

Effective forces and pseudopotential wells and barriers in the linear Paul trap

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Abstract. The paper presents the numerical studies of effective forces acting on a charged microparticle inside the linear Paul trap in gas media. The locations of the microparticle trapping as the dependence on microparticle and trap parameters have been studied.

1. Introduction

The theory of motion of a nonrelativistic charged particle in an alternating electric field was developed in [1]. The effective force acting on a charged particle is called Gaponov–Miller force [4]. The generalizations of the theory of charged particle motion in an alternating electric field in a gaseous medium with the friction force proportional to the particle velocity was derived in [5].

The phenomenon of charged microparticles trapping by an alternating electric field is used in Paul traps [6]. The alternating electric field in the trap is generated by the alternating voltage of specific frequency that is applied to the trap electrodes. This alternating electric field may result in arising of pseudopotential wells and barriers in various areas of the trap and the physics of trapping as well as the particle behavior are not similar to those for traps like [2, 3]. Pseudopotential wells and barriers do not depend on the sign of microparticle charge but on its magnitude.

The purpose of this work is to use the approach developed in [4] for studying the effective forces that act on a charged microparticle in the linear Paul trap and identification of areas of pseudopotential wells and pseudopotential hills inside the trap. The dependencies of microparticle charge, mass, alternating field magnitude and frequency on areas of pseudopotential wells and barriers were studied.

2. Numerical calculations of the effective force acting on a charged microparticle in the linear trap

The sketch of the linear Paul trap is presented in figure 1. The trap consists of four cylindrical electrodes with radius $R_1 = 1$ mm and length $L = 10$ cm. The distance between the axes of the electrodes is $L_b = 2$ cm. The alternating voltage $U_\omega \sin(\omega t)$ is applied to a pair of electrodes number 1 and $-U_\omega \sin(\omega t)$ is applied to pair of electrodes number 2, where $\omega = 2\pi f$, f is the voltage frequency, U_ω is AC voltage amplitude.



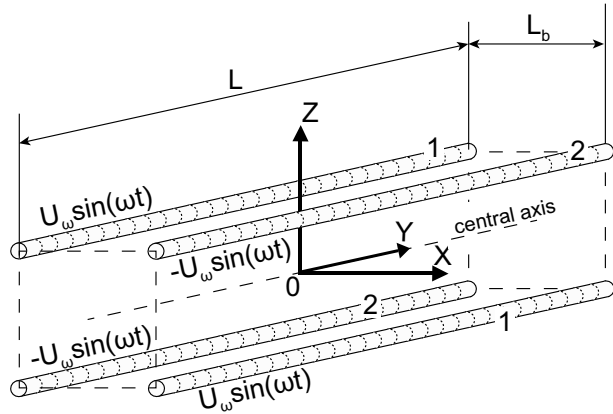


Figure 1. The sketch of the linear Paul trap.

The microparticle motion in the alternating electric field is described by the equation

$$m_p \ddot{\vec{r}} = m_p \vec{g} + \sum_e \vec{F}_e(r) + 6\pi\eta r_p \dot{\vec{r}}, \quad (1)$$

where m_p is the microparticle mass, $\ddot{\vec{r}}$, $\dot{\vec{r}}$ and \vec{r} are microparticle acceleration, velocity and vector respectively, g is the free fall acceleration, $F_e(r)$ is an electric force acting on the microparticle from each electrode e , η is the dynamic viscosity of gas medium ($\eta = 18 \mu\text{Pa s}$), r_p is a microparticle radius.

The electric force acting on the microparticle from each electrode can be represented as the sum of Coulomb forces of point-like charges uniformly distributed along the electrode positioned along the axis of the surrounding grounded cylindrical shell [7–9]:

$$\vec{F}_e(r) = \sum_t \frac{LU q_p (\vec{r}_t - \vec{r})}{2N \ln \frac{R_2}{R_1} (r_t - r)^3},$$

where, U is the electrode voltage ($U \sin(\omega t)$ or $-U \sin(\omega t)$), q_p is a microparticle charge, N is the number of point-like charges presenting the charges of each trap electrode, R_2 is the radius of the grounded cylindrical shell surrounding the trap, r_t is the vector of a point-like charge.

