Similarities in Dielectrophoretic and Electrophoretic Traps

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Abstract In this study we present a universal theoretical formulation of the particle motions in electrophoretic and dielectrophoretic traps. It is extended from the well-known Mathieu equation based theories for Paul trap. The white noise random force model is utilized to form the Brownian motion of particle in the traps and the instantaneous dielectrophoretic force is employed rather than the time-averaged ponderomotive expression. The new approach enables many interesting properties of dielectrophoretic traps about stability and random motion. This study will be expected to provide a concrete protocol for the design of nanoscale traps which is essential in single molecule analysis.

Keywords: Dielectrophoretic trap, Paul trap, Random motion, Universality

1. Introduction

Electrophoresis (EP) and Dielectrophoresis (DEP) are two representative object-manipulation principles used in various biological applications including trapping, sorting, separation of cells, viruses, nanoparticles, etc. (Hughes and Morgan, 1998; Hughes, 2000; Voldman et al., 2006, Guan et al., 2011; Park et al., 2012). EP is the motion of charged particles due to the electric field by following Columbic law while DEP is the movement of the suspended particles in solvent resulting from polarization forces induced by an inhomogeneous electric field. Due to the difference in fundamentals, DEP is usually applied to the neutral particles while EP is utilized to handle the charged particles.

In the present study, we consider the planar quadrupole dielectrophoretic trap (planar QDT, see Figure 1), in which four electrodes are aligned mutually perpendicular and pointing towards the trap center. Oscillating (AC) electric fields are applied to the electrodes such that the phase angle of the field between adjacent electrodes is 180°. Such geometrical configuration is same as that of planar Paul trap (planar PT) which is typically used to trap the charged atom and ions in low pressure environment (Hughes, 2000).

Although both planar QDT and PT employ the quadrupole electrodes with AC field, their analyses are quite different: For DEP traps, people have mostly been interested in the static characteristics, which is governed by the ponderomotive components. However, for PT the rigorous understanding of dynamic features (e.g. stability) including static ones has been established with the aid of Mathieu function theory. It enables an accurate estimation of particle random motion at long-time limit.

Conventionally, the stability of DEP trap has been known to be determined by the sign
of real part of Clausius-Mossotti factor, \( \Re \left( \frac{\sigma_p - \sigma_m}{\sigma_p + 2\sigma_m} \right) \), where \( \sigma = \varepsilon \) the product of dielectric constant of material and vacuum permittivity \( (\varepsilon_0 = 8.854 \times 10^{-12} \text{ F/m}) \), \( \sigma \) is electric conductivity, \( j \) is the imaginary unit, \( j = -1 \), \( \omega \) is AC frequency. The subscripts \( p \) and \( m \) indicate particle and medium, respectively. \( \Re(f_{CM}) \) has the value of \( \frac{\sigma_p - \sigma_m}{\sigma_p + 2\sigma_m} \) at low frequency limit (\( \omega \to 0 \)) and \( \frac{\varepsilon_p - \varepsilon_m}{\varepsilon_p + 2\varepsilon_m} \) at high frequency limit (\( \omega \to \infty \)) (see Figure 2). \( \Re(f_{CM}) \) becomes zero at the critical frequency of \( \omega_{crit} = \sqrt{\frac{\sigma_p - \sigma_m}{\sigma_p + 2\sigma_m}} \). If the particle is less polarizable than the medium (\( \omega > \omega_{crit} \)), then \( \Re(f_{CM}) \) becomes negative, and the particles experience the force towards field minima (negative DEP, or nDEP). If the relative polarizability is greater than that of the medium (\( \omega < \omega_{crit} \)), then \( \Re(f_{CM}) \) will be positive (positive DEP, or pDEP), and the particle moves to field maxima (Voldman, 2006). In PQDT, nDEP makes the trap stable by localizing the targets towards the center, whereas pDEP pushes the particles towards the electrodes and the trap becomes unstable.

At low AC field frequencies, the ions have enough time to follow each change in sign of the field direction, so the conductivity effect is dominant. However, At high frequency the ions do not have enough time to follow the change in sign of the field. Thus the permittivity dominates (Orlin et al, 2009). The polystyrene is known as good dielectric material even at high AC frequency, so its electric conductivity can be assumed constant regardless of the change of AC frequency. The electric properties of electrolyte vary with frequency (Jones et al., 2004). However, the AC frequencies utilized in electrophoretic and dielectrophoretic traps are sufficiently high (> 100 kHz) in which the electric properties do not change any more. Considering this, the variation of electric properties with AC frequency is not included in this study.

