Outside localization around a toroidal electrode of a Paul trap

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Abstract
Here we describe and experimentally confirm the localization of charged microparticles outside the area of a radio-frequency Paul trap. We consider the nonlinear effective potential formed by the trap, treating the field independently for different electrodes of the trap. To approach the proposed model to reality, we also consider the nonlinear effects originating from the viscosity of surrounding medium. Proposed approach allows to conduct an analytical description of the effective potential and define quasi-equilibrium points both inside and outside the trap. Predictions of the proposed model are in full compliance with obtained experimental results.

1. Introduction
As of today, the combination of a toroidal electrode and two end-cap electrodes referred to as a Paul trap. It is a widely used tool for radio-frequency localization of charged particles. A lot of devices utilized for trapping [1, 2], transferring [3, 4], analyzing [5, 6], and cooling [7, 8] of charged particles are derived from the Paul trap, which makes this tool a universal platform for particle manipulation [9].

Plenty of work was performed to study, develop, and modify the classical Paul trap. These works can be assigned to several classes. First comes the consideration of nonlinear trapping fields, for example, anharmonic [10], octapole [11], and hexapole [12] fields. Second class of works comprises all possible modifications of the trap geometries, like triangular [13, 14] and cylindrical [15] shapes, geometrical perturbations [16], microfabrication-compatible trap geometries [17]. There are works on the tuning of the trap voltages, for instance, AC voltage parametrizations [18, 19]. Trapping can be considered not only in vacuum, but also in viscous gases [20].

All the above-mentioned works are constrained to analyze the field inside a trap, while the radio-frequency field outside the toroidal electrode, even for the classical Paul ion trap, is still unexplored. In this work, we propose a new way to describe the electric field of the radio-frequency quadruple Paul trap. We show that its field distribution is sufficiently different from the usual model distribution given by harmonic higher-order polynomials [16, 21, 22]. The proposed model of the effective potential also considers the corrections due to viscosity of the medium and, moreover, allows to obtain the potential minima not only inside the trap, but outside the toroidal electrode as well. We have conducted an experimental verification of our model by localizing charged borosilicate glass microparticles in the Paul trap. The results of the experiment confirm theoretically predicted points of quasi-equilibrium.

The paper is organized as follows. In section 2, we provide a theoretical description of the fields formed by the Paul trap with one toroidal and two end-cap electrodes. In section 3, we numerically simulate an effective potential that originates from the trap field distribution. Finally, in section 4 we demonstrate an experimental confirmation of the existence of quasi-equilibrium points outside the trap, highlight the main regimes of trapping, for which we provide the estimates on the depth of potential minima.

2. Theory
In this part of the paper, we calculate the spatial distribution of a field around a Paul trap using the superposition principle of the fields from different trap electrodes (section 2.1). After that, utilizing the resulting field we derive the effective potential of a charged trapped particle (section 2.2).
2.1. Calculation of electrical field

Spatial distribution of a potential formed by a Paul trap is described by the solution of Dirichlet problem with boundary conditions \[23\]. Widely implemented model solution that describes the field distribution inside the trap is given by the following homogeneous second-order polynomial \[24\]:

\[
U = \frac{R^2 - 2z^2}{(R_0 - r_0)^2 + 2z_0^2},
\]

where \(R\) and \(z\) are the spatial coordinates, \((R_0 - r_0)\) is the inner radius of the toroidal electrode of the trap shown in figure 1, and \(2z_0\) is the distance between end-cap electrodes, for which the relation \(2z_0^2 = (R_0 - r_0)^2\) holds [9]. As can be seen from (1) and figure 1, this model is inaccurate in case when \(\sqrt{R^2 + z^2} \gg R_0\). In addition, the model does not consider the thickness of electrodes.