To calculate the effective force acting on a charged microparticle the equation (1) should be solved at the initial conditions $s(r_0, \dot{r}_0)$ at $t = 0$ and the velocity of a microparticle as a time-varying function $v_p(t, s)$ should be found [4]. To derive the microparticle velocity $v_p(t)$ the equation (1) was solved numerically by the Runge-Kutta method of order $N_{rk} = 4$.

Let's consider kinetic energy of a microparticle moving with the velocity $v_p(t, s)$. The averaged kinetic energy of a microparticle over the period of the electric field oscillation ($T = 1/f$) is described by the equation

$$\overline{W(r_0)} = \frac{1}{2} m_p \frac{\int_0^T v_p(t, s)^2 dt}{T}$$

and the effective force acting on a charged microparticle can be derived from the equation

$$F_{\text{eff}} = - \nabla_{r_0} \overline{W(r_0)}.$$

The equation (1) was solved separately for projections of $v_p(t, s)$ on the axes x , y and z . At calculating a velocity projection on one axis, velocity projections on another two axes were considered as 0 m/s. The following initial conditions s were taken in the numerical calculations: the initial microparticle velocity $r_0 = 0$ m/s and the initial microparticle position r_0 was taken as

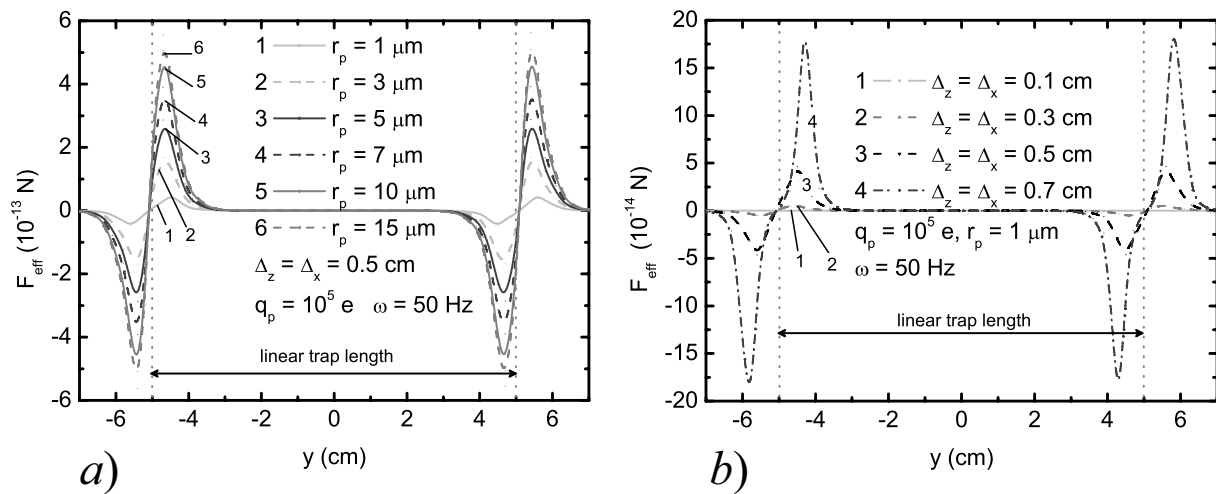


Figure 2. The dependences of F_{eff} on the position of microparticle along the y axis at different microparticle radii r_p (a), at different initial microparticle shifts Δ_x and Δ_z (b).

a shifts Δ_x , Δ_y and Δ_z from the coordinate origin (point 0 in figure 1). In numerical calculations, a microparticle moved along one axis from the initial position while other two coordinates were fixed.

In the numerical calculations the microparticle with mass density $\rho_p = 3990 \text{ g/cm}^3$ was used. The microparticle charge and the initial microparticle position are shown in the following figures. The voltage magnitude was set $U_\omega = 1 \text{ kV}$.

The results of the effective force calculations along y axis are presented in figure 2 where the y axis is directed to the right. Figure 2a presents the dependences of F_{eff} on the position of microparticle along the y axis at different microparticle radii r_p . In figure 2a and following figures microparticle is dragged to the right in areas with positive value of the effective force and dragged to the left in areas with negative value of the effective force. It means that the microparticle is dragged to the point where F_{eff} changes its sign from positive to negative. Also in figure 2a and following figures vertical dot lines demonstrate the borders of the trap.

