Numerical comparison between Maxwell stress method and equivalent multipole approach for calculation of the dielectrophoretic force in octupolar cell traps.

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Abstract— **This paper presents detailed numerical calculations of the dielectrophoretic force in octupolar traps designed for single-cell trapping. A trap with eight planar electrodes is studied for spherical and ellipsoidal particles using an indirect implementation of the boundary element method (BEM). Multipolar approximations of orders one to three are compared with the full Maxwell stress tensor (MST) calculation of the electrical force on spherical particles. Ellipsoidal particles are also studied, but in their case only the dipolar approximation is available for comparison with the MST solution. The results show that the full MST calculation is only required in the study of non-spherical particles.**

Keywords: Dielectrophoresis, microelectrodes, boundary element, dieletrophoretic trap.

I. INTRODUCTION

When a dielectric particle is suspended in a medium of different electrical properties, and is subjected to a spatially non-uniform electric field, a force actuates on the particle. This force is called the dielectrophoretic (DEP) force [1], and depending on whether the particle is forced to move towards the minimum or the maximum of the external field, it is denominated negative or positive dielectrophoresis. A recent review of the theory behind DEP can be found in [2].

The DEP force is of great interest because biological cells and macromolecules behave as dielectric particles in external AC fields, and thus their movement can be controlled by using an appropriately designed electric field. Applications of DEP today include sorting [3], separation [4], and characterization [5] of biological particles. Manipulation of viruses [6] and DNA molecules [7] has already been demonstrated using this technique.

The conventional theory of dielectrophoresis uses a dipolar approximation to calculate the DEP force [1]. In this approximation, it is assumed that only a dipole is induced on the particle and that the particle is small enough compared to the characteristic variation length of the external electric field, that this can be considered constant in the region surrounding the particle. In the case of single-cell traps the field changes

rapidly, and it is of interest to find out precisely what level of accuracy can be expected from this approximation. Also if the particle is situated near a field null, higher order moments will be of importance in comparison with the first order (dipole) moment, and the approximation will fail to predict correctly the behavior of the particle.

The predictions made by the dipole model can be significantly improved by the application of a more complete model that includes higher order moments. The general expresions for the multipolar approximation for a homogeneous sphere in an arbitraty electric field was developed in the works by Washizu [8], and Jones and Washizu [9], [10]. Schnelle *et al* [11] were the first to study the influence of higher order moments on particle behavior in dielectrophoretic traps.

Although the multipolar approximation has been fully developed for the case of a spherical particle, there are no available expressions for the higher order multipolar contributions to the force for ellipsoidal particles —that could be used to approximate many biological particles. Furthermore, the multipolar method can not be used with irregularly shaped particles, such as the biconcave shape adopted by erythrocytes. This leaves open the question of how good the dipolar approximation is when applied to realistic systems where the particle is of a size comparable to the trap size and has a non-spherical shape.

A precise calculation of the force can be obtained numerically without resorting to the multipolar approximation, by considering the particle's presence in the external field calculation and then using the Maxwell stress tensor method [12] to obtain the force. Initial comparative studies by Benselama *et al* [13] show that even higher order multipolar calculations fail to predict accurately the electrical forces on a spherical particle when it is positioned close to the electrodes.

Because a full MST calculation is more involved and takes a much longer computational time —a complete multidomain numerical calculation must be done for each position of the particle in the trap—, it is of interest to compare it with the multipolar approximation for particles of different shapes and

sizes to find out if the increment in complexity is justified by the difference in the results. It is our objective to clarify the issue of whether the dipolar approximation or the equivalent multipole approach used by most authors can predict accurately the electrical force in dielectrophoretic single-cell traps.

In the following sections the theory of the dipolar and multipolar approximations is briefly introduced, followed by the complete MST solution, and then results from each of these approaches are shown and analysed.

II. EQUIVALENT MULTIPOLE MODEL OF THE DEP FORCE

In this approach the particle under consideration is substituted by a series of multipoles that account for the local changes of the electric field in the region surrounding the particle. This approximation is strictly valid only when the external field is not changing rapidly in the region containing the particle.

