J. At. Mol. Sci.
doi: 10.4208/jams.012513.042013a

Vol. **5** , No. 1, pp. 26-33
February 2014

Geometric optimization of hybrid ion trap

Jafar. Kamalirad*

Department of Physics, Marvdasht Branch, Islamic Azad University, Marvdasht, Iran

Received 25 January 2013; Accepted (in revised version) 20 April 2013
Published Online 18 November 2013

Abstract. In this study we determined the effect of geometry of ring electrode on the operation of a new ion trap with cylindrical ring electrode and hyperbolical end cap electrode. This model indicated how adjusting the geometric cell parameters could reduce the impact of presence of higher order fields. Our work also illustrated the possibility of improving other desired properties of a trap. For example we found how these adjustments could minimize the non-linear effects. We also noticed the possibility of increasing the time of ion storage in a trap by the effect of one field in a hybrid ion trap. In this study we have obtained all of the equations of motion in a trap analytically.

PACS: 37.10.Ty, 07.75.th

Key words: hybrid ion trap, quadrupole, equation of motion, coefficients of field, geometric parameters

1 Introduction

An ion trap is a device which confines ions in a particular area of a space. Hybrid ion trap is a combination of two ion traps, quadruple and cylindrical traps which both of them are well known traps and also have numerous uses. In this study, we grounded the end cap electrode and connected the ring electrode to the v_0 potential as common for the standard hyperbolic trap. And then in similar theoretical case, we have calculated the equations of motion for a single ion too [1].

$$v_0 = v_{dc} + v_{rf}\cos\Omega t \tag{1}$$

Ions follow the different trajectories under the influence of the applied field. If ions oscillate on the x-y plane with limited amplitude, they will be revealed at end. Otherwise

*Corresponding author. *Email address:* `jafar_kamalirad@yahoo.com` (J. Kamalirad)

the amplitude of motion increases exponentially and thus ions will be destroyed due to the collision with electrodes. We will study these conditions in our work. On the other hand deviation of hyperbolic geometry leads to nonlinear effects that we will also discuss it later. We have replaced the standard hyperbolic ring electrode with a cylindrical ring electrode in this study and also we have calculated the motion equations for a single trapped ion as mentioned earlier.

2 Calculation of the electric field and potential inside the trap

The following equations govern in the Hybrid ion trap:

$$\begin{cases} \frac{z^2}{z_0^2}-\frac{r^2}{r_0^2}=1 \\ r=r_1 \end{cases} \tag{2}$$

Where r is radial displacement and z is axial displacement. r_1 is inner radius of the ring electrode and z_0 is vertex of the end cap electrode. Also θ is the asymptotic angle.

In the Eq. (1) V_{dc} is direct current component of the applied potential, V_{rf} is amplitude of the oscillating component of the applied potential, the parameter Ω is frequency of the oscillating potential and t is time. We assumed that electrodes have been extended to infinity. Also the trap is free from any background ion gas.

$$\nabla^2\phi=0 \tag{3}$$

The separating method of variables and riddance from azimuthal dependency leads to following equation:

$$\phi(r,z)=\phi(r)\phi(z) \tag{4}$$

Boundary conditions says that potential of trap is v_0 where $r=r1$ and potential is Zero where points belong to hyperbolic electrode. The separating technique of variables leads to the following equation eventually:

$$\phi(r,z)=\sum_{n=0}^{\infty}A_nI_0(p_nr)\cos(p_nz) \tag{5}$$

Where I_0 is modified Bessel function in the zero order which is also a first kind function. The potential value is being obtained by applying the Boundary conditions:

$$\phi(r,z)=4v_0\sum_{n=0}^{\infty}\frac{(-1)^n}{(2n+1)}\frac{I_0(p_nr)}{I_0(p_nr_1)}\cos(p_n\frac{z}{\rho}) \tag{6}$$

$$\rho=\sqrt{1+\frac{r^2}{z_0^2tg^2\theta}} \tag{7}$$

3 Equation of motion in the HIT (Hybrid Ion Trap)

For a charged ion which its mass is m and its charge is e, we can write the following equation

$$\frac{d^2\overrightarrow{r}}{dt^2}=-\frac{e}{m}\overrightarrow{\nabla}\phi \tag{8}$$

