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Field optimization of toroidal ion trap mass analyzers using toroidal multipoles

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ABSTRACT

Toroidal ion traps show promise for miniaturized mass spectrometers. However, because of the geometry of the trap, there remains a lack of understanding about the electric field and its effect on the motion of trapped ions. As an approach to this problem, solutions to the Laplace equation in a toroidal coordinate system can be used to characterize the electric potential distribution. The symmetric 2nd order solution of the second kind, or toroidal quadrupole, was previously explored for an ion trap. Non-ideal features in the stability diagram were similar to that for conventional ion traps with higher-order field contributions. To eliminate or reduce these non-ideal features, other solutions to the Laplace equation, including higher-order solutions, can be added to the toroidal quadrupole. The toroidal hexapole (T3) improves the stability diagram by reducing the jagged features at the stability apex and reducing the $\beta_r + 2\beta_z = 2$ resonance line when the A_3 coefficient of the toroidal hexapole is in the range of 2.75. The $\beta_r = 1/2$ resonance line is eliminated by the A_3 coefficient of 1 or greater for the toroidal hexapole. The $\beta_r = 2/3$ resonance line is not present in the viewed voltage range when the A_3 coefficient is between 3.5 and 4.75, and the $\beta_r + \beta_z = 1$ resonance line becomes evident in this same range with the toroidal hexapole contribution is greater than 4.25. The toroidal octopole (T4) and decapole (T5) give no clear trend in variation of the non-ideal features in the stability diagram. The electrode geometry and stability diagram were very sensitive to small additions of the toroidal dipole (T1). The addition of a toroidal hexapole component to the toroidal quadrupole provides improvement in ion trapping, and is expected to play an important role in optimizing the performance of all types of toroidal ion trap mass spectrometers.

1. Introduction

Ion traps use radiofrequency (RF) fields to trap ions for several purposes. For instance, spectroscopic studies have used ion traps to obtain spectra from ions in the gas phase [1,2]. Quantum optics can observe fluorescence resulting from macroscopic quantum jumps of trapped ions [3]. Ion traps can also be used as logic gates for quantum computing [4]. Gas phase reactions involving trapped ions can explore pathways of collisionally induced dissociation (CID) reactions [5]. While these applications can use various ion trap designs, only devices based on a quadrupolar potential distribution have proven to be useful for mass analysis and mass spectrometry.

Paul [6,7] developed the quadrupole ion trap (QIT) for ion storage and mass analysis. Various trap designs have been developed since then to accomplish increased ion capacity and/or ease in fabrication. The linear ion trap (LIT) confines the ions about a line as opposed to about a single point, thereby increasing the number of ions that can be trapped and analyzed [8]. The cylindrical ion trap (CIT) used cylindrical and planar electrodes, which are simpler to machine than the hyperbolic electrode shapes of the QIT [9]. The rectilinear ion trap (RIT) also uses planar electrodes while increasing the ion capacity like the LIT [10].

Lammert et al. [11] recently developed a toroidal ion trap to increase ion capacity by trapping the ions in a ring (or torus). They started with a "symmetric" toroidal ion trap design whose trapping region had the same cross section as the QIT. This design showed poor mass resolving power due to the fields introduced by the curvature of the trap. Another design, the "asymmetric" toroidal ion trap, adjusted the electrode shapes to have different asymptotic slopes for the central electrode and the outer ring electrode in order to correct the fields. This design has been miniaturized [12], and it has been used in a commercial, portable GC–MS system [13]. In 2012 Taylor and Austin [14] simplified the electrode shapes of the

