaccurate first and second stability diagrams reported by Sadat Kiai et al. [10]. The error in the second diagram lies in shifting the stability region to the right, which corresponds to higher values of *q*; whereas, in the first diagram, the lower part of the diagram has been shifted to lower values of *a*.

The purpose of this paper is to accurately compute five stability regions for a quadrupole ion trap in the *a*–*q* plane using the RK5 method [11] rather than the simpler and most popular algorithm, the so-called fourth-order Runge–Kutta method. The RK5 method simulates the accuracy of the Taylor series method of order 5; whereas, the more common RK4 method simulates it as the order of 4. In this computation, except for the first region, the stability diagrams have been computed for the positive values of the Mathieu parameters, namely $a > 0$ and $q > 0$.

2. Theory

Theoretical treatment of a Paul trap as well as the related formulas is well-established, and can be found in the literature [12]. Fig. 1 shows a schematic view of a quadrupole ion trap. It composed of a ring metallic electrode located symmetrically between two metallic end-cap electrodes. In the figure, the ring electrode has been grounded; whereas, the electric potential applied to the end-cap

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doi:10.1016/j.ijms.2008.12.016

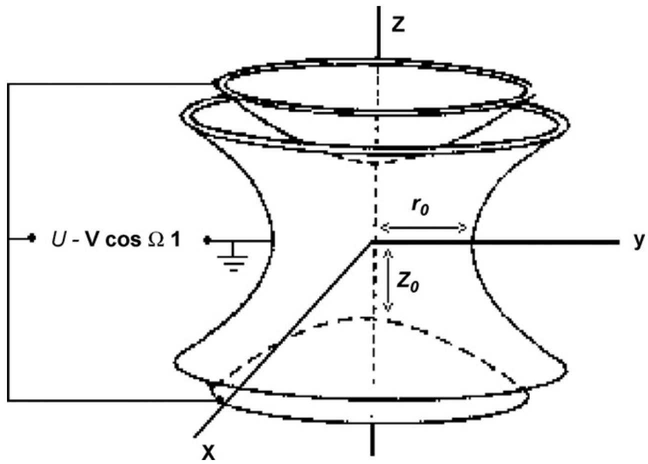

Fig. 1. A schematic view of a Paul trap.

electrodes is

$$\varphi_0 = U - V\ \cos\ \Omega t, \tag{1}$$

where U and V are dc and ac potentials, respectively, and Ω stands for the trapping rf angular frequency in rad/s. Considering that $r_0^2 = 2z_0^2$, the electric field components into the trap become

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

$$E_r = \frac{(U - V\ \cos\ \Omega t)}{2z_0^2} r. \tag{3}$$

Consequently, the equations of motion of a particle with mass M and charge Q in this field can be expressed by the set of Mathieu differential equations

$$\frac{d^2z}{d\xi^2} + (a_z - 2q_z\ \cos\ 2\xi)z = 0 \tag{4}$$

$$\frac{d^2r}{d\xi^2} + (a_r - 2q_r\ \cos\ 2\xi)r = 0. \tag{5}$$

The a and q parameters for z and r components as well as the dimensionless parameter ξ are defined as follows:

$$\xi = \frac{\Omega t}{2} \tag{6}$$

$$a_z = -2a_r = \frac{4QU}{Mz_0^2\Omega^2} \tag{7}$$

$$q_z = -2q_r = \frac{2QV}{Mz_0^2\Omega^2}. \tag{8}$$

3. Computational results

To compute the stability regions of the Paul trap, the Eqs. (4) and (5) were solved by using the Runge–Kutta algorithm with higher order derivative approximations, namely the RK5 method. Computations were made for all the values of the Mathieu parameters a and q lying in the selected interval for each region. For this purpose, the small and equal steps for a and q parameters were considered. The steps were selected as 0.005, 0.002, 0.0002, 0.0002 and 0.0001 for the five stability regions. Figs. 2–6 show the five stability regions in the a–q plane obtained from our computation for a quadrupole ion trap using the fifth-order Runge–Kutta method. Because different conventions are used for the second, the third and other higher stability regions, we have labeled the five regions on a separate figure shown as Fig. 7. Moreover, the values of the lower and upper tips of