With converting t (time) to the dimensionless parameter, we will have

$$\begin{cases}\frac{d^2z}{d\tau^2}+(\alpha_z-2\xi_z\cos(2\xi))Z(r,z)=0\\ \frac{d^2r}{dt^2}+(\alpha_r-2\xi_r\cos(2\xi))R(r,z)=0\end{cases} \tag{9}$$

where

$$\tau=\frac{\Omega t}{2} \tag{10}$$

$$\alpha_z=\frac{-16ev_{dc}}{mz_0^2\Omega^2},\quad \xi_z=\frac{8ev_{rf}}{mz_0^2\Omega^2} \tag{11}$$

$$\alpha_r=\frac{8ev_{dc}}{mz_0^2\Omega^2},\quad \xi_r=\frac{-4ev_{rf}}{mz_0^2\Omega^2} \tag{12}$$

$$R(r,z)=z_0\sum_{n=0}^{\infty}\frac{(-1)^n}{I_0(p_nr_1)}[I_1(p_nr)\cos(\frac{p_nz}{\rho})-\frac{2r}{\rho^3z_0^2tg^2\theta}I_0(p_nr)\sin(\frac{p_nz}{\rho})] \tag{13}$$

$$Z(r,z)=\frac{z_0}{2\rho}\sum_{n=0}^{\infty}(-1)^n\frac{I_0(p_nr)}{I_0(p_nr_1)}\sin(\frac{p_nz}{\rho}) \tag{14}$$

Where $I_1(x)$ is the modified Bessel function in first order which is also a first kind function.

4 Calculation method

To solve the motion equations analytically we must expand the $R(r,z)$ and $Z(r,z)$ series at first. Using MATLAB software and Runge Kutta Method of Order 4, we continue to calculate with expanding the above series until 6 terms. If we assume the ions are more likely to be trapped into the center of trap and if $z<<z_0$, we can write the Taylor series of trigonometric functions. When we expanded the terms of $Z(r,z)$ and after expanding sinus in Eq. (14) until two terms, We will have:

$$\frac{d^2Z}{d\tau^2}+(\alpha_z\eta-2\eta\xi_z\cos(2\xi))z=0 \tag{15}$$

where

$$\eta=\frac{\pi}{4\rho}A-\frac{\pi^3z^2}{96\rho^3z_0^2} \tag{16}$$

and

$$A=\sum_{n=0}^{5}\frac{(-1)^n(2n+1)I_0(p_n r)}{I_0(p_n r_1)} \tag{17}$$

These equations are similar to Mathieu equation for quadrupole ion trap.

$$\frac{d^2Z}{d\tau^2}+(\alpha_z-2q_z\cos(2\xi))z=0 \tag{18}$$

We can change the Eq. (15) to the canonic form (18) by defining the parameters of hybrid ion trap like below:

$$\alpha_{zHIB}=\alpha_z\eta,\quad q_{zHIB}=\xi_z\eta \tag{19}$$

These equations is just confirmed in $z<<z_0$ conditions. If an ion is not located in center of the trap, we must consider higher order terms in the expansion. Now in center of the trap where $z\approx 0$ and $r\approx 0$ besides the conditions mentioned above, we can obtain the equations below immediately

$$\rho=1,\quad I_0(0)=1, \tag{20}$$

and

$$\eta=\frac{\pi}{4},\quad A=const \tag{21}$$

This value is constant. First this means that q_{zhit} and a_{zhit} are just dependent to the DC voltages and RF radio frequencies. Second this means that η also gives the unique geometry of the quadrupole ion trap corresponding with the hybrid ion trap. It is evident if ions are not located in the center of HIT, value of η would not be constant anymore rather it will be varied based on the ion position in the trap. But in our current situation η is approved in the condition of $z<\frac{z_0}{10}$ which is a good physical approximation. For each a,q (or each α,ξ) one specific trajectory is being predicted for a single trapped ion . Some of trajectories are stable and others are unstable. The relation between QIT and HIT is interesting too. By these calculations in the center of a trap along with usage of the Eqs. (20) and (21) we obtain:

