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Radiofrequency trapping of ions in a pure toroidal potential distribution

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ABSTRACT

Although toroidal ion traps are being used more widely in miniaturized mass spectrometers, there is a lack of fundamental understanding of how the toroidal electric field affects ion motion, and therefore, the ion trap's performance as a mass analyzer. Toroidal harmonics, which represent solutions to the Laplace equation in a toroidal coordinate system, may be useful to understand these devices. This paper reports on SIMION simulations of ion trapping and ion motion in a time-varying electric potential representing the symmetric, second-order toroidal harmonic of the second kind—the solution most analogous to the conventional, Cartesian quadrupole. Simulations show that this potential, which we call the toroidal quadrupole, is similar to that of the Cartesian quadrupole in its ability to trap ions. The stability diagram for the toroidal quadrupole shares similarities with that of both the quadrupole ion trap (QIT) and the quadrupole mass filter (QMF), but has several minor differences including a series of chasms and a portion of the boundary that is diffuse.

1. Introduction

Radiofrequency electric fields have been used to trap ions for many applications including spectroscopy, quantum computing, time and frequency metrology, and mass spectrometry. For example, trapped ions have enabled infrared spectra [1] and fluorescence measurements [2] to be obtained from molecular species using both a conventional Paul (quadrupole) trap and also a Paul–Straubel trap [3]. For quantum computing, trapped ions were used as quantum ion gates controlled by laser light [4,5]. In improving frequency metrology, Be^+ ions have been trapped for a 303 MHz frequency standard [6]. Ion-neutral collisions were studied with a 22-pole trap and measured by a quadrupole mass spectrometer [7]. While higher-order multipole potentials, such as the hexapole and octopole, have been used for ion storage and ion transport (as, e.g., ion guides [8] [9]), they are not suitable as mass analyzers because of poor resolution [10,11]. For this reason, only ion traps that are based on quadrupolar potentials have previously been or are currently used for mass analysis.

Quadrupole devices used in mass spectrometry come in two basic geometries depending on whether the potential varies quadratically in three or two dimensions. The former is the basis of quadrupole [12] and cylindrical [13] ion traps, and the latter forms the basis of linear [14] and rectilinear [15] ion traps. Another type of trapping device is the toroidal ion trap [16], which can be regarded either as a linear trap curved back onto itself to form a ring, or as a rotation of the cross-section of a 3-dimensional quadrupole about an axis outside the trapping region (Fig. 1).

A motivation behind the development of the toroidal ion trap [16] was to maintain a large trapping capacity in a device that would be miniaturized for portable mass spectrometry applications. In a toroidal trap, the trapping center is a ring, allowing more ions to be stored than in a conventional quadrupole ion trap (QIT), where the trapping center is just a point. The initial report of the toroidal trap included two designs. The first had a cross-section that was identical to the cross-section of the QIT, but with an external rotational axis. However, this device, termed the "symmetric" toroidal ion trap, gave poor performance due to electric field perturbations resulting from the toroidal curvature. A second design remedied the curvature effects by using an asymmetric cross-section—with different electrode asymptotes on the inner vs. outer electrodes. This geometric correction allowed mass resolution and accuracy

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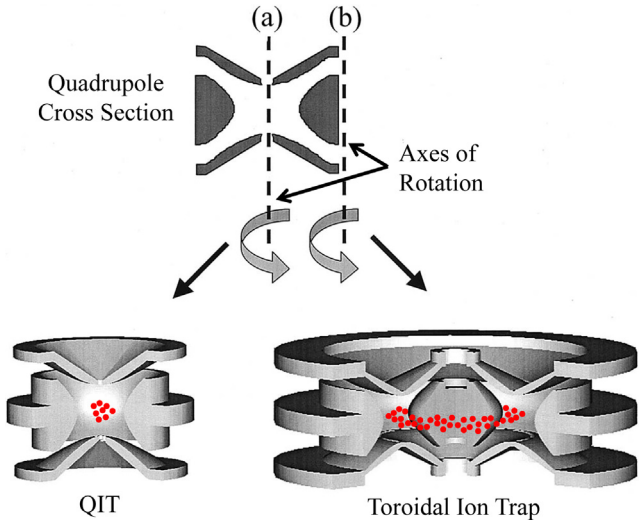

Fig. 1. Comparison of the QIT and the toroidal ion trap. For the QIT, the rotational axis passes through the trapping center. For the toroidal ion trap, the rotational axis is offset to outside the trapping region.

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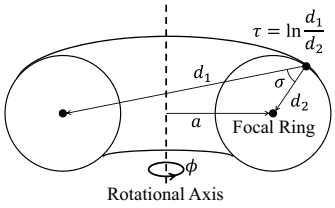

Fig. 2. Toroidal coordinate system, (σ, τ, ϕ), with a torus containing a focal ring of a radius of a.

similar to other ion traps. A miniaturized version of the "asymmetric" toroidal ion trap has now been used as the basis of a portable GC–MS system [17,18]. Taylor and Austin [19] presented a simplified version of the toroidal ion trap using only cylindrical and planar electrodes, which are easier to fabricate than hyperbolic electrodes.

