Single-phase ion trap with cylindrical zero-potential surface

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Abstract. In the present article, we discuss an electrostatic field around four-bar trap, where in-phase AC voltage is applied to all electrodes. We consider shielding effect on trap’s field distribution. The ideal octupole field is obtained using a cylindrical grounded surface. Single-phase trap gives an opportunity to form an $n$-order multipole field within $n + 1$ number of electrodes. This approach reduces the number of electrodes in comparison with the classical case.

1. Introduction

Multipole traps are widely applied as devices for trapping and manipulation of charged particles [1,2]. For example, multipole ion guides are part of the particle accelerator [3–5] and the mass-analyzer Orbitrap [6]. An octupole trap can be coupled with photoelectron-photofragment coincidence (PPC) [7]. 22-pole trap can be used in laser spectroscopy [8,9], IR-spectroscopy [10,11] and chemical reactions studying [12,13].

A concept of multipole ion trap is the same as for quadrupole ion trap (QIT), using additional pairs of electrodes. In both cases, the electric potential spatial distribution is given in term of $n$-order harmonic polynomials ($n = 2$ for QIT and $n > 2$ for multipole ion trap) [14]. The need for a high-precision installation of each electrode makes the experimental implementation of a multipole ion trap a big challenge [15–17].

The shape of the electrostatic field and effective potential are strongly depended on electrode’s displacement, phase delay and amplitude jumps [18]. The use of a large number of physical electrodes in the design of multipole ion traps leads to a critical deformation of the trap field; as a result, artifact potential minima may appear [19]. Reducing the number of physical electrodes without decreasing the order of the multipole field could eliminate these issues.

Article [20] shows the possibility of realization an octupole field with four-bar trap (“single-phase” trap). In contrast to the classical scheme of connection a quadrupole ion trap, the authors of the work use a single-phase connection of all electrodes, where the equations of motion still satisfy the Earnshaw’s theorem. Mathematical simulation and experimental implementation show the formation of three stable equilibrium points. The observed effect correlates with effective potential symmetry breaking in octupole trap with electrode’s displacement [16]. Symmetry breaking can also occur due to asymmetric zero-potential shielding.

In this work we provide a numerical simulation of potential distribution in single-phase trap with external cylindrical zero-potential shielding. As a result, an ideal octupole field forms with $4 + 1$ electrode trap. In general, we can achieve $n$-order multipole field with $n + 1$ number of electrodes instead of $2n$ electrodes in classical case.
2. Results and discussion

In most researches with trapped charged particles, the QIT is usually an object of interest. Potential energy of particle in four hyperbolic electrodes trap in classical case is given by

\[ E(x, y) = \frac{e(V_0 + U_0 \cos(\omega t))}{2r_0^2}(x^2 - y^2) \]  

(1)

where \( e \) is particle’s charge; \( U_0, V_0 \) are AC and DC amplitudes; \( \omega \) is AC frequency; \( r_0 \) is trap’s radius.

In general case, the electrical potential spatial distribution of multipole ion trap is given in the form of an \( n \)-order harmonic polynomials

\[ U(x, y) = \frac{V_0 + U_0 \cos(\omega t)}{n r_0^n} \Re[(x + iy)^n] \]  

(2)

The classical design of an ion trap consists of \( N = 2n \) electrodes where neighboring electrodes have \( \pi \) phase delay. Thus, equation (1) is a special case of (2) where \( N = 4 \).

It is important to note that there is no fundamental limit on the even number of electrodes and the value of the phase delay. Indeed, it is possible to construct an ion trap with odd number of electrodes with in-phase voltage applied.

The principal opportunity to obtain stable trapping in the case of a single-phase trap is given in [20]. This paper demonstrates the possibility of stable trapping in four-bar trap with the same phase of AC voltage applied to each electrode. The described setup leads to symmetry breaking due to the asymmetric zero-potential surface shielding. The zero-potential surface is at the distance \( L \) from the center of the trap (Fig. 1a). Since symmetry is broken, the effective potential of such trap has only three potential minima instead of four.

To avoid this issue, we propose external cylindrical zero-potential shielding (Fig. 1b).

\[ \Delta U(x, y) = 0 \]  

(3)

where \( x, y \in \Omega \).