A. Spherical particles

In the simplest possible approximation, the time-averaged DEP force for a spherical particle is given by the expression:

$$\left\langle \vec{F}_{\text{DEP}} \right\rangle = 2\pi R^3 \varepsilon_{\text{f}} Re\left[K\left(\omega\right)\right] \nabla(E^2) \tag{1}$$

where R is the particle radius, ε_f is the permittivity of the fluid suspending medium, E is the rms magnitude of the local electric field, and $Re[K(\omega)]$ is the real part of the Clausius-Mossotti factor, given by:

$$K(\omega) = \frac{\tilde{\varepsilon}_{\text{p}} - \tilde{\varepsilon}_{\text{f}}}{\tilde{\varepsilon}_{\text{p}} + 2\tilde{\varepsilon}_{\text{f}}} \tag{2}$$

where ω is the angular frequency of the external applied field and $\tilde{\varepsilon}_{\text{f}}$ and $\tilde{\varepsilon}_{\text{p}}$ are the complex dielectric permittivities of the fluid and the particle respectively. The complex permittivities are given by $\tilde{\varepsilon}_{\text{i}} = \varepsilon_{\text{i}} - j\sigma_{\text{i}}/\omega$, where ε_{i} is the dielectric permittivity of medium i, σ_{i} is the electric conductivity of medium i, and j is $\sqrt{-1}$.

This is the dipolar approximation for the DEP force on a sphere, and it is used extensively in the literature to predict the characteristics of DEP cell traps.

The general expression of the DEP force in terms of its multipolar components was obtained by Washizu and Jones [9], [10], and the expression of the time averaged nth force order contribution is:

$$\left\langle \vec{F}_{\text{DEP}}^{(n)} \right\rangle = \frac{1}{2} \frac{\mathbf{p}^{(n)} [\cdot]^n \left(\nabla\right)^n \vec{E}}{n!} \tag{3}$$

where $[\cdot]^n$ and $(\nabla)^n$ represent n dot products and gradient operations, and $\mathbf{p}^{(n)}$ is the multipolar induced tensor of order n:

$$\mathbf{p}^{(n)} = \frac{4\pi\varepsilon_{\text{f}} R^{2n+1} n}{(2n+1)!!} K^{(n)}(\omega) \left(\nabla\right)^{n-1} \vec{E} \tag{4}$$

with $K^{(n)}$ the nth order Clausius-Mossotti factor given by:

$$K^{(n)}(\omega) = \frac{\tilde{\varepsilon}_{\text{p}} - \tilde{\varepsilon}_{\text{f}}}{n\tilde{\varepsilon}_{\text{p}} + (n+1)\tilde{\varepsilon}_{\text{f}}} \tag{5}$$

Note that a factor $1/2$ is included in (3) in order to account for the time average, under the assumption that the external field oscillates harmonically.

A BEM calculation is used to find the external field produced by the electrode arrangement, and its derivatives, in order to find the force using this approximation. Once the field and its derivatives are calculated on the centre of the sphere, a simple application of the formulas above gives the total DEP force on the particle.

B. Ellipsoidal particles

The induced effective moment for an ellipsoidal particle with principal radii a, b, and c, can be found by examining the limit of the electrostatic potential at a point far from the ellipsoid, where ellipsoidal coordinates degenerate into spherical coordinates. Following Jones [14] the x component of the effective dipole moment due to a dielectric ellipsoid is given by:

$$p_{\text{x}} = \frac{4\pi\text{abc}}{3}\varepsilon_{\text{f}}\left[\frac{\varepsilon_{\text{p}} - \varepsilon_{\text{f}}}{\varepsilon_{\text{f}} + (\varepsilon_{\text{p}} - \varepsilon_{\text{f}})L_{\text{x}}}\right]E_{\text{x}} \tag{6}$$

The other two components of the effective moment, p_{y} and p_{y}, are of similar form. The time-averaged dielectrophoretic force produced by a harmonically oscillating external field on the ellipsoid is then given by the following expression:

$$\left\langle \vec{F}_{\text{DEP}}^{\text{ellipsoid}} \right\rangle = \frac{2\pi abc}{3}\varepsilon_{\text{f}}\left[p_{\text{x}}\partial_{\text{x}} + p_{\text{y}}\partial_{\text{y}} + p_{\text{z}}\partial_{\text{z}}\right]\vec{E} \tag{7}$$

Where the depolarization factors L_{x}, L_{y}, and L_{z}, are all positive and interrelated as follows:

$$0 \leq L_i \leq 1, \qquad i = x, y, z \tag{8}$$

$$L_{\text{x}} + L_{\text{y}} + L_{\text{z}} = 1 \tag{9}$$

The value of L_{x} is given by an elliptic integral:

$$L_{\text{x}} = \frac{abc}{2}\int_0^\infty \frac{ds}{(s+a^2)\sqrt{(s+a^2)(s+b^2)(s+c^2)}} \tag{10}$$

Similar expressions apply for y and z by simply changing the $(s + a^2)$ outside the square root by $(s + b^2)$ or $(s + c^2)$.