Previously, we have reported simulation studies with the symmetric, asymmetric, and simplified designs for toroidal ion traps [20]. These simulations determined the electric fields in the trapping region as well as the effects of higher-order fields on ion motion. These results confirmed that the asymmetric design had the least amount of higher-order fields compared to the other two designs. The findings also showed that the fields of the simplified design more closely resemble that of the symmetric design even though its reported performance is closer to the asymmetric design.

However, it was also observed [20,21] that neither the conventionally defined quadrupole nor Cartesian multipoles generally are adequate to completely describe the potentials in toroidal traps. If the potential distribution in a toroidal trap was quadrupolar, the potential must vary as the square of the distance from the trapping center. This would result in the following inconsistencies:

(1) The potential cannot indefinitely increase quadratically because it will run into the rotational axis—at that point the potential would be non-differentiable;
(2) Moving in any linear direction from the trapping center, the potential will be perturbed by curvature effects;
(3) There is no a priori reason for the multipoles to all be centered at the same radial distance (e.g., at the trapping center).

This first point may be considered by using the Poisson Equation for a closed volume with a contained charge (the central electrode), but the other two effects cannot be handled this way. The second point will be the case for all higher-order multipoles as well as the quadrupole. Thus the potential in a toroidal ion trap cannot be described by a quadrupole or by a sum of Cartesian multipoles except in the local vicinity of the trapping center.

It may be possible to evaluate the local field using a perturbation approach [22], but for a toroidal ion trap, a solution based on a toroidal coordinate system may be more appropriate and useful.

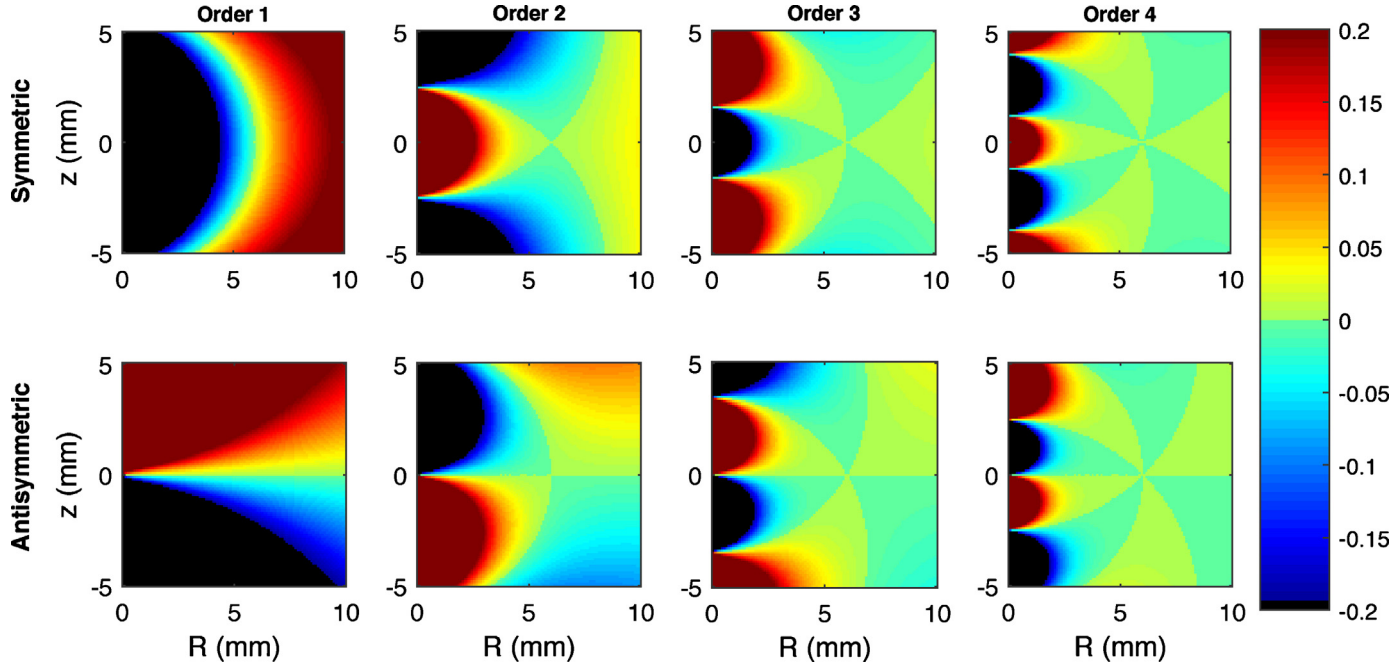

Fig. 3. Symmetric and antisymmetric toroidal harmonics of the second kind.