The steady states of dielectric particles with Quincke rotation under ion traps

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Abstract. The dynamics of dielectric particles with Quincke rotation under nonuniform electric fields generated by ion traps are researched. Based on a recently proposed model, I make a further discussion about a quadrupole electric field with numerical simulation. According to the results, the steady state of a single particle under different field strength can be classified into several stages. Some more complicated electric fields are considered too. But the dynamics of particle under other multipole fields can’t be simulated well with the model, which indicates that the model still needs to be improved. A more complicated 3D electric fields are considered too, the evolution of steady states under this 3D electric field is similar to the quadrupole field.

1. Introduction
When a single dielectric particle is suspended in a slightly conducting liquid with a strong uniform electric field, it will rotate spontaneously. This phenomenon called Quincke rotation was first discovered in the late nineteenth century by Quincke [1]. The electrorotation of a single particle in a uniform electric field has been well discussed [2-4]. With a strong enough electric field the rotation can exhibit chaotic behaviours [5, 6]. In addition, Quincke rotation can happen on cylindrical object like ellipsoidal particle. In this case the particle’s cylindrical axis would either parallel or perpendicular to the electric field direction. It was researched with both numerical [7] and experimental [8] methods. The deformation of liquid drop in the state of electrorotation [9] and size effect [10] are also studied numerically. When subjected in a nonuniform electric field, the rotational particle can move through complicated trajectories. Certain forms of electric field can induce the particle to the place where the field is minimum, in which the particle can reach several kinds of steady states [11]. In the case of multiple particles, hydrodynamic [12] and electric [13] interaction between the particles should be taken into account. For several particles the changes of motion state with time can be computed and displayed [11, 14]. The self-assembly of a large number of particles under electric field was also observed [11, 15]. The mathematical models of Quincke rotation were developed and corrected for many years [2]. Based on previous studies [2, 16], Das and Saintillan derived a model simulating two either fixed or free spheres in a uniform electric field [14]. Subsequently Hu improved the model with considering quadrupole moments so that the model can be used in nonuniform electric field [11].

Hu’s model is applicable to arbitrary number of spherical particles and electric field, he considered various steady states of particles under an electric field generated by 4 parallel electrodes spaced symmetrically from a central axis. This electric field generated by 4 electrodes usually exists in
a linear or two-dimensional (2D) quadrupole ion trap. It’s often used for studying ion properties or as a mass spectrometer [17]. In this paper I will make a more in-depth discussion of this electric field and research the motion and rotation of particles under some more complicated electric fields within ion traps.

2. Model and problem
The derivation of the model can be found in Hu’s paper [11], which considers some colloidal spherical particles suspending in a dielectric fluid with an applied electric field. In this paper the parameters of particles and fluid, including permittivity \( \varepsilon_p \) and \( \varepsilon_r \), conductivity \( \sigma_p \) and \( \sigma_r \), and viscosity of fluid \( \eta_f \) comes from the same experiment [18].

Here I give a simple version of the model only to solve the case of single particle. The dimensionless equation can be written as:

\[
\frac{d\mathbf{P}}{dt} = \mathbf{\Omega} \times \left[ \mathbf{P} - \varepsilon_{cm} G \nabla \bar{\phi}_a(\mathbf{r}) \right] - \frac{1}{D} \mathbf{P} - \sigma_{cm} G \nabla \bar{\phi}_a(\mathbf{r}) \\
\frac{d\mathbf{Q}}{dt} = A + A^T - \frac{1}{D'} \left[ \mathbf{P} - \sigma_{cm} G \nabla \bar{\phi}_a(\mathbf{r}) \right]
\]

(1)

where

\[
A = \mathbf{\Omega} \times \left[ \mathbf{Q} - 2\varepsilon'_{cm} G \nabla \bar{\phi}_a(\mathbf{r}) \right] \\
\frac{d\mathbf{r}}{dt} = \mathbf{U} = \frac{2}{3} G \mathbf{P} \cdot \nabla \bar{\phi}_a(\mathbf{r}) + \frac{1}{9} G \mathbf{Q} \cdot \nabla \nabla \bar{\phi}_a(\mathbf{r}) \\
\mathbf{\Omega} = \frac{1}{2} G \left( \mathbf{P} \times \nabla \bar{\phi}_a(\mathbf{r}) + (\mathbf{Q} \cdot \nabla) \times \nabla \bar{\phi}_a(\mathbf{r}) \right)
\]

(2)

(3)

(4)

Here \( \mathbf{P} \), \( \mathbf{Q} \), \( \mathbf{U} \) and \( \mathbf{\Omega} \) are respectively dimensionless dipole moment, quadrupole moment, velocity and angular velocity. \( \bar{\phi}_a \) is the applied electric potential. The parameters \( \varepsilon_{cm} \), \( \varepsilon'_{cm} \), \( \sigma_{cm} \), \( \sigma'_{cm} \), \( D \) and \( D' \) are derived from the permittivities and conductivities and their definition can be found in the paper [11]. In this model there is another important parameter \( G \) measuring the electric field strength, which was proposed in the equation (19) of the reference [11]. Although the definitions of \( G \) vary according to the forms of electric fields, it’s always proportional to the strength of electric field. So this model is appropriate to research the dynamics of particles under a certain form of field with different strength.