$$r_1=z_0\sqrt{\frac{2}{\pi 4}} \tag{22}$$

Where z_0 and r_1 are coordinates for HIT and QIT respectively. Considering previous mentioned assumptions this equation is signifying the relation between geometries of QIT and HIT, stability in QIT (Paul Trap) with parameter of r_1 is equivalent to stability in HIT with parameter of z_0.

Now we can simulate the ion trajectories by computer software (MATLAB). Our boundary conditions are $r=z=10^{-6}m$, $r=z=0$ and dimensionless parameter of τ is in the range of zero to 1000. After solving the system of coupled differential equations (9) we can plot the trajectory of an ion in the HIT in the coordinates of $z-t$ and $r-t$.

Now we can obtain the trajectory of the ion in the coordinate of $r-z$ by eliminating the parameter of τ in coordinates of $r-\tau$ and $z-\tau$. We used MATLAB software to do these calculations.

5 Coefficients of field and geometric optimization

Now we expand the potential to the terms based on extent of the poles. We can express a distribution with cylindrical symmetry by the following equation:

$$\phi(r,z)=\sum_{n=0}^{\infty}A_n(r^2+z^2)^{n/2}P_n(\frac{z}{\sqrt{r^2+z^2}}) \tag{23}$$

Where A_n is the coefficient to specify orders of the Poles (e.g. n=0-4 corresponds to the monopole, dipole, quadrupole, hexapole and octopole, respectively).

$P_n(x)$ is the Legendre polynomial zeros. The z axis of the electric field with mirrored symmetry is being represented by below equation:

$$(\frac{\partial\phi}{\partial z})_{z=0}=\sum_{n=1}^{\infty}(-1)^n(2n)A_{2n}z^{2n-1} \tag{24}$$

In a perfect quadrupole hyperbolic ion trap (Paul Trap), the only terms which would be nonzero are monopolar (A_0) and quadrupolar (A_2). However practically it would be inevitable that some higher orders fields are present in a real ion trap. One reason for this presence of higher orders fields is the electrodes which are being truncated. In fact the cylindrical ring electrode and the hyperbolic end cap electrode do not extend to infinity. This factor as well as the impact of machining and manufacturing processes leads to presence of the higher order fields too. Now we optimize the ratio of (r_1/z_0) so that for $(n>2)$ A_n terms tend to zero. In Eq. (24) we see an independency from asymptotic angle (advantage of trap).

We use Eq. (7) to calculate the ratio of $(\frac{\partial\phi}{\partial z})_{z=0}$ and then put it equal to Eq. (24). As a result, terms include of odd coefficients of fields (e.g. A_0,A_1,A_3,A_5) tend to zero and terms include of even coefficients (e.g. A_2,A_4,A_6) will be obtained. In the following equations we calculate the hexapole, octopole and dodecapole respectively.

$$A_2=\frac{\pi v_0}{2z_0^2}\sum_{k=0}^{\infty}\frac{(-1)^k(2k+1)}{I_0(\frac{(2k+1)\pi}{2(z_0/r_1)})} \tag{25}$$

$$A_4=\frac{\pi^3 v_0}{96z_0^4}\sum_{k=0}^{\infty}\frac{(-1)^k(2k+1)^3}{I_0(\frac{(2k+1)\pi}{2(z_0/r_1)})} \tag{26}$$

$$A_6=\frac{\pi^5 v_0}{96\times 5!z_0^6}\sum_{k=0}^{\infty}\frac{(-1)^k(2k+1)^3}{I_0(\frac{(2k+1)\pi}{2(z_0/r_1)})} \tag{27}$$

Precise calculations indicate the expansion of terms of (A_4,A_6) is not extending to infinity. By expanding the above equations so that n is been in range of zero to maximum 300, we can find the numerical values of coefficients of field.