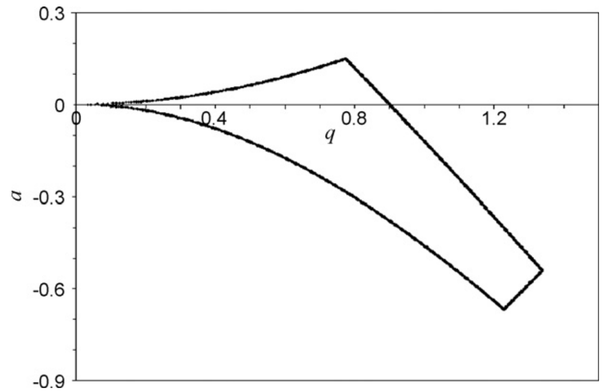

Fig. 2. The first stability region for a Paul trap obtained from our RK5 method.

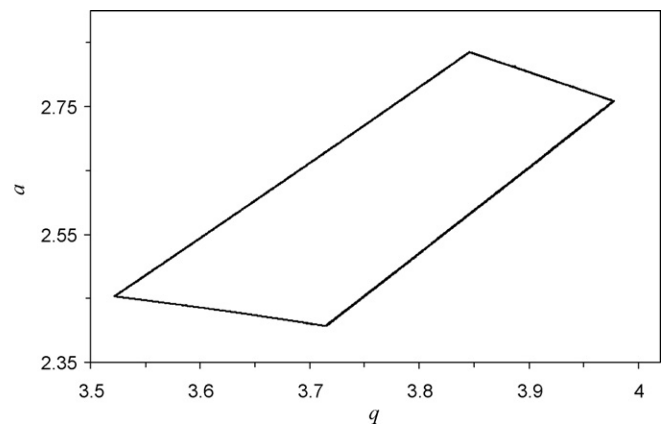

Fig. 3. The second stability region for a Paul trap obtained from our RK5 method.

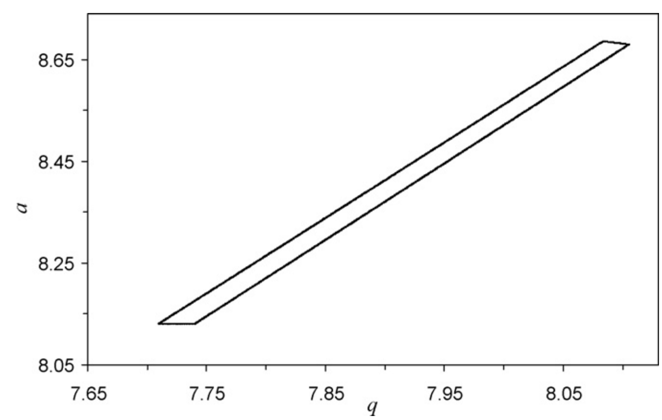

Fig. 4. The third stability region for a Paul trap obtained from our RK5 method.

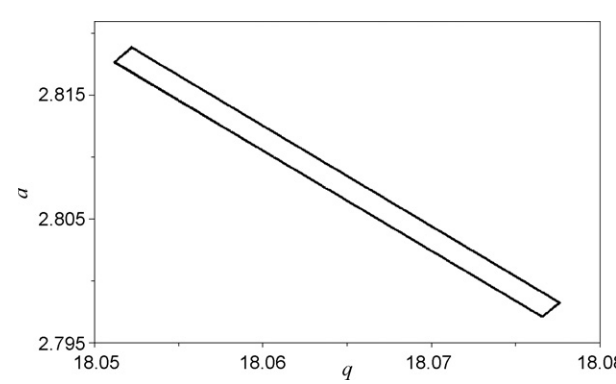

Fig. 5. The fourth stability region for a Paul trap obtained from our RK5 method.