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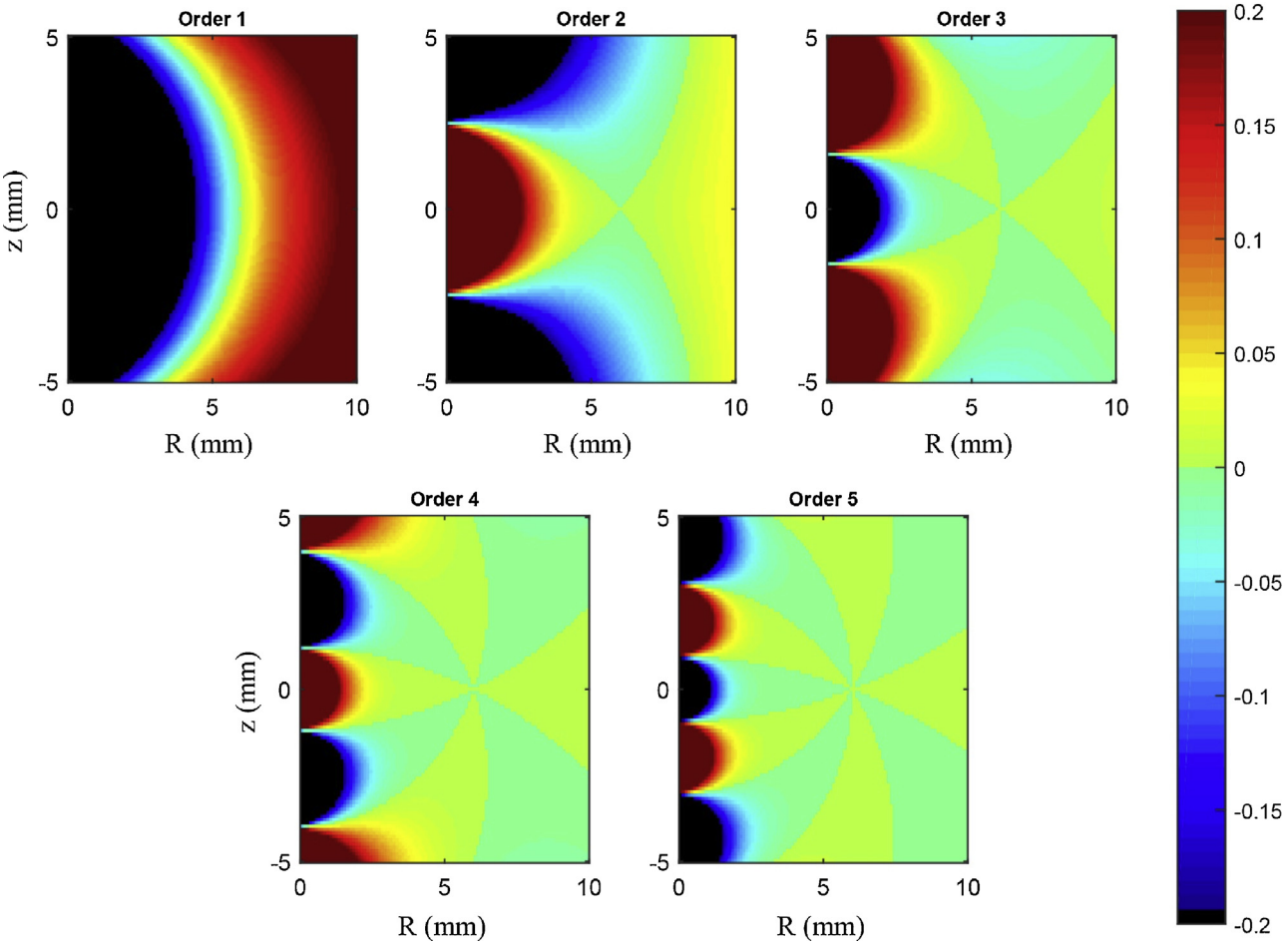

Fig. 1. Symmetric toroidal harmonics of the second kind.

toroidal ion trap so that all the electrodes were cylindrical or planar, analogous to the CIT.

Simulations to quantify the fields and observe their effects on ion motion have been used for comparing performance and improving conventional ion trap designs. Fields that deviate from the linearity found in a perfect QIT can result from imperfections in the electrode shapes such as electrode truncation, exit slits, and manufacturing tolerances. These may have both beneficial and detrimental effects on the performance of the trap as a mass analyzer. For the QIT, CIT, LIT, and RIT, the trapping potential can be expressed as the sum of different multipole contributions added to the dominant quadrupolar potential. These contributions can be calculated by taking a high-ordered polynomial fit of the potential distribution where each term represents a specific multipole contribution (A_1: dipole, A_2: quadrupole, A_3: hexapole, A_4: octopole. . .) [15]. For ion traps with a toroidal geometry, this method is not mathematically valid [16]. To be defined as a quadrupole in a Cartesian coordinate system, the potential distribution must vary as the square of the distance from the trapping center. This is not possible in toroidal devices because the potential cannot continue increasing when it meets the axis of rotation, and also because the potential does not increase quadratically when measured in a linear direction other than axially or radially.

In order to analyze the fields for these toroidal devices, we have previously compared the electric fields and simulated ion motion in three designs of ion traps: the symmetric toroidal ion trap, the asymmetric toroidal ion trap, and the cylindrical-electrode toroidal ion trap [17]. The study concluded that the asymmetric design had the best performance because its fields were closest to an ideal quadrupole. Interestingly, the cylindrical-electrode design had fields closer to that of the symmetric design even though its reported performance was as good as the asymmetric design. As an additional approach, we have also simulated ion motion in a potential distribution of a mathematically pure harmonic in a toroidal coordinate system [18]. After mapping the potential distributions of several of the orders of the symmetric toroidal harmonics of the second kind (Fig. 1), we used the second order for simulations, referred to as the toroidal quadrupole. In the immediate vicinity of the trapping region, the potential of this toroidal quadrupole closely resembles the potential in a LIT. In mapping the stability diagram of this toroidal quadrupole, there were several resonance lines and jagged edges that would possibly make this design difficult to use in mass analysis. These resonance lines may correspond to those seen in QITs with significant higher order fields superimposed such as the hexapole and octopole.

Kotana and Mohanty [19] used three methods of computing the multipole coefficients in a toroidal coordinate system for various ion traps of toroidal geometry, and all three methods gave similar results. They also presented Mathieu stability parameters and compared the secular frequencies of what they calculated and what they observed. Kotana and Mohanty [20] have also mapped out stability diagrams for the two toroidal ion trap designs first presented by Lammert's group. They found resonance lines at $\beta_r = 2/3$ and $\beta_r + 2\beta_z = 2$ (labeled as $\beta_z = 2/3$) with the stability diagrams of both designs and $\beta_r + \beta_z = 1$ for the symmetric toroidal ion trap. Lines like these are indicative of non-linear (higher-order) fields being present in the trap, and ions are ejected at the resonance line rather than the boundary during mass analysis [21]. For the QIT, resonance