More rigorous and accurate approach is a direct solution of the electrostatic problem of potential around the trap electrodes (figure 1). In order to solve the exact electrostatic problem, let us firstly consider the field around the toroidal electrode of the trap and introduce new toroidal coordinates \((\mu, \theta, \phi)\), shown in figure 1:

\[
R = \frac{C_0 \sinh \mu}{\cosh \mu - \cos \theta}, \quad z = \frac{C_0 \sin \theta}{\cosh \mu - \cos \theta},
\]

where \(C_0\) is the scaling constant, \(r_0 = C_0/\sinh(\mu_0)\) and \(R_0 = C_0 \coth(\mu_0)\). The third toroidal coordinate, \(\phi\), does not change, which is due to the symmetry of a torus in toroidal coordinate system.

We consider a surface of the toroidal electrode as equipotential one, thus the following boundary conditions must be satisfied:

\[
U_{\text{ring}}(\mu, \theta, t)|_{\mu_{\Theta}} = V_{\text{ring}} \cos(\Omega t),
\]

where \(V_{\text{ring}}\) and \(\Omega\) are the AC voltage amplitude and frequency, correspondingly, and \(\mu_{\Theta}\) is the surface coordinate of a torus, given by

\[
\mu_{\Theta} = \log \left[ \frac{R_0}{r_0} \sqrt{\left( \frac{R_0}{r_0} \right)^2 - 1} \right].
\]

Laplace equation in toroidal coordinate system has the following form [25]:

\[
\frac{\partial^2 U_{\text{ring}}}{\partial \mu^2} + \frac{\partial^2 U_{\text{ring}}}{\partial \theta^2} + \frac{\partial U_{\text{ring}}}{\partial \mu} \coth \mu + \frac{U_{\text{ring}}}{4} = 0.
\]
After applying the standard separation of variables [23, 25, 26], the final solution reads:

\[
U_{\text{ring}}(\mu, \theta, t) = \frac{\sqrt{2}}{\pi} V_{\text{ring}} \cos(\Omega t) \sqrt{\cosh \mu - \cos \theta} \times \sum_{n=-\infty}^{\infty} \frac{P_{n-1/2}(\cosh \mu)}{P_{n-1/2}(\cosh \mu_0)} e^{i n \theta},
\]

where \(P_{n-1/2}\) and \(Q_{n-1/2}\) are Legendre polynomials of the first and second kind, respectively.

Now consider independently the field of the end-cap electrodes. The field potential can be approximately described by a solution of the Dirichlet problem. For end-cap electrode of radius \(r_0\), this potential has a form of an integral around the electrode surface area with coordinates \((r, \phi)\), for which \(0 < r < r_0\), \(0 < \phi < 2\pi\), and around the horizontal coordinate \(R\) respective to the end-cap plane:

\[
U_{\text{end}}(R, \phi, t) = \frac{V_{\text{end}} \cos(\Omega t)}{2\pi} \int_0^{2\pi} \int_0^{r_0} \frac{r \, dr \, d\phi}{z^2 + r^2 + R^2 - 2rR \cos \phi},
\]

Integrating by \(r\), we can obtain

\[
U_{\text{end}}(R, \phi, t) = \frac{V_{\text{end}} \cos(\Omega t)}{2\pi} \int_0^{2\pi} \xi \, d\phi,
\]

where \(\xi = \frac{\sqrt{z^2 + R^2}}{z^2 + R^2 \sin^2 \phi} - \frac{z^2 + R^2 - R \, r_0 \cos \phi}{z^2 + R^2 \sin^2 \phi} \times [z^2 + R^2 + r_0^2 - 2R \, r_0 \cos \phi]^{1/2} \).

Let us introduce new variables

\[
\begin{align*}
\hat{p}_\pm &= \sqrt{R^2 + (z \pm L/2)^2}, \\
n_1^\pm &= 2R/(\hat{p}_\pm + R), \\
n_2^\pm &= -2R/(\hat{p}_\pm - R), \\
C &= 4r_0/R/[(z \pm L/2)^2 + (R + r_0)^2],
\end{align*}
\]

and determine the areas of half-space along the \(z\)-axis for lower end-cap electrode as \((-L/2, \infty)\) and for upper end-cap electrode as \((-\infty, L/2)\), where \(L\) is the trap dimension along the \(z\)-axis. By doing this, one obtains the expression for the field around the end-cap electrodes:

\[
U_{\text{end}}^\pm(R, z, t) = V_{\text{end}} \cos(\Omega t) \left\{ \frac{1}{\pi \sqrt{(z \pm L/2)^2 + R^2}} \right. \times \left. \left[ \frac{r_0}{\hat{p}_\pm + R} \Pi(n_1^\pm, C) + \frac{r_0}{\hat{p}_\pm - R} \Pi(n_2^\pm, C) \right] \right\},
\]

where \(\Pi((n_1^\pm, n_2^\pm), C)\) are full elliptical integrals of the third kind. Thus, the model of the end-cap potential is valid only for \(z \in [-L/2, L/2]\).