Note that this is only a first order approximation and therefore it will predict zero force for any particle position such that the ellipsoid's centre corresponds to a field null.

III. MAXWELL STRESS TENSOR DERIVATION OF THE DEP FORCE

A different approach to the calculation of the DEP force is to use the Maxwell stress tensor formulation and integrate the stress tensor $\mathbf{T}$ over the surface of the particle:

$$\vec{F}(t)_{\text{DEP}}^{\text{MST}} = \oint \left(\mathbf{T} \cdot \vec{n}\right) dA \tag{11}$$

where $\vec{n}$ is the unit vector normal to the surface and t is time. This is regarded as the most rigurous approach to derive field-induced forces [15].

The general expression for the DEP force obtained by Wang et al [12] is used in order to find out how precise the multipolar approximation is when compared to this more rigurous calculation.

The time-averaged net DEP force on a particle using MST is given by:

$$\left\langle \vec{F}_{\text{DEP}}^{\text{MST}} \right\rangle = \frac{\varepsilon_{\text{f}}}{4} \oint \left\{ \left[\left(\vec{E}_{\text{f}} \vec{E}_{\text{f}}^{*} + \vec{E}_{\text{f}}^{*} \vec{E}_{\text{f}} \right) - |\vec{E}_{\text{f}}|^2 \mathbf{I} \right] \cdot \vec{n} \right\} dA \quad (12)$$

Note that in this case the presence of the particle is included directly in the calculations, and that no assumptions are made regarding the external field homogeneity. This means that even when strong field inhomogeneities are present, the values of the DEP force obtained using this method will be correct. It is expected that the results obtained using the multipolar approximation described in the previous section will worsen as the field gradient increases, and will depart from the values predicted by the MST method. It is of interest to find out how significant is the difference between the two methods for different particle sizes and positions inside a dielectrophoretic trap.

IV. NUMERICAL CALCULATION OF THE ELECTRIC FIELD

In order to calculate the electric field created by the electrode setup shown in figures 1 and 2, Laplace's equation, $\nabla^2 \phi = 0$, must be solved in a system with conductors - the electrodes- and piecewise homogeneous dielectrics -the fluid and the particle. The potential is given on the electrodes, and the conditions of continuity of the potential and the normal component of the electric displacement across different dielectrics provide the boundary conditions at dielectric interfaces.

In order to calculate the electric field the indirect formulation of the boundary element method (IBEM) with only sources is used [15], [16]. In this formulation the surfaces separating different dielectrics are replaced by equivalent polarization surface charge densities, and the surfaces between a dielectric and a conductor are replaced by a total surface charge corresponding to the sum of the free surface charge of the conductor and the polarization charge of the dielectric. Using the collocation method a system of linear equations is obtained. The surfaces are discretized with six-noded, higher order, isoparametric triangular elements. For a node on a conductor the equation to solve is:

$$\phi_i(\vec{r}) = \frac{1}{4\pi\varepsilon_0} \sum_j \int_{A_j} \sum_{k=1}^{k=6} \frac{q_{jk}(\vec{r}')N_{jk}(\vec{r}')}{|\vec{r} - \vec{r}'|} dA \quad (13)$$

For a node in a dielectric interface the equation to solve is:

$$q_i(\vec{r}) = \frac{\varepsilon_{\text{f}} - \varepsilon_{\text{p}}}{2\pi(\varepsilon_{\text{f}} + \varepsilon_{\text{p}})} \sum_j \int_{A_j} \sum_{k=1}^{k=6} q_{jk}(\vec{r}')N_{jk}(\vec{r}')\frac{(\vec{r} - \vec{r}') \cdot \vec{n}}{|\vec{r} - \vec{r}'|^3} dA \quad (14)$$

where N_{jk} and q_{jk} are the basis function and the total surface charge density of the kth node in the jth element

respectively. The system of equations is solved using the GMRES iterative solver [17] with a Jacobi preconditioner [18] to improve convergence.

Once the charge densities q_i have been obtained the electric field can be calculated exactly anywhere by applying $\vec{E} = -\nabla\phi$ to equation (13):

$$E_i(\vec{r}) = \frac{1}{4\pi\varepsilon_0} \sum_j \int_{A_j} \sum_{k=1}^{k=6} q_{jk}(\vec{r}')N_{jk}(\vec{r}')\frac{(\vec{r} - \vec{r}') \cdot \hat{i}}{|\vec{r} - \vec{r}'|^3} dA \quad (15)$$

where $\hat{i}$ is the unitary vector in the i direction. Higher order derivatives can also be calculated in an exact manner by applying directly the derivative to the above equation.