In figure 2a the maximum magnitude of the force F_{eff} is proportional to microparticle radius, not the microparticle mass. Also in figure 2a the areas of positive and negative values of F_{eff} overlap the linear trap ends. It means that outside the trap near the ends of it there are regions about 1 mm aside where the microparticle is attracted by the trap.

In figure 2b the dependences of F_{eff} on the position of the microparticle along the y axis at different initial microparticle shifts Δ_x and Δ_z are shown. The closer the microparticle to the central trap axis (figure 1) the smaller magnitude of F_{eff} will be because the value of the peak to peak of the electric field strength during an oscillation period will be smaller near the central axis. At the central axis F_{eff} becomes zero.

The behavior of F_{eff} across the linear trap electrodes is presented in figures 3 and 4, where the x axis is directed to the right. In figure 3a the dependences of F_{eff} on the position of the microparticle along the x axis at different initial shift Δ_z are shown. The closer the microparticle to the central trap axis the smaller magnitude of F_{eff} will be. At central axis F_{eff} becomes zero. Also from figure 3a one can see that trapping area lies in the narrow region with a width of about a half of the distance between the trap electrodes.

In figure 3b the dependences of F_{eff} on the position of the microparticle along the x axis at different microparticle radii r_p are shown. Lines 1, 2 and 3 for the small microparticle ($r_p = 1$ – $5 \mu\text{m}$) show that the effective force instead of trapping it inside the trap throws it out. The

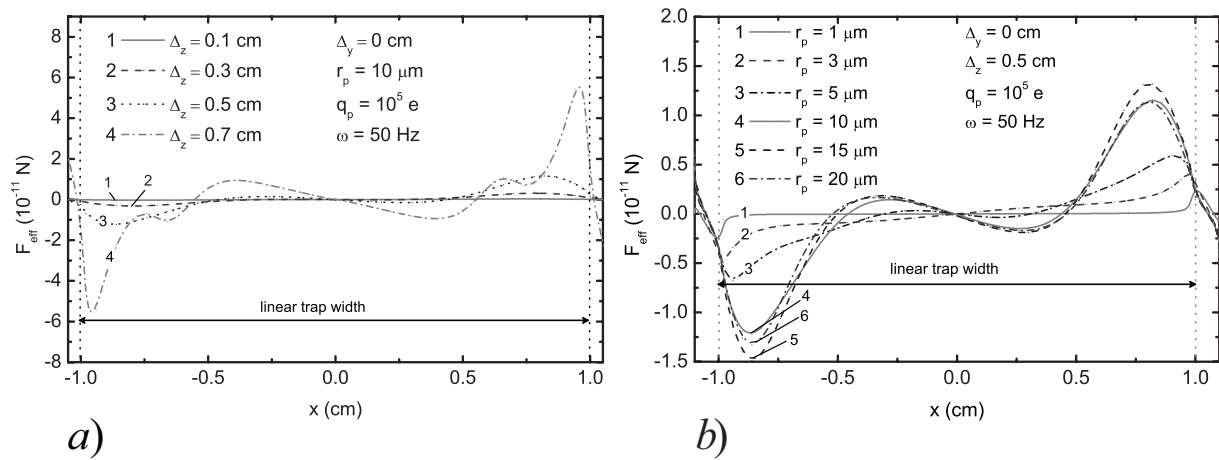


Figure 3. The dependences of F_{eff} on the position of the microparticle along the x axis at different initial shift Δ_z (a), at different microparticle radii r_p (b).

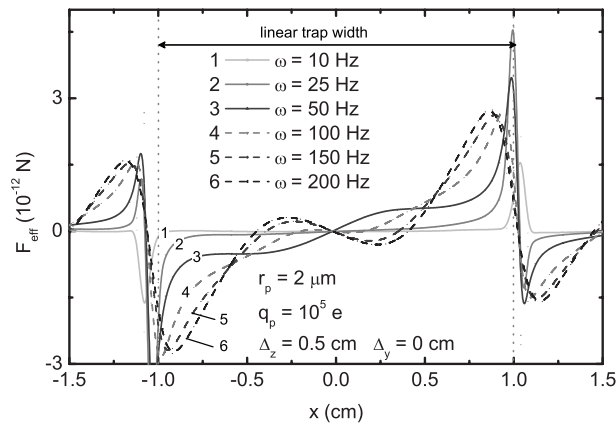


Figure 4. The dependences of F_{eff} on the position of the microparticle along the x axis at different alternating voltage frequencies ω .

microparticle trapping starts at a microparticle radius bigger than $r_p = 5 \mu\text{m}$. The width of trapping area becomes wider with the growth of microparticle radius.

