



Multipole expansion in quadrupolar devices comprised of planar electrode arrays

Daniel E. Austin^{a,*}, Brett J. Hansen^{a,b}, Ying Peng^a, Zhiping Zhang^a

^a Department of Chemistry and Biochemistry, Brigham Young University, Provo, UT 84602, United States

^b Department of Electrical and Computer Engineering, Brigham Young University, Provo, UT 84602, United States

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ABSTRACT

Ion trap mass analyzers made using arrays of independent electrodes allow unprecedented control and variability of electric field shapes. We present a method to select and implement specific values for higher-order multipoles, which are known to affect ion trapping and mass analysis in quadrupole ion traps. Electrode arrays are amenable to microfabrication techniques, hence this method can be used to improve performance in miniaturized ion trap mass spectrometers. With ion traps made using two opposing electrode array plates, both even- and odd-order multipoles can be independently adjusted.

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1. Introduction

Quadrupole electric potentials find widespread use in containing, guiding, and analyzing charged particles. Most commercial mass spectrometers include quadrupole mass analyzers, mass filters, or ion guides. Quadrupoles are also used to trap ions for spectroscopic studies [1], for quantum computing applications [2], and for study of chemical reaction dynamics [3]. Despite the long history and wide application, purely quadrupolar potential distributions have never been created—all quadrupolar devices contain higher-order multipoles [4,5]. For some applications, including ion trap mass spectrometry, these higher-order multipoles can have a significant effect on performance [6,7]. A classic example is the original Finnigan ion trap mass spectrometer, which was manufactured with a “stretched” geometry to correct the negative octopole that interfered with mass analysis [4]. Other ion traps have also seen dramatic changes in mass resolution resulting from small changes in the magnitude and sign of higher-order multipoles [8].

Changing the shape and/or position of electrodes is commonly done to optimize the electric fields of quadrupole ion traps [5]. Additional “compensation” electrodes (positioned between the primary electrodes) have also been suggested as a method to modify the trapping fields [9,10]. However, these techniques have a simultaneous effect on all the components of the field. For example,

increasing the separation between hyperbolic electrodes in an ion trap changes not only the quadrupole field, but also the other even, higher-order field components. Several studies have reported configurations that optimize a single component in linear ion traps and quadrupole mass filters (e.g., optimizing only the 12-pole), or that optimize a linear combination of higher-order fields [11,12], but individual field components cannot be independently optimized.

Higher-order multipoles are of particular concern for miniaturized and microfabricated quadrupole-based mass analyzers. Efforts to miniaturize ion trap mass analyzers have typically relied on simplified electrode geometries. For instance, the cylindrical ion trap—a geometrically simplified version of the quadrupole ion trap—has been the basis for many miniaturized and microfabricated mass analyzers [13–18]. Similarly, the rectilinear ion trap uses electrodes that are simpler, and therefore easier to miniaturize, than the linear ion trap from which it is conceptually derived [19,20]. However, with geometrical simplification comes a decrease in the quality of electric fields and the resulting mass resolution.

Our lab has previously introduced a new way of making radiofrequency ion traps, in which the trapping fields are created between two ceramic plates [21]. A series of independently-adjustable electrodes are lithographically deposited onto each plate. The first of these devices, the Halo ion trap, creates a toroidal trapping potential using a series of 15 concentric electrode rings per plate [22]. The planar Paul trap (a 3-D quadrupole) was later demonstrated using plates with 25 electrode rings [23]. Trapping fields in both devices were determined by the RF amplitude applied to each electrode ring. Although this approach allows significant control over the field shape, including control of multipole components, no method was

* Corresponding author at: Department of Chemistry and Biochemistry, Brigham Young University, C-310 BNSN, Provo, UT 84602, United States.
Tel.: +1 801 422 1551.

E-mail addresses: austin@chem.byu.edu, dea@byu.edu (D.E. Austin).

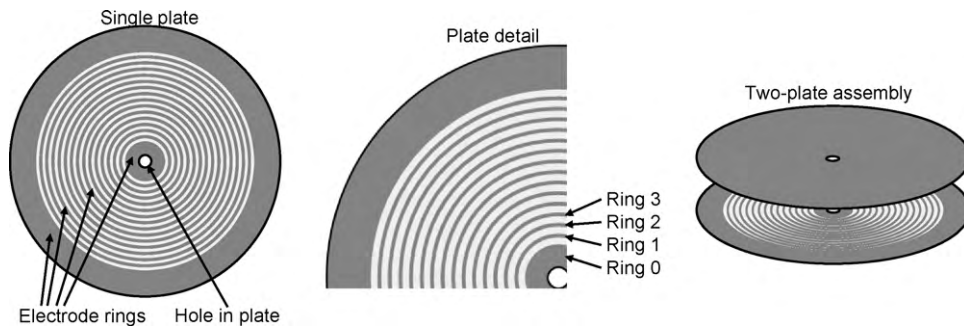


Fig. 1. Quadrupole ion trap made using two plates, each with lithographically-defined electrode rings, and overlaid with a resistive layer (not shown).

reported for determining what potentials should be applied to each ring in order to produce a given field.