V. NUMERICAL RESULTS

The numerical code was validated by both comparison with simple analytical problems in 2D and 3D and direct comparison with available experimental values of the dielectrophoretic force on micron-sized polystyrene beads.

Once the code had been validated, several numerical tests were caried out with two spheres of radius 5 μm and 10 μm, as well as with an oblate ellipsoid of axes $a = b = 10$ μm and $c = 2.5$ μm.

In each case the calculation of the potential with an empty trap was performed first and then the solution was used as initial guess for the calculations that included the particle. This produced converged results to an accuracy of 10^{-6} in the GMRES solver in a very small number of iterations. Typically the solution is obtained after 14 to 18 iterations depending on the position of the particle within the trap.

It was observed that when the particle surface was close to the electrode surface a fine mesh was necessary in order to obtain converged results. This was expected due to the near-singular behavior of some of the integrals in that case, but it is something to consider when doing comparisons of the accuracy of different methods when the particle is close to the electrodes.

A. Influence of the relative particle/trap size

In this section the results for two spherical latex beads of radius 5 and 10 μm in the eight electrode trap shown in Fig. 1 are presented. The trap used has an interelectrode distance of 50 μm, as shown in Fig. 2, and therefore the particle to trap size ratios are 0.2 for the 5 μm sphere and 0.4 for the 10 μm sphere. It will be shown that for spherical particles with a particle to trap size ratio equal or less than 0.2 the quadrupolar term is the highest order multipole with a significant influence in the force, and that the octupolar term has only a significant importance in the determination of the force for particles with higher particle to trap size ratios. It will also be shown that using a high multipolar order the predicted force values are very close to the force values calculated using the MST method.
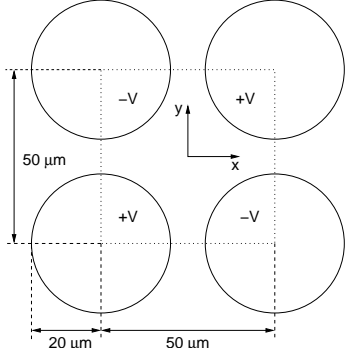
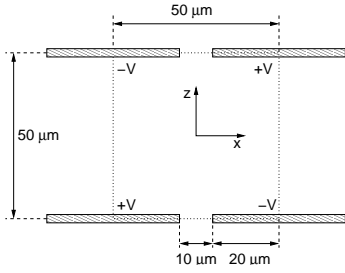Fig. 1. Top view of the geometry used for the dielectrophoretic trap.

Fig. 2. Frontal view of the geometry used for the dielectrophoretic trap.

Fig. 3. Force on a sphere of radius 5 μm moving away from the center of the trap.

Fig. 4. Surface density plot of $|\vec{E}|$ for a sphere of radius 5 μm in the plane $z = 17.5$ μm. Notice the significant disturbance of the field around the particle.

1) Sphere of radius 5 μm: In this case a series of calculations for positions along axes x, z, and $x = y$ have been made with the particle moving away from the centre of the trap. Also the force with respect to the distance from the electrodes has been investigated at a point in the middle of one of the quadrants of the trap, $x = y = 12.5$ μm.

The comparison between the results obtained using the multipolar model and the Maxwell stress tensor calculation are shown in Fig. 3.

It is clear that for the symmetry axes x and z, where the field intensity is zero, the dipolar model fails to predict the force on the particle —Fig. 3(A) and 3(B). Although the dipolar approximation fails completely in these cases, the higher order multipolar approximations show the correct trends and values in the evolution of the force with the distance from the centre of the trap. Note that the contribution from the octupolar term is of small importance.

When the comparison is made away from axes x and z, the agreement between the dipolar approximation and the MST calculation is much better. Still, as shown in Fig. 3(C) and 3(D), the dipolar approximation incurs significant error, but using a quadrupolar order of approximation improves the solution so much that it never differs from the MST solution by more than 5%. This is a remarkable accuracy for a very simple method of calculating the force.