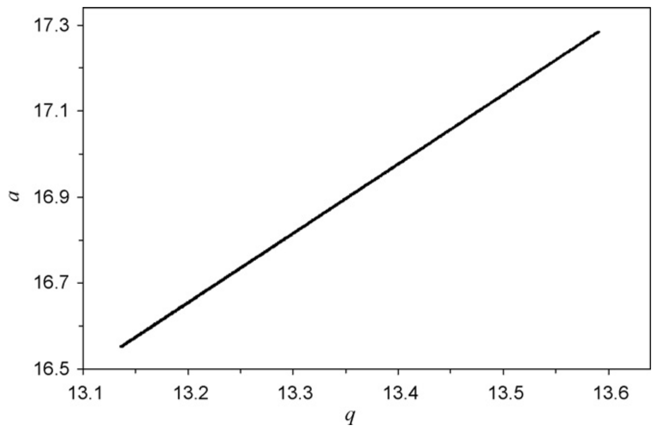

Fig. 6. The fifth stability region for a Paul trap obtained from our RK5 method.

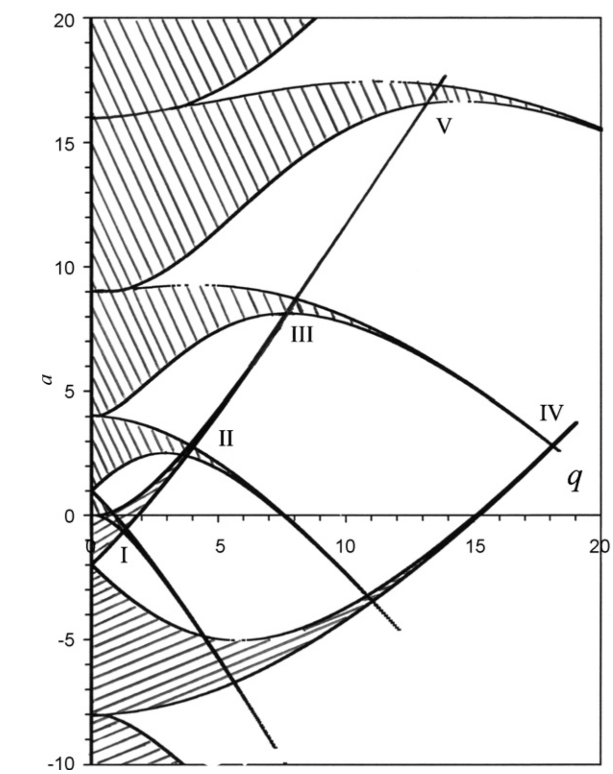

Fig. 7. The stability regions I, II, III, IV and V of the Paul trap computed in this work using the RK5 method.

the stability diagrams computed in this paper are listed in Table 1. One can see the significant difference between Figs. 2 and 3 with the corresponding results reported by Sadat Kiai et al. [10], which show that the first and second stability regions are not quite accurate. In that article, the Mathieu differential equations were solved by matrix techniques using a finite difference method.

Table 1
The values of (a, q) at the lower and upper tips of the five stability regions of a Paul trap computed in this work.

Region no.	Tip	a	q
I	Upper	0.15	1.35
	Lower	−0.67	0
II	Upper	2.84	3.98
	Lower	2.41	3.52
III	Upper	8.69	8.11
	Lower	8.13	7.71
IV	Upper	2.818	18.077
	Lower	2.797	18.051
V	Upper	17.28	13.59
	Lower	16.55	13.14

4. Conclusion

Five stability regions in a Paul trap were accurately computed by using a numerical algorithm based on the RK5 method. In this computation, the size of the integration step was considered as 0.02. Also, the computation was repeated for the integration step size, 0.05, and no significant effects on the final results were found. The first stability region obtained in this work is in excellent agreement with that published by Dawson [12].

In general, the Runge–Kutta method with any order is the same as integration by Simpson's rule. For the same step size in the RK5 and RK4 algorithms, if the only error at each step is attributed to the Simpson's rule, the accumulated error for the RK5 method would be less than that of the RK4 method. However, it should be noted that it is not easy to obtain the accuracy of a Runge–Kutta solution, and it is also beyond the scope of this paper.

The results obtained from our computation show that the first and second stability regions published in 2005 [10] do not have enough accuracy. Furthermore, the regions of stability obtained in this paper have been computed for the first time using the fifth-order Runge–Kutta method.

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