This article presents a solution to this problem using standard matrix algebra. The multipole expansion of each independent electrode and the desired overall trapping field form a set of linear equations which can be solved to determine the needed potentials for each electrode. This method can be used to create fields in which the higher-order terms are independently variable. For instance, a quadrupole ion trap in which the octopole, 12-pole, and 16-pole terms are all exactly zero, can be experimentally realized. Using this approach, miniaturized mass analyzers can be produced in which the electric fields are not compromised by simplification of electrode geometry. This solution applies to all quadrupole devices consisting of arrays of electrodes on one or two plates [24]. This paper discusses the basis for and implementation of this solution.

where P_n is the Legendre polynomial of order n , and ρ_0 is the characteristic dimension (for ion traps this is typically the inner radius of the ring electrode). The set of terms with $n=0$ (monopole), $n=1$ (dipole), $n=2$ (quadrupole), $n=3$ (hexapole), etc., are referred to as the multipole expansion of a given potential distribution. The A_n -terms in this equation represent the magnitude of each pole. The A_0 -term does not affect the behavior of charged particles within the potential distribution because it produces no electric field. For primarily quadrupolar devices, the A_2 -term dominates. Odd-order terms (A_1, A_3, A_5 , etc.) are zero for systems with symmetry about a plane perpendicular to the rotational axis, including conventional quadrupole ion traps. Even, higher-order multipoles (i.e., A_4, A_6, A_8 , etc.) sometimes have significant effect on the behavior of trapped ions, and are therefore of particular concern for quadrupole-based mass analyzers. Eq. (2) can be expanded for terms $n=2, 4$, and 6 in cylindrical coordinates as follows:

$$\Phi(r, z, \phi, t) = \Phi_0(t) \left[A_2 \frac{r^2 - 2z^2}{2r_0^2} + A_4 \frac{3r^4 - 24r^2z^2 + 8z^4}{8r_0^4} + A_6 \frac{5r^6 - 90r^4z^2 + 120r^2z^4 - 16z^6}{16r_0^6} \right] \quad (3)$$

The potential along the z axis (the axis of rotation) can be found by evaluating the above equation at $r=0$:

$$\Phi(z, \phi, t)_{r=0} = \Phi_0(t) \left[A_2 \frac{-z^2}{r_0^2} + A_4 \frac{z^4}{r_0^4} + A_6 \frac{-z^6}{r_0^6} \right] \quad (4)$$

The system under consideration does not possess a characteristic radial dimension, so it is more convenient to define the A -terms based on z_0 , which is half the plate spacing:

$$\Phi(z, \phi, t)_{r=0} = \Phi_0(t) \left[A_2 \left(\frac{z}{z_0} \right)^2 + A_4 \left(\frac{z}{z_0} \right)^4 + A_6 \left(\frac{z}{z_0} \right)^6 + \dots \right] \quad (5)$$

For convenience, the signs of some of the terms in Eq. (5) have been switched, such that the dependences of all terms on z have the same sign. In this case, all A -terms of even-order multipoles will have the same sign when the poles themselves have the same sign with respect to z . A superlinear field under this convention is one in which the higher-order multipoles have the same sign as the primary quadrupole. This latter equation is the definition that will be used throughout this paper.

Because of the superposition principle, the multipole expansion of an ion trap made with an array of electrodes is equal to the sum of the multipole expansions created by each individual electrode in such an array. For instance, the quadrupole content, A_2 , of an ion trap made using an array of m rings is

$$A_2 = A_{2,1}\Phi_{01} + A_{2,2}\Phi_{02} + A_{2,3}\Phi_{03} + \dots + A_{2,m}\Phi_{0m} \quad (6)$$

where Φ_{0m} is the applied RF amplitude (Φ_0) to ring m , and $A_{2,m}$ is the quadrupole ($n=2$) term created by ring m alone. Similar equations can be written for each of the higher-order multipoles. This process leads to n equations in m variables, the $A_{n,m}$ -terms of which

2. Theory

Consider a quadrupole ion trap made using two rigid, insulating plates, as shown in Fig. 1. Each plate contains a 1-mm hole in the center, and includes electrode rings (with width 100 μm) centered at radii 2, 2.5, 3, 3.5, ..., 12 mm. An additional electrode spans the distance between the 1-mm hole and a radius of 1.8 mm. Electrodes are numbered as shown. The plates are separated by 5 mm. These dimensions are similar to those of the planar Paul ion trap reported by Zhang et al. [23]. The potential on each ring is independently adjustable. A thin layer of germanium, providing a uniform surface resistance, is deposited on top of the array of electrode rings. The potential of the germanium layer directly above an electrode ring is equal to the potential applied to that ring, while the potential of the germanium between electrode rings can be solved using Ohm's Law. The same solution would be obtained if the substrate was made of a resistive material.

The potential distribution in the region between the plates is constrained by the Laplace equation:

$$\nabla_{x,y,z}^2 \Phi = 0 \quad (1)$$

The system being considered has cylindrical symmetry, so this equation is satisfied by the following potential distribution in spherical polar coordinates:

$$\Phi(\rho, \theta, \phi, t) = \Phi_0(t) \sum_{n=0}^{\infty} A_n \frac{\rho^n}{\rho_0^n} P_n(\cos \theta) \quad (2)$$

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