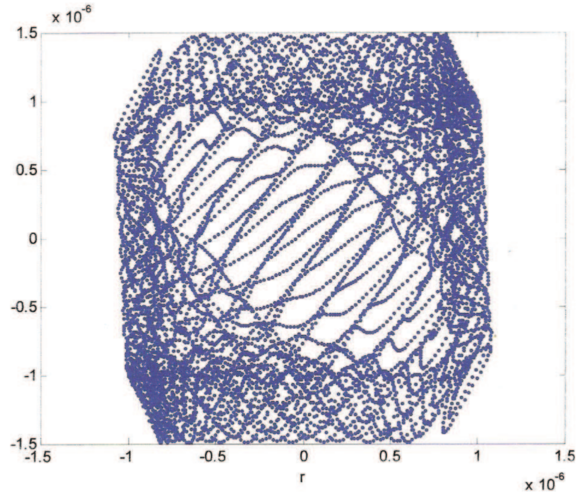

Figure 1: This figure shows the stable trajectory of an ion motion with selecting the boundary conditions so that ($r = z = 10^{-6} m$), ($\frac{dz}{dt} = \frac{dr}{dt} = 0$) and τ is in the range of 0 to 1000 and θ is also asymptotic angle ($\theta = 50°$) thus we gain (z_0=0.956 cm) and (r_1= 1 cm).

In our typical calculations the term of order (220) is zero .We can test it typically by selecting the potential magnitude equal to 10 units and by using definite aspect ratio of ($\frac{z_0}{r_1}$).

This is very important because the field coefficients in Eqs. (24-26) are independence from the asymptotic angle which leads to geometric optimization. Here we evaluate the superposition of higher orders coefficients (A_4, A_6) on the quadrupole term (A_2). This means that plotted curves variations of (A_4/A_2), (A_6/A_2) could be evaluated based on aspect ratio of (z_0/r_1). For this purpose we consider r_1 as a constant value (e.g. 1.661 cm) and also we assume z_0 is a variable. Thus, different diagrams would be plotted by choosing the trap geometric parameters of r_1, z_0 and experimental parameter of v_0. Not only all diagrams of (A_4/A_2), follow the certain gradient, but also the diagrams of (A_6/A_2) follow the same gradient.

As the calculations confirm the octapole term of (A_4) is stranger than others and dodecapole term of (A_6) should be weaker than it logically, which is so. Intuitive values were obtained practically confirm this claim too. Coefficients of even terms with $n > 6$ are unimportant. But the interesting point is that in HIT the obtained term signs of octapole and dodecapole fields are negative.

We know the hyperbolic ion trap with pulled cap and optimized asymptotic angle has stronger octapole field with the same sign with quadrupole field. But when we apply QIT which have electrodes with finite length, the sign of octapole field would be opposite of the sign of basic quadrupole field [6]. Negative octapole field is a response to negligible separation of Paul Trap mass with truncated electrodes. On the other hand octapole field with negative sign can delay the ejection of ion from the trap which is very important matter for experimentalists.

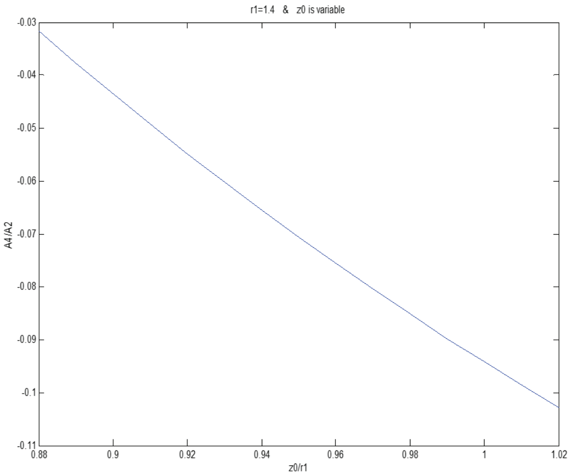

Figure 2: This diagram shows the superposition of fractional octapolar component on the basic quadrupole field (A_4/A_2) based on aspect ratio of (z_0/r_1); where r_1 is equal to 1.4 cm and z_0 is a variable for this interval. Expansion of the terms of A_4, A_2has been done to 300 terms. X-axis and y-axis represent the aspect ratio and octapolar component respectively.