Finally, according to the superposition principle, the full trap potential is formed by toroidal \(U_{\text{ring}}\) (equation (6)) and end-cap \(U_{\text{end}}\) (equation (10)) potentials:

\[
U(R, z, t) = U_{\text{ring}}(\mu(R, z), \theta(R, z), t) + U_{\text{end}}^+(R, z, t) + U_{\text{end}}^-(R, z, t),
\]

Expansion of the field (11) in the center of toroidal electrode fully corresponds to the potential distribution described in equation (1).

2.2. Calculation of effective potential

Particle motion in the trap field is usually described by the Lagrange formalism. Since the amplitudes \(V_{\text{ring}}\) and \(V_{\text{end}}\) are harmonically modulated, the motion is non-autonomous, i.e. explicitly time-dependent. Nevertheless, using widely implemented averaging methods, one can analyze the averaged model that is very close to the dynamical one, except for lack of the explicit time-dependence.

If there is no DC voltage applied to the electrodes, the secular motion of a particle with averaged coordinates \((\bar{R}, \bar{Z})\) is defined by the average kinetic energy of the fast oscillations [27]. If one neglects the Coulomb interaction between charged particles, the equations of motion of the field result in the following effective potential [27]:

\[
\phi_{\text{eff}}(\bar{R}, \bar{Z}) = \frac{e^2}{2\pi m} \int_0^{2\pi} dt \frac{\bar{Z}}{\bar{Q}} \int \frac{d}{dQ} U(\bar{R}, \bar{Z}, t) dt \left[ \int \frac{d}{dQ} U(\bar{R}, \bar{Z}, t) dt \right],
\]
where $Q$ is the generalized coordinate, $\tau = \Omega t/2$ is the dimensionless time. Interpretation of the effective potential (12) in terms of real radio-frequency fields (11) fully describes the secular motion of the charged particles. We note that the proposed model is in good agreement with the existing model of the effective potential for the ideal radio-frequency traps [24].

However, this estimation is valid only for localization in very high vacuum, when the interaction with residual gas is very weak. In sufficiently dense medium, the motion of a charged particle is damped. For instance, it was reported that particles of the size bigger than 10 $\mu$m undergo a strong nonlinear friction upon the localization in air, which results in unusual expanded orbits [20].

To generalize our model, let us consider the effective potential in the presence of a strong friction. In a simplified one-dimensional model case [29], the particle motion is described by

$$m\ddot{x} = \frac{eV}{(R_0 - r_0)^2} \cos \left(\Omega \frac{t}{2}\right) - \gamma \dot{x} - \alpha \dot{x} \dot{x}^2,$$

(13)

where $\gamma$ and $\alpha$ are the linear and nonlinear friction coefficients, respectively. Let us introduce fast ($\dot{x}$) and slow ($X$) motion [27]:

$$m\ddot{X} = \frac{eV}{(R_0 - r_0)^2}(\dot{x} + X) \cos \left(\Omega \frac{t}{2}\right) - \gamma (\dot{x} + X) - \alpha (\dot{x} + X) \sqrt{\dot{x}^2 + X^2}.$$

(14)

Let us approximate the fast-motion (micromotion) amplitude as an infinitely small quantity, $\dot{x}_0 \approx 0$. Since the micromotion can be described as $\epsilon \approx \epsilon_0 \cos \Omega t$, the corresponding derivatives $\dot{\epsilon}$ and $\dot{\epsilon}_0$ are in proportion with $1/\Omega^2$ and thus are not negligible for great frequencies [28], [29]. Therefore the equations of motion of the slow component $X$ have the form:

$$m\ddot{X} = \gamma (X) - \alpha \dot{X} \dot{X}^2 - \frac{\alpha \dot{X}^2}{X} \dot{\epsilon}^2 - \frac{d}{dx} \left(\frac{m}{2} \dot{\epsilon}^2\right).$$