The equation of the quadrupole potential can be written as \( \phi_a = a(x^2 - y^2) \) where the constant \( a \) is the measurement of the field strength [figure 1(a)]. Other 2D multipole fields can be easily derived [19]. Examples of pattern of electric potentials generated by 6 and 8 electrodes, or hexapole potential and octupole potential, are shown in figure 1(b) and (c). By introducing the field radius \( r_0 \), their potential can be written as \( \phi_6 = a(x^3 - 3xy^2)/r_0 \) and \( \phi_8 = a(x^4 - 6x^2y^2 + y^4)/r_0^2 \). In these fields the particles tend to be trapped in the central area with the lowest electric potentials. However, as the field strength increasing, the particles will move around the center rather than stay in the central point. Sometimes the particles will finally move through stable orbits.

![Figure 1](image1.png)

**Figure 1.** (a) The contour of quadrupole potential. (b) The contour of hexapole potential. (c) The contour of octupole potential. These contours reflect the distributions of potentials in various magnitudes.
3. Results: 2D fields
Since all the particles tend to move towards the area with lowest electric potential, generally the spherical particles in 2D electric fields will stay in a straight line perpendicular to the direction of field gradient so that all of them are in the center of the field, and that’s how linear ion traps store ions. For example, if the 2D electric field changes in x and y direction, then the chain formed by particles will be parallel to z direction. Figure 2 shows the initial (red points) and final (blue points) steady positions of 7 particles under 2D quadrupole potential perpendicular to z direction, which can be written as \( \phi_4 = a(x^2 - y^2) \). The final steady positions of the particles are on the z axis.

![Figure 2. Initial (red points) and final steady (blue points) positions of 7 particles under 2D quadrupole field perpendicular to z direction. The final steady positions are on the z axis.](image)

If the field strength becomes too strong, the particles will not stay in the center of electric field but move respectively in really complicated and unregular trajectories.

For single particle, its trajectory can be easily observed. By displaying the trajectory of the steady states, we can get some interesting patterns and classify the dynamics of particles into several stages as the field strength increasing.

3.1. Quadrupole field
Let’s consider the electric field generated by 4 electrodes first. The dynamic of particle within it when the field strength is small has been thoroughly discussed [11]. But the final trajectories under strong fields were only roughly researched. In the first stage, the particle will stay statically at the center without any rotation [figure 3(a)]. Because the electric field is too small to generate Quincke rotation. In the second stage with a stronger field, the particle will not only stay in the origin but also rotate with a stable angular velocity, which is Quincke rotation. The magnitude of angular velocity increases with the field strength. In stage 3, the stable trajectory of particle will reach into a special case. The steady state of the particle will be a circular orbit with its angular velocity still stay unchanged [figure 3(b)]. With even stronger field, in stage 4, the angular velocity of particle will fluctuate periodically, correspondingly the trajectory will not a circle but a periodic pattern too. Figure 3(c) gives an example of stage 4. Because the period of particle motion (T1) is generally not divisible by the period of each fluctuation (T2), the trajectory will cover an annular region after enough time. In other words, the particle will not move within a steady orbit. With an appropriate field strength, however, T1 is divisible by T2 so that steady state is a steady orbit. For the electric field generated by 4 electrodes, 3 special field strength are found, under which the ratios of T1 and T2 are 3, 4, and 7 [figure 4(a)-(c)]. When the electric field is too strong, there will be no steady state. The trajectory will become chaotic and irregular, which can be classified to stage 5 [figure 4(d)].
Figure 3. In this paper all the blue trajectories are from $t=0$ to $t=700$, and the red trajectories are from $t=600$ to $t=700$, which show the steady states. (a) Stage 1 and stage 2 under quadrupole field: in both of the stages the particle will approach and stay at the center, while there is no Quincke rotation in stage 1. (b) Stage 3: a steady circular orbit. (c) Stage 4: a periodic trajectory.

Figure 4. (a)-(c): 3 Special cases of stage 4 under quadrupole field, in which the particle will reach a steady state moving along a stable orbit. (a) $T_1/T_2=3$. (b) $T_1/T_2=4$. (c) $T_1/T_2=7$. (d) An example of stage 5 under quadrupole field: the trajectory is no longer regular and steady.
Figure 5. Fluctuation range of angular velocity vs $G$ reflecting 5 stages (S1-S5).

A graph of the fluctuation range of angular velocity in steady states vs the parameter $G$ [figure 5] can explicitly show the development of five stages (S1-S5). We can see only from the second stage with enough field strength can the Quincke rotation be generated. In stage 2 the steady angular velocity increases almost linearly with field strength while in stage 3 the angular velocity decreases with field strength. In stage 4 the angular velocity begins to fluctuate. The amplitude increases with $G$ first and then decreases with $G$. The chaotic rotation in stage 5 cannot be appropriately reflected on this graph.