The quadrupole electrode configuration is also used for the Paul trap (planar quadrupole Paul trap, PQPT) which traps charged particles (e.g. atoms and ions) (Paul, 1990). Although both PQDT and PQPT use the quadrupole electrodes with AC-field, their analyses are quite different from each other: The particle motions in DEP trap have been investigated with the period-averaged ponderomotive DEP force (Hughes et al, 1998 and Voldman et al, 2001), whereas for PQPT the dynamics is understood based on the instantaneous electrophoretic force (Arnold et al, 1993, Hasegawa et al, 1995, Major et al, 2005 and Park et al, 2012). Such difference gives rise to the following question: Does a universal theory for the electrical traps exist? Also, the random motion in DEP trap has not been attracted so far possibly because the DEP usually traps the micro-objects whose size is sufficiently larger than the thermal noise. However, if the size of particle is in nanoscale, its random motion becomes prominent. The current rapid development of single molecule analysis (Gupta, 2008 and Walter et al, 2008) highly demands the trapping of nanometer-and/or sub-nanometer-sized biological objects (DNA, proteins, etc.).

Considering all the above, in this study we employ the equation of motion (EOM) with instantaneous DEP force, and then investigate the stabilities in analogue with the theories for PQPT. Also, the random fluctuations in PQDT are rigorously examined.

2. Equation of Motion (EOM)

EOM for the particles in EP trap (x-direction) is given by:
\[
\frac{d^2 x}{d t^2} = -\gamma \frac{dx}{dt} + F_{\text{DEP},x} + \sqrt{2k_B T \gamma W(t)}
\]

(1)

where \( \gamma \) is the viscous friction coefficient formulated as \( \gamma = 6\pi r \eta \). \( r \) is the particle radius and \( \eta \) is the medium viscosity. \( \sqrt{2k_B T \gamma W(t)} \) is the fluctuation force due to random impulse from the neighboring fluid molecules and \( W(t) \) is the white noise with (mean, variance) = (0,1). The DEP force, \( F_{x,\text{DEP}} \) can be expressed with the multi-pole expansion in quadrupole electric field (Washizu et al, 1996):

\[
F_{\text{DEP},x} = 2A_{\text{DEP}} \times \left[ \text{Re}(f_{\text{CM}}) + |f_{\text{CM}}| \cos(2\omega t - \phi) \right] x
\]

(2)

where

\[
A_{\text{DEP}} = \frac{n_0 r^3 V_0^2}{R_0^4} \ ,
\]

(3)

\[
|f_{\text{CM}}| = \sqrt{\left[ \text{Re}(f_{\text{CM}}) \right]^2 + \left[ \text{Im}(f_{\text{CM}}) \right]^2} \ ,
\]

(4)

\[
\tan \phi = \frac{\text{Im}(f_{\text{CM}})}{\text{Re}(f_{\text{CM}})} \ .
\]

(5)

Considering the correspondence between \( x \)- and \( y \)-directional DEP forces, it is sufficient to examine the EOM in \( x \)-direction in identifying the dynamic features of PQDT. Therefore, the subscript \( x \) for \( F_{\text{DEP}} \) is dropped for simplicity hereafter.

As a first step to understand the dynamic features of PQDT, we consider the case without both fluidic damping and random force, i.e. The first and second terms in Eq. (1) are neglected.

### 3. Results and Discussion

#### 3.1 No fluidic damping, no random motion

When the fluidic damping and random fluctuation are not considered, Eq. (1) becomes

\[
m \frac{d^2 x}{d t^2} - 2A_{\text{DEP}} \times \left[ \text{Re}(f_{\text{CM}}) + |f_{\text{CM}}| \cos(2\omega t - \phi) \right] x = 0
\]

(6)

By introducing a dimensionless time of \( \tau = \omega t \)

\[
d^2 x \over d\tau^2 + \left[ a_{\text{DEP}} - 2q_{\text{DEP}} \cos(2\tau - \phi) \right] x = 0
\]

(7)

Now, the above expression is quite similar to the governing equation for PQPT (Mathieu equation). Although the DC field is not applied, the term mimicking DC effect naturally appears as \( a_{\text{DEP}} \) (pseudo-DC effect). This term is equivalent to the \( a_{\text{PT}} \)-parameter (\( a_{\text{PT}} = \frac{2QU}{mR_0^3 \omega^2} \), where \( U \) is DC voltage and \( Q \) is particle charge) expressing DC contribution to Paul trap. Due to the mathematical similarity, all the theoretical approaches for PQPT are expected to be still valid for PQDT (Paul, 1990; Major et al, 2005). Following the general procedure of the stability analysis for PQPT (Hasegawa et al, 1995) we can construct the stability chart for PQDT as illustrated in Figure 3.