(15)

As was shown recently in [27], the pseudopotential is defined by the kinetic energy of fast oscillations, which can be estimated as

$$\Phi_{\text{eff},11} = \frac{m}{2} \left(\dot{\epsilon}^2\right) = \frac{m}{4\pi} \int_0^{2\pi} \frac{e^2V^2}{m^2\Omega^2(R_0 - r_0)^4} X^2 \sin^2(\Omega t) \, dt = \frac{e^2V^2}{8m\Omega^2(R_0 - r_0)^4} X^2.$$

(16)

Substituting (16) in (15), we get the first-order approximation:

$$m\ddot{X} = -\frac{e^2V^2}{4m\Omega^2(R_0 - r_0)^4} X - \gamma (X) - \alpha \dot{X} \dot{X}^2 - \frac{\alpha \dot{X}^2}{X} \dot{\epsilon}^2.$$  

(17)

And putting (16) in (17), one can define a final formula for the secular motion:

$$m\ddot{X} = -\frac{e^2V^2}{4m\Omega^2(R_0 - r_0)^4} X - \gamma (X) - \alpha \dot{X} \dot{X}^2 - \frac{\alpha \dot{X}^2}{X} \dot{\epsilon}^2.$$  

(18)

Ariasing additional cubic nonlinearity is fully characterized by nonlinear damping coefficient $\alpha$. Thus, for $\alpha \to 0$, only linear damping affects the stability regions, and the general pattern of motion does not change [30].

3. Simulation

Here we consider the numerical results of calculation of the effective potential. Since the field $\Phi_{\text{eff}}(\vec{R}, \vec{Z})$ considered in this work is of potential type, accurate solutions around the quasi-equilibrium areas can be found from the following equation system:

$$\begin{cases} 
\partial_{\vec{x}} \Phi_{\text{eff}} = 0, \\
\partial_{\vec{Z}} \Phi_{\text{eff}} = 0.
\end{cases}$$

(19)

Figure 2(a) features the effective potential distribution $\Phi_{\text{eff}}(\vec{R}, \vec{Z})$ for an ideal Paul trap with the potential distribution from equation (1). Figure 2(b) illustrates the derived effective potential distribution, as in equation (11). Both existing ideal (1) and proposed expanded (11) models firmly describe the stability in the center of the trap (indicated by green). In addition to this, our model predicts new unstable quasi-equilibrium points (indicated by red) that arise around saddle-shaped potential. The depth of this potentials defines the ion localization force along the axial direction.

Let us introduce the ratio between the end-cap and toroidal electrode voltage amplitudes, $k = V_{\text{end}}/V$. For $k \to 0$, the resulting potential (Figure 2(b)) is in full equivalence with the ideal case (figure 2(a)). However, when increasing $k$ up to $\approx 3$, one can observe both the deepening of the main quasi-equilibrium point and formation of a new quasi-equilibrium area situated outside the trap toroidal electrode (figure 2(c)). Due to toroidal symmetry,
this new area is as well of toroidal shape, which indicates the possibility of orbiting of particles outside the trap area. External localization is a manifestation of the symmetry breaking of the effective potential \[31, 32\]. Nevertheless, the existing deviation from the quadrupole configuration is not due to the displacement of the position of electrodes \[32\]. The deviation is due to the superposition of pseudopotentials that originate from the interaction with the field of the toroidal electrode and two end-cap electrodes. In classical configuration of the Paul trap, the field of the end-cap electrodes is constant, thus their pseudopotential is equal to zero \[9\]. In our configuration, the field of the end-cap electrodes oscillates with the same frequency \(\Omega\) as of the toroidal one.