Boundary conditions are given by

\[ U(x, y)|_{\partial \Omega} = f(x, y) \]  

(4)
The function \( f(x, y) \) describes the potential distribution on bar and shielding electrodes. In terms of the task, boundary conditions on shielding correspond to \( U = 0 \) and on electrodes to \( U = U_0 \). Defining \( R \) as shielding radius, \( r \) as trap’s radius and \( d \) as electrodes radius (Fig. 1b), boundary conditions \( f(x, y) \) for \( N \) – electrodes single-phase trap with cylindrical zero-potential shielding take the following form

\[
f(x, y) = \begin{cases} 
0, & x^2 + y^2 = R^2 \\
V_0 + U_0 \cos(\omega t), & \left[x + r \cos\left(\frac{2\pi j}{N}\right)\right]^2 + \left[y + r \sin\left(\frac{2\pi j}{N}\right)\right]^2 = d^2
\end{cases}
\]

where \( j \in [1, N] \).

The number of electrodes \( N \) can be odd, unlike the classic case. The stable trapping is potentially possible for \( N \geq 2 \).

Dirichlet problem with determined boundary conditions can be solved numerically via finite elements method (FEM). Inner space of trap triangulates with any convenient method if approximation near the boundary (5) and geometrical center of the trap is accurate enough. The numerical simulation for \( U_0 = 1 \text{V}, R = 10d, r = 5d, t = 0 \) is shown on Fig. 2a.

Figure 2. The results for numerical simulation for electrical potential spatial distribution with \( U_0 = 1, R = 10d, r = 5d \). a) \( x^2 + y^2 < 10^2 \); a) – cross section of the electric potential; b) section of the effective potential near the trap’s center. The red line corresponds to the equivalent ideal octupole effective potential, the blue line corresponds to the numerically calculated values single-phase trap with cylindrical shielding effective potential. Here, effective potential normalized to the potential well depth.

The distribution obtained match the ideal octupole field (2) in a special case \( n = 4 \). It should be noted that total number of electrodes in the proposed configuration is \( n + 1 \) instead of \( 2n \) electrodes in case of classic configuration. At the same time electric field value in the center of the trap is not zero, \( U(x,y)_{|0,0} > 0 \) in instead of the classical case. So, considering (2) in the special case \( n = 4 \), we can approximate the result on Fig.1a with the model

\[
U_m(x, y) = \left[ U(0,0) - \frac{1}{4r_{\text{eff}}^4}(x^4 - 6x^2y^2 + y^4) \right] \cos(\omega t)
\]

where \( r_{\text{eff}} \) is radius of ideal octupole trap, which corresponds to \( r_0 \) in equation (2).
Considering the given geometry of the electrodes \( r_{\text{eff}} = 4.939 \) and \( U(0,0) = 0.8747 \). The approximation (6) has physical sense in the inner area of electrodes. We can describe this area by trap’s radius \( r_{\text{in}} \):

\[
 r_{\text{in}} = R - 1 
\]

where \( R \) is normalized shielding radius.

Consider the configuration of a single-phase trap where trap’s radius \( r_{\text{in}} = 4d \), the cross-section of the electric potential is shown on Fig. 2a. In this case, accuracy of approximation can be defining as standard deviation \( \sigma \) of \( [U(x,y) - U_m(x,y)] \) for \( x^2 + y^2 < r_{\text{in}}^2 \) region. Thus, the value of accuracy does not exceed \( 10^{-14} \) near the trap’s center \( (x,y < 0.5r_{\text{in}}) \) and \( 10^{-6} \) on the periphery \( (x,y \equiv r_{\text{in}}) \).

The shape of effective potential is also approximated to the ideal pseudopotential with cylindrical model [14]. Blue line on Fig. 2b indicate the section of time-averaged effective potential [19] for the given electrode’s geometry and the approximated pseudopotential model (6) for \( r_0 = r_{\text{eff}}, V_0 = 0 \). The green line corresponds to \( x < r_{\text{in}} \) region. The standard deviation does not exceed \( 10^{-10} \) from absolute value of potential well depth for \( x, y < 0.5r_{\text{in}} \) region.

3. Conclusion

In this paper, we demonstrate the effect of shielding on field formation in single-phase ion trap. We showed that single-phase four-bar trap with external cylindrical zero-potential shielding lead to true octupole field. This field is equivalent for the field of classic eight-bar ion trap. Forming a \( n \)-order multipole field by the method proposed in the work requires only \( n + 1 \) electrode, in contrast to \( 2n \) electrodes in the classic case. Reducing the number of electrodes in multipole trap decreases the possibility of trap’s field deformation due to electrodes displacement.

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