International Journal of Mass Spectrometry 408 (2016) 62–76

Contents lists available at ScienceDirect

International Journal of Mass Spectrometry

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

Determination of multipole coefficients in toroidal ion trap mass analysers

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ARTICLE INFO

Article history:
Received 6 May 2016
Received in revised form 28 June 2016
Accepted 29 June 2016
Available online 4 August 2016

Keywords:
Toroidal ion trap
Mathieu parameters
Secular frequency
Toroidal harmonics
Toroidal multipole coefficients

ABSTRACT

In this paper, we present methods to determine multipole coefficients for describing the potential in toroidal ion trap mass analysers. Three different methods have been presented to compute the toroidal multipole coefficients. The first method uses at least square fit (LS) and is useful when we have ability to compute potential at a set of points in the trapping region. In the second method we use the Discrete Fourier Transform (DFT) of potentials on a circle in the trapping region. The third method uses surface charge distribution obtained from the Boundary Element Method (BEM) to compute these coefficients. Using these multipole coefficients we have presented (1) equations of ion motion in toroidal ion traps, (2) the Mathieu parameters in terms of multipole coefficients and (3) the secular frequency of ion motion in these traps. It has been shown that the secular frequency obtained from our method has a good match with that obtained from numerical trajectory simulation.

1. Introduction

In this paper, we discuss three different methods to determine multipole coefficients suitable for describing the potential in toroidal ion trap mass analysers.

A toroidal ion trap mass analyser can be viewed as a linear ion trap curved around and connected at the ends or as a cross section of a quadrupole ion trap (QIT) rotated on edge to form the toroid [5,13]. This produces a circular ion trapping region [4]. These are axi-symmetric devices. In the literature the toroidal ion trap was originally presented as a storage device [2,3]. Later, the use of toroidal ion traps as mass analysers was demonstrated by Bier and Syka [4] and Lammert et al. [5]. These analysers have large trapping region and less space charge effect in comparison to quadrupole ion trap mass analysers in which trapping occurs at a point [4]. These analysers are now available commercially in a miniaturized structure [36].

Toroidal ion trap mass analysers have received the attention of several researchers [6–15]. These studies include design and simplification of toroidal ion trap mass analysers [5–10] and miniaturization of toroidal mass analysers [6,11–13]. Another direction to this investigation were simulation studies of ion trajectories in toroidal ion trap mass analysers [7,8].

Efforts to optimize the performance of toroidal ion trap mass analysers require the evaluation of potentials and fields within the device. Lammert et al. [5] have made toroidal ion trap mass analyser by optimizing the electric field obtained numerically. Taylor and Austin [10] have designed a simplified and optimized toroidal ion trap geometry by setting desired percentage of multipole coefficients. These multipole coefficients are obtained by polynomial fitting to the numerically obtained potential along its axis. This is same as multipole expansion in axially symmetric ion trap mass analysers such as QIT, in which potential around trapping point is expressed in series form of Legendre polynomials [30,16,18]. Higgs and Austin [7] have taken a polynomial fit to the numerically obtained potential in the trapping region of the toroidal ion trap and have used this polynomial to compute the trajectory of ion motion.

Some shortcomings of these approaches have been highlighted in the literature. For instance Higgs and Austin [7] pointed out that there is a lack of understanding of higher order field contributions and their effects on ion motion in toroidal ion traps. Further, Higgs et al. [8] suggested that a solution based on a toroidal coordinate system may be more appropriate and useful. It is at this point that our study hopes to contribute. We will take up for investigation the determination of multipole coefficients in the toroidal coordinate system. Such studies are not available in the mass spectrometry

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http://dx.doi.org/10.1016/j.ijms.2016.06.011
1387-3806/

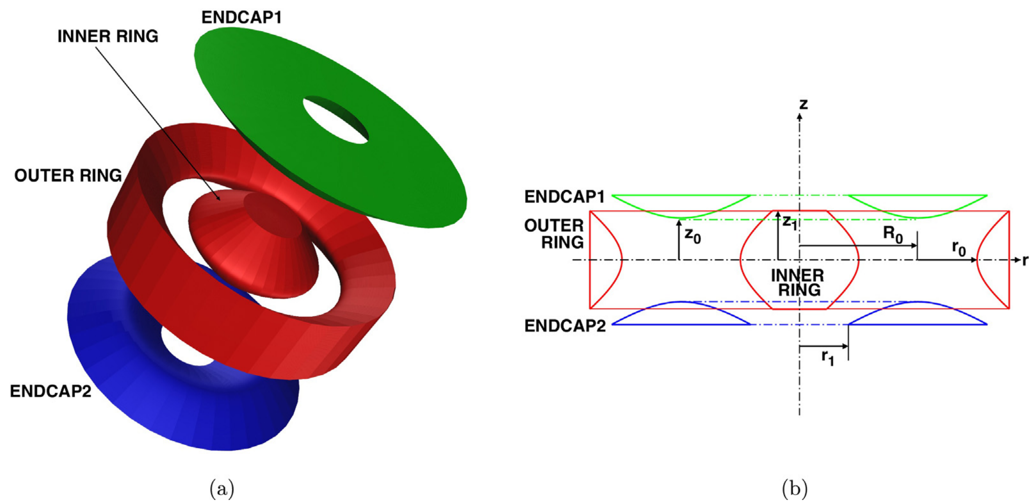

Fig. 1. Schematic view of HypTorTrap obtained from a quadrupole ion trap rotated on edge to form the toroid. (a) Three dimensional view and (b) cross section in *xz*-plane.

literature and to our knowledge it is not readily available in the mathematical literature too.