Figure 2 (c) takes into account the correction due to the nonlinear friction \(18\) discussed in section \(2.2\). This nonlinear friction does not affect the stability areas except for the deepening of the trapping potential. This allows the stable localization in medium with a wider range of initial conditions, whilst in vacuum, finite orbiting around the quasi-equilibrium areas is possible only for small initial velocities.

The stability areas are affected mainly by the ratio of the voltage amplitudes \(k\) and the trap geometry. An illustrative comparison between the effective potential distributions for different \(k\) calculated using the proposed model is given in figure 3. The potential well depth ratio \(D_{\text{out}}/D_{\text{in}}\) varies from 0:1 = 0 (for \(k = 0\)) to 0.06: 0.94 \(\approx 15.6\) (\(k = 1\)), and the relation \(D_{\text{in}}k=0.3/D_{\text{in}}k=0 = 0.94\), i.e. the depth of the central quasi-equilibrium point decreases in proportion to \(k\).

4. Experimental confirmation of outside localization

Here we describe the experimental confirmation and demonstration of the predicted effect of localization around a toroidal electrode of a trap. We have constructed a radio-frequency trap, toroidal and end-cap electrodes of which were supplied with voltages \(V = 10^3\) V and \(V_{\text{end}} = 3.2 \cdot 10^3\) V correspondingly of
oscillation frequency $\Omega = 50$ Hz. We trapped the hollow beads of borosilicate glass with the size of $(50 \pm 5) \times 10^{-6}$ m. For these parameters, the voltage ratio $k$ is equal to 3.2, which indicates transition to the case of outside localization. We performed the localization in air and used a low-frequency AC voltage to compensate the gravitational force. Since the depth of the effective potential is inversely proportional to the frequency, $\Phi_{eff} \propto 1/\Omega^2$ from (16), this configuration is suitable to localize even particles of more than $10^{-5}$ m size [20, 33, 34]. Localization dynamics of such particles is in agreement with the model of nonlinear damping [20], which allows to estimate the quasi-equilibrium points taking into account cubic nonlinearities (discussed in section 2.2).

Figure 4(a) illustrates the experimental realization of a particle localization inside and outside of the Paul trap, which is indicated by areas A and B, correspondingly. Figure 4(b) shows the detected characteristic positions of trapped particles. The central cluster of points (area A) is distinguishably shifted towards bottom end-cap electrode, which is primarily due to the effect of gravitation. The collateral clusters of points (area B) correspond to the quasi-equilibrium outside the toroidal electrode of the trap.

The trajectories of the trapped particles are of a ring shape (figure 4(a), area B), which can be viewed as extended orbits with a rotational period of $2\Omega$. This is due to the nonlinear friction upon a strong damping in the air medium [20]. Radial position of the additional area of quasi-equilibrium can be estimated as $R_{exp} \approx 64 \times 10^{-3}$ m (figure 4(b), area B), which is in good agreement with the proposed model (see figure 2(c)), where $R_{max} = 55 \times 10^{-3}$ m for the same trap parameters. In addition to orbiting around quasi-equilibrium area, particles in area B float around the toroidal electrode of the trap. We have observed this float occurring only in the counter-clockwise direction, which can be explained by either unification of initial injection velocities or inhomogeneity of the inner structure of the particles.

5. Conclusion

In this paper we proposed a model of a spatial distribution of the effective potential formed by a quadruple Paul trap. In accordance with our model, we find two regimes of particle trapping, which we parametrize using the electrode voltage ratio $k = V_{end}/V$. Conventional regime appears when $k \sim 1$. In this regime, the localization of a particle happens only in the trap center. Outside-localization regime is in action for $k \gg 1$, for which the quasi-equilibrium points are present outside the trap. The proposed model considers the nonlinearity of the air medium and demonstrates high agreement with the experiment we conducted for the trap in outside-localization regime ($k = 3.2$). Proposed approach can be used to describe fields in the traps of complex geometry, like asymmetric traps and traps with displaced electrodes. Moreover, the proposed experimental setup can serve as a basis for ‘radio-frequency tweezers’, which, unlike optical tweezers, are not limited by the properties of localized object (i.e. transparency for a given wavelength) and require only a non-zero charge of a trapped particle.
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