Notice that in all cases the changes introduced by adding increasingly higher order multipolar terms is limited, and that including multipolar terms of order higher than the quadrupole produces no significant improvement in the solution. This can be ex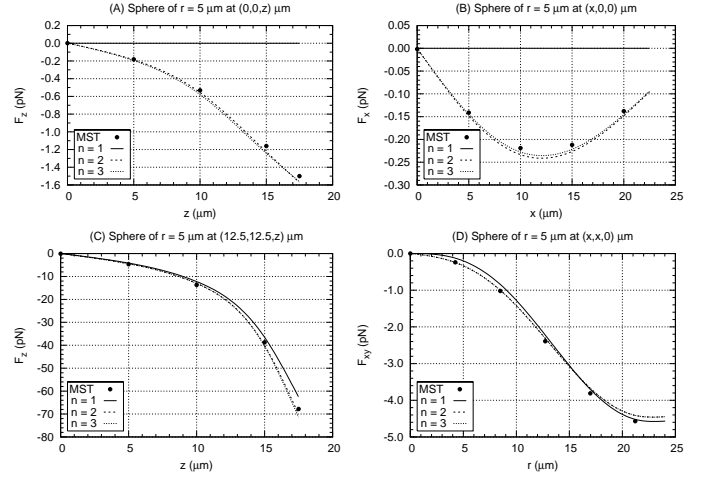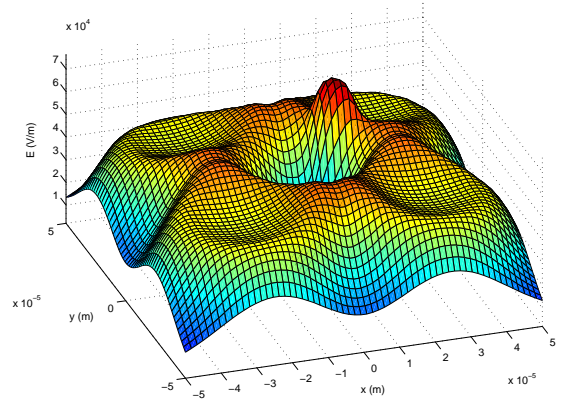plained by recalling that the different multipolar terms represent with increasingly accuracy the deformation of the electric field produced by the presence of the particle. Although the change in the field intensity in the region surrounding the particle is significant for positions close to the trap electrodes, as shown in Fig. 4, the simple geometry of the particle and its relatively small size make the inclusion of multipolar terms of order higher than 2 unnecessary.

2) Sphere of radius 10 μm: The same cases were investigated for a larger sphere, in order to compare results directly. Again, the comparison between the results obtained using the multipolar model and the Maxwell stress tensor calculation are shown in Fig. 5.

As expected the force predicted by the dipolar approximation when the particle is in positions along axes of symmetry in the trap is zero —Figs. 5(A) and 5(B). In the same manner as in the previous case, the dipolar approximation fails completely in these regions, but the higher order terms show
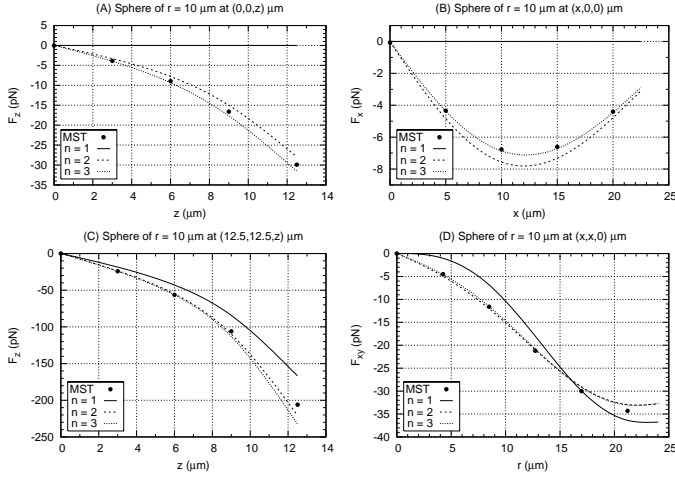
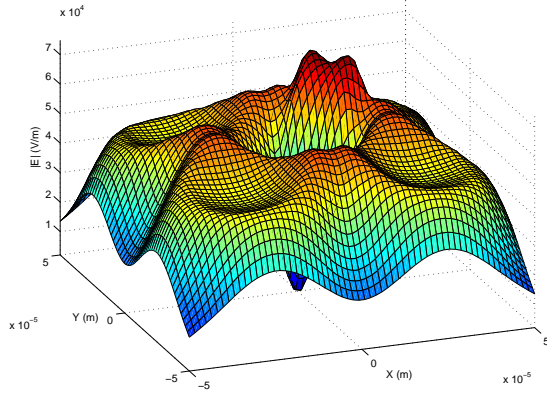Fig. 5. Force on a sphere of radius 10 μm moving away from the center of the trap.

Fig. 6. Surface density plot of $|\vec{E}|$ for a sphere of radius 10 μm in the plane $z = 10$ μm. The significant disturbance of the field around the particle has a more complicated shape than in the case of the smaller sphere.

Fig