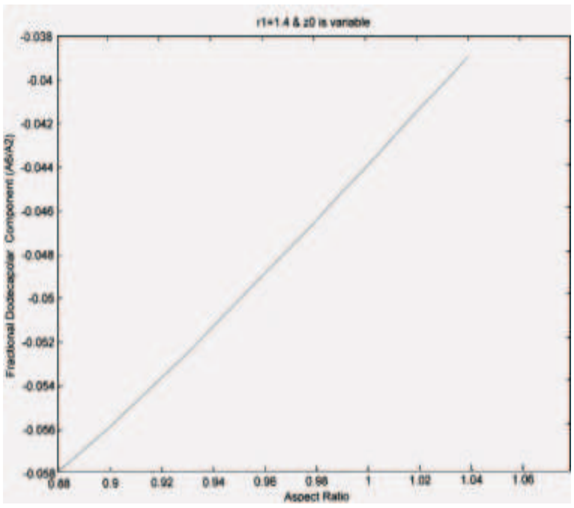

Figure 3: This diagram shows the superposition of fractional dodecapolar component on the basic quadrupole field (A_6/A_2) based on aspect ratio of (z_0/r_1); where r_1 is equal to 1.4 cm and z_0 is a variable for this interval. Expansion of the terms of A_6, A_2 has been done to 300 terms. X-axis and y-axis represent the aspect ratio and dodecapolar component respectively.

Now we can exactly plot the trajectory of an ion in the HIT. Also we can plot fractional dodecapolar components as well as fractional octapolar components per aspect ratio for the parameters of HIT.

6 Conclusion

Although electrodes in the studied HIT extended to infinity but negative sign is obtained for octapolar field. This occurred due to the deviation from hyperbolic standard geometry (however in practice, the actual ion traps are non-linear). In fact this is how cylindrical ring electrode shows its effect on the coefficients of field. In this trap (HIT) octapolar field of (A_4) is stranger than other resonance fields and also the dodecapolar field is obtained with negative sign and it takes smaller values than the octapolar field. Our goal was to optimize the parameters of the HIT such that coefficients of the field tend to zero for higher order fields ($n > 2$) and also we wanted to bring the non-linear effects down to the possible minimum. We reached these purposes at end. However, finally it must be mentioned that the octapolar field of a HIT increases the time of ion storage in the trap so that it can have many practical applications in the branches of physics and chemistry such as mass spectrometry, nuclear physics, spectroscopy and vacuum technology.

Acknowledgments I gratefully acknowledge the support of my supervisor professor A. R. Doroudi for his support in both research work and for all the fruitful discussions that I have had with him.

References

[1] Peter. H. Dawson, Quadrupole mass spectrometry and its applications.
[2] G. Arfcan, Mathematical methods for physicist (1982).
[3] J. D. jackson, Classical electrodynamics (1962).
[4] M. Abramowitz, I. A. stegun, Handbook of mathematical Functions (1965).
[5] R. Alheit, F. Vedel, M. vedel, Higher order non-linear resonances in a Paul trap (1966).
[6] J. Franzen, The non-linear ion trap part 4 (1993).
[7] Y. Wang, J. Franzen, K. P. Wanczek, The non-linear resonance ion trap part 2 (1992).
[8] Y. Wang, J. Franzen, The non-linear ion trap part 3 (1993).
[9] J. Franzen, The non-linear ion trap part 5 (1993).
[10] C. Richard.Arkin, Brian. Goolsby, D. A. Laude, Characterization of the hybrid ion trap (1999).