For a typical micro-sized polystyrene bead (\( r = 1.0 \mu m \), density is \( \rho_p = 1050 \text{ kg/m}^3 \)) in a micro-trap (\( R_0 = 4.0 \mu m \) and \( V_0 = 1.2 \text{ V} \)), \( A_{\text{DEP}} \) has the value of \( 1.228 \times 10^{-5} \text{ N/m} \). Also, \( a_{\text{DEP}} \) and \( q_{\text{DEP}} \) are expressed as

\[
a_{\text{DEP}} = -\frac{A_{\text{DEP}}}{m \omega^2} \text{Re}(f_{\text{CM}}) \quad \text{and} \quad q_{\text{DEP}} = \frac{A_{\text{DEP}}}{m \omega^2} |f_{\text{CM}}| \ ,
\]

respectively. Since \( \frac{e_p + e_n}{e_p + 2e_n} \frac{\sigma_p - \sigma_n}{\sigma_p + 2\sigma_n} \) and \( 0 < \cos \phi < 1 \), in practical applications \( a_{\text{DEP}} \) and \( q_{\text{DEP}} \) generally fulfil the condition of \( |a_{\text{DEP}}| \ll 1 \) and \( 0 < q_{\text{DEP}} \ll 1 \). This condition is
valid for nano-particle in nano-trap as well, because the value of $A_{\text{DEP}}$ is still quite small as $1.228 \times 10^{-4}$ N/m for ($r$, $R_0$) = (100, 400) nm and $1.228 \times 10^{-2}$ N/m for ($r$, $R_0$) = (1, 4) nm. As seen in Figure 3(b), in the very vicinity of $(a_{\text{DEP}}, q_{\text{DEP}}) = (0, 0)$ the slope of the stability border becomes zero. It indicates that for the condition of $0 < q_{\text{DEP}} \ll 1$ which commonly happens in practical applications, the stability of PQDT is purely determined by the sign of $a_{\text{DEP}}$. The trap is stable when $a_{\text{DEP}} > 0$ and $\text{Re}(f_{\text{CM}}) < 0$ while it becomes unstable for $a_{\text{DEP}} < 0$ and $\text{Re}(f_{\text{CM}}) > 0$. This is exactly identical to the well-known conventional stability condition that PQDT is stable when $\omega > \omega_{\text{crit}}$ whereas unstable with $\omega < \omega_{\text{crit}}$. For example, the particle in water and that in n-hexane have the same stability feature. This is a unique property of PQDT, distinguished from PQPT. This observation still holds for the nanoparticles in nano-trap as illustrated in Figure 5. For a nano-particle, the value of $b_{\text{DEP}}$ is further increased and as a result, the region of stability is hugely enlarged (see Figure 5(a)), while maintaining the tangent of stability border near $(a_{\text{DEP}}, q_{\text{DEP}}) = (0, 0)$ as zero. It is because the stability features of PQDT are all determined by the first island in the stability chart, and the first island is known to be robust to the change of system parameters for PQPT (Major et al, 2005; Zerbe et al, 1994).

### 3.2 With fluidic damping, no random motion

If we consider the fluidic damping without random force, Eq. (1) is expressed as

$$m \frac{d^2 x}{dt^2} + \gamma \frac{dx}{dt} - 2A_{\text{DEP}} x \left[ \text{Re}(f_{\text{CM}}) + \left| f_{\text{CM}} \right| \cos(2\omega t - \phi) \right] x = 0$$

(8)

In order to non-dimensionalize Eq. (8), a parameter $b_{\text{DEP}} = \frac{\gamma}{m\omega}$ needs to be introduced in addition to $a_{\text{DEP}}$ and $q_{\text{DEP}}$:

$$\frac{d^2 x}{dt^2} + b_{\text{DEP}} \frac{dx}{dt} + [a_{\text{DEP}} - 2q_{\text{DEP}} \cos(2\tau - \phi)] x = 0$$