3.2. Other multipole fields

With even more electrodes, like hexapole and octupole field, the result of particle trajectory is quite different from what we would expect. With any magnitude of field strength, the particle will move forward to the center without rotation [figure 6]. And the particle will stay near the origin point rather than accurately on the origin point, which indicates that the model can still be improved. In fact, when dealing with the electric potentials of the particle, the author of reference [11] made a multipole expansion for the disturbance potential and linearized the applied potential. The first two terms are included in the equations, which corresponds dipole moment $\tilde{P}$ and quadrupole moment $\tilde{Q}$. So adding other multipole moments like octupole moment is a direction to improve this model.

Figure 6. An example of the result under hexapole field: (a) the trajectory (b) the development of angular velocity. The particle will finally stay at the origin and the angular velocity will always fall to zero in this model.
4. Results: a 3D field

Obviously in a 3D electric field the particles will move along three-dimensional trajectories. This part will consider a simple 3D electric field whose potential equation can be written as $\phi_{3d} = \alpha(x^2 + y^2 - 2z^2)$. Looked from x-z plane and y-z plane [figure 7(a)], the potential is a deformation of quadrupole potential. Looked from x-y plane with a constant z coordinate [figure 7(b)], the potential can be written as $\alpha(x^2 + y^2 + \phi_0)$. This kind of field can also trap the particle into the center where the potential is minimum but can’t form a stable orbit. So the dynamics of the particles under this 3D field is somewhat similar to the quadrupole field but with the influence of the third dimension.

![Figure 7](image7.png)

**Figure 7.** (a) The contour of the 3D potential looked from x-z or y-z plane. (b) The contour of the 3D potential looked from x-y plane. These contours reflect the distributions of potentials in various magnitudes.

![Figure 8](image8.png)

**Figure 8.** (a) Stage 1 under the 3D field: the particle will stay at the center without Quincke rotation. (b) Stage 2: the particle will stay at the center with steady rotation. (c) Stage 3: the particle will move in a periodic trajectory. (d) Stage 4: the trajectory is no longer regular and steady.
Figure 9. Fluctuation range of angular velocity vs \( G \) reflecting 4 stages (S1-S4).

The trajectories and steady states of a single particle change with the field strength and can be classified into several stages like the quadrupole field. The first two stage is the same as the quadrupole potential. In the stage 1 when the field strength is too small to trigger Quincke rotation, the particle will stay at the center without rotation [figure 8(a)]. In the stage 2 the particle will stay at the center with a stable rotation velocity [figure 8(b)]. What is different is that there is no stage with a circular orbit like the stage 3 of quadrupole field. In the stage 3 of this 3D field, the particle will move along a 3D periodic trajectory. The trajectory will just cover a tubular region with its wall getting thicker and thicker [figure 8(c)]. This stage corresponds to the stage 4 of quadrupole field but there are still no special cases with stable orbit. In stage 4 the trajectory will become chaotic and irregular too [figure 8(d)]. A graph like figure 5 can show the development of the stages (S1-S4) and its similarity with the quadrupole field [figure 9].

This 3D electric field can also be used in an ion trap. Figure 10 shows the initial (red points) and final (blue points) steady positions of 7 particles under the 3D potential. No matter where the particles initially are, all of them eventually gather and stay near the center. When there are a large number of particles, there will be always some particles failing to stay near the center because the space nearing the central area is finite. In fact, its acknowledged that when used as ion trap, 2D electric fields are more efficient and have better capacity [20].

Figure 10. Initial (red points) and final steady (blue points) positions of 7 particles under the 3D electric field. The final steady positions are around the origin.
5. Conclusion
We researched the steady states of the particles under different electric fields with the effect of Quincke rotation. Under the electric fields of ion traps, the particles tend to stay around the center of the fields where the electric potentials are minimum. For multiple particles, we only considered their steady locations under small field strength. For a single particle, we can observe their steady trajectories. We first considered the quadrupole electric field. The development of steady states can be classified into 5 stages as the electric field strength increasing. In the stage 1, the field is too small to generate Quincke rotation. The particle will just stay at the center without rotation. In stage 2, the particle will stay at the center with a stable angular velocity, which is so-called Quincke rotation. The speed of rotation increases almost linearly with field strength. In stage 3, the particle will finally move around the origin along a stable orbit. For quadrupole field the orbit is a perfect circle. In stage 4, the orbit will not be stable. Both the motion and rotation of the particle will respectively oscillate and finally the trajectory will cover an annular region. However, there are some special cases in this stage. When the period of particle motion is divisible by the period of rotation, the particle can move along some interesting steady orbits. Theoretically there are more special cases than I showed above, the reason I didn’t find them may be that the step of field strength increasing is not small enough, or I have shown all the cases. It’s still discussible. When the electric field is too strong, the trajectory will be irregular and not worth study. The steady states under a 3D electric field are similar to the quadrupole field. The particle will evolve from staying at the center to moving along 3D trajectory.

Besides, the results of electric fields with more electrodes seem to be unreasonable, the particles will always stay at the origin without Quincke rotation. To get better results under these more complicated fields, we may need to improve this model by adding more multipole moments into the model to describe the electric potential more accurately.

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