Three approaches have been adopted in this study for three different circumstances. In the first method, a least square fit is used. This method is useful when we have ability to compute potential at a set of points in the trapping region. We call this method as LS method in this paper. This method is analogous to the method used to compute multipole coefficients for cylindrical ion traps (CIT) by Wu et al. [18], in which a least square fit of potential with polynomial has been used. In the second method, we use Discrete Fourier Transform (DFT) of potential on a circle (having a particular property which will be discussed later) in the trapping region. This method has greater accuracy with less computational effort, in comparison to the LS method. We call this method as the DFT method in our discussion. This method is analogous to computation of Laurent coefficients using the DFT [27]. The third method is used when the surface charge distribution has been determined using the boundary element method. We call this method as the Surface Charge BEM (SC-BEM) method. This method is analogous to the method used by Beaty [30] to compute multipole coefficients for the QIT.

Having obtained toroidal multipole coefficients, the Mathieu parameters [1] will be shown in terms of these coefficients. Although the formulae for Mathieu parameters in terms of multipole coefficients for nonlinear ion traps, such as CIT, have been presented in the literature [17], similar formulae do not exist for toroidal ion traps. Having obtained the Mathieu parameters in terms of toroidal multipole coefficients, we will show how these can be used to estimate secular frequencies [1] in these traps.

Five separate toroidal trap geometries have been taken up for investigation. Of these, two are similar to the geometries reported in the literature, while the other three are chosen to demonstrate that our method can handle the variety of complexities that may arise. However, the methods presented in this paper are applicable to toroidal ion traps in general, and not restricted to the example geometries discussed here.

Geometries considered in the study are presented in Section 2, and Section 3 presents the computational methods. Required theory will be discussed in Section 4 and results are presented in Section 5.

2. Geometries considered

In this section we present five geometries that have been taken up for investigation.

2.1. The geometry HypTorTrap

The first geometry considered will be referred to as HypTorTrap. This geometry has four electrodes, each electrode cross section is hyperbolic. This geometry is similar to the symmetric version of the geometry considered by Lammert et al. [5]. We have considered this for simplicity, although the asymmetric version that they have investigated has better performance than the symmetric one. Fig. 1(a) shows its three dimensional view. This trap is obtained from QIT rotated on edge to form the toroid. Its cross section in *xz*-plane is shown in Fig. 1(b). The distance R_0, from origin to the mid point between ring electrodes on *x*-axis is 20 mm. The half distance r_0, between ring electrodes is taken as 10 mm and the half distance z_0, between endcap electrodes is taken as 7.07 mm. The truncation of ring electrodes as well as endcap electrodes is done such that the trap has top bottom symmetry. The truncation of endcap electrodes are done such that the least distance between *z*-axis and truncation point is r_1, which is taken as 8.24 mm. The ring electrodes are truncated at height z_1 from radial plane (or *xy*-plane) and is taken as 8.31 mm.

The parametric equations of the hyperbolic surfaces are given as follows: INNER RING: $r(t) = R_0 - r_0\cosh(t)$ and $z(t) = z_0\sinh(t)$; OUTER RING: $r(t) = R_0 + r_0\cosh(t)$ and $z(t) = z_0\sinh(t)$; ENDCAP1: $r(t) = R_0 + r_0\sinh(t)$ and $z(t) = z_0\cosh(t)$; ENDCAP2: $r(t) = R_0 + r_0\sinh(t)$ and $z(t) = -z_0\cosh(t)$. In all cases t changes from -1 to 1.

2.2. The geometry CylTorTrap

The second geometry considered will be referred to as CylTorTrap. It is obtained by replacing hyperbolic electrodes of the trap shown in Fig. 1(a), with flat electrodes. This too, like HypTorTrap discussed above, is a symmetric version of the trap reported by Lammert et al. [10]. Fig. 2(a) shows its three dimensional view. The electrodes are obtained by replacing hyperbolic surfaces of ring electrodes shown in Fig. 1(a) with cylinders and endcap electrodes with annuli. Its cross section in *xz*-plane is shown in Fig. 2(b). The distance R_0, from origin to the mid point between concentric cylinders on *x*-axis is 20 mm. The half distance r_0, between concentric cylinders is taken as 10 mm and the half distance z_0, between endcap electrodes is taken as 10 mm. The half height z_1, of cylinders forming ring electrodes is taken as 6 mm. The thickness d, of cylinders forming ring electrodes is taken as 4 mm. The hole radius r_1, of annuli forming endcap electrodes is taken as 6 mm. The thickness d, of annuli forming endcap electrodes is taken as 4 mm.