(9)

Figure 4 shows the stability chart for the micro-particle ($r = 1 \mu m$) in the micro-trap ($R_0 = 4 \mu m$) with viscous medium. The $b_{\text{DEP}}$ values in the figure are typical ones for the micro-traps. With inclusion of viscous damping, the stable area is enlarged and it further widens with increase in $b_{\text{DEP}}$. However, near $(a_{\text{DEP}}, q_{\text{DEP}}) = (0, 0)$, the tangent of stability border is still zero. It indicates that the stability condition of PQDT is not affected by the medium viscosity: stable with $\omega > \omega_{\text{crit}}$ whereas unstable with $\omega < \omega_{\text{crit}}$.

### 3.3 With fluidic damping, with random motion

Rewriting Eq. (1) with random force as well as fluidic damping,

$$m \frac{d^2 x}{dt^2} + \gamma \frac{dx}{dt} - 2A_{\text{DEP}} \times \left[ \text{Re}(f_{\text{CM}}) + \left| f_{\text{CM}} \right| \cos(2\omega t - \phi) \right] x = \sqrt{2k_BT/\gamma} W(t)$$

(10)
The particle trajectory $x(t)$ from Eq. (10) consists of the deterministic part, $x_{\text{det}}(t)$, and the random oscillation, $x_{\text{ran}}(t)$. Two different numerical methods of conventional 4th-order Runge-Kutta method and Euler-Maruyama method (Yuan et al, 2004; Cohen et al, 2012) were applied to numerically compute $x_{\text{det}}(t)$ and $x_{\text{ran}}(t)$, respectively. A typical trajectory for micro-particle in micro-trap is illustrated in Figure 5(a). The magnitude of random fluctuation was measured by averaging $x_{\text{ran}}(t)$ over 10 repetitions with different random seeds. Figure 6 reveals the detailed trajectories and phase plots for micro-particle ($r = 1 \mu m$) in micro-trap ($r = 4 \mu m$) at various frequencies of $f = f_{\text{crit}}, 1.2f_{\text{crit}}$, and $1.5f_{\text{crit}}$. For the stable traps, at long-time limit ($t \to \infty$) only the random part remains while the deterministic part in the motion vanishes. If the system is not stable, the mean motion itself diverges regardless of the random motion, i.e. the system stability can be determined by the EOS without random motion (Park et al, 2012). The magnitude of random fluctuation at long-time limit, $\sqrt{\langle x^2 \rangle}$, is estimated from the average over 10 repetitions.

For the micro-particle in micro-trap, $\sqrt{\langle x^2 \rangle}$ decreases as $82.8 \to 46.7 \to 33.6$ nm, as $\omega / \omega_{\text{crit}}$ increases as $1.0 \to 1.2 \to 1.5$. The random motion is less than 8% of particle size at most. When only the particle size is reduced by 1/10 (100 nm) with maintaining the trap size, the random fluctuation decreases as 26.2 nm and it remains almost unchanged with the change of frequency (25.8 nm at $\omega = 1.5\omega_{\text{crit}}$). However, when the particle with the radius of 100 nm is placed in a nano-trap whose size is $R_0 = 400$ nm, the random fluctuation is observed as 24.8 nm at $\omega = \omega_{\text{crit}}$, which is further reduced as 12.2 and 8.8 nm with increase in frequency as 1.2 and 1.5 $\omega_{\text{crit}}$, respectively. Thus, $\sqrt{\langle x^2 \rangle}/r$ is increased as 24% at maximum. These observations indicate that the trapping of nano-particle can be successful only with the nano-sized trap, however its random motion becomes comparable to the particle size.
5. Conclusions

In conclusion, in the present study a universal theoretical approach has been developed for the analysis of dynamics of electrical traps such as PQDT and PQPT. The instantaneous formulation for DEP force was employed rather than the ponderomotive expression. This approach leads us to several interesting properties in addition to the reproduction of conventional key properties of PQDT. For example, the stability of PQDT was not affected by the degree of medium viscosity. Also, the quantification of random fluctuation in PQDT was possible. In near future, PQDT is expected to further miniaturize to nanoscale to trap biomolecules (e.g. DNA, RAN, protein, etc.) for single-molecule analysis. The current study will be a milestone for such endeavor.

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References


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