To trap a small particle the frequency of the alternating voltage should be increased. In figure 4 the dependences of F_{eff} on the position of the microparticle along the x axis at different frequencies f are shown. While at frequencies lower than 50 Hz the trap tends to throw the small microparticle ($r_p < 5 \mu\text{m}$) out, at high frequencies greater than ~ 100 Hz the trap holds the microparticle inside. Also in figure 4 one can see that outside the trap there are regions where the sign of F_{eff} value changes from positive to negative in the x axis direction and microparticle can be trapped in these areas.

All results presented above were derived in the absence of gravity.

The behavior of the effective force F_{eff} in the case of gravity across the linear trap electrodes is presented in figure 5, where the z axis is directed to the right and the gravity to the left. In figure 5a the dependences of F_{eff} on the position of the microparticle along the z axis at different microparticle radii r_p are shown. The behavior of F_{eff} in the case of gravity becomes complex, i.e. inside the trap two areas of the microparticle capturing appear: one above the central axis of the trap and the other one at the border of the trap.

The dependences of F_{eff} on the position of the microparticle along the z axis at different initial microparticle shift Δ_x are shown in figure 5b. Figure 5b shows that the greater microparticle is shifted aside in the x axis the more areas of the microparticle capturing appear. For example

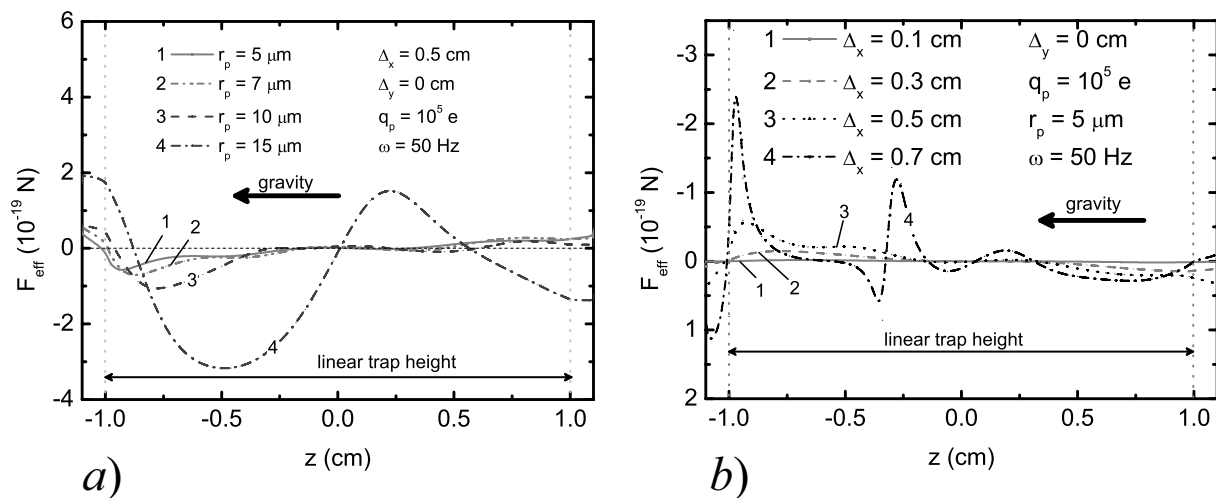


Figure 5. The dependences of F_{eff} on the position of microparticle along the z axis at different microparticle radii r_p (a), at different initial microparticle shift Δ_x (b).

line 4 ($\Delta_x = 0.7$ cm) in figure 5b changes the sign from positive to negative 3 times inside the trap while line 1 does the same change only once.

3. Conclusion

The effective forces acting on the charged microparticle inside the linear Paul trap were studied. The effective force behavior appeared to be complex which is expressed in the appearance of the pseudopotential wells and barriers at different areas inside and outside the trap.

In the presence of gravity, it appears to be from 1 to 3 pseudopotential wells in the vertical direction depending on the microparticle radius. The presence of the stopping potential along trap electrodes was shown. To confine small particles with radius less than 5 μm the frequency of the alternating voltage of the trap needs to be higher than 100 Hz.

The numerical calculations predict the possibility of the microparticle trapping outside the trap.

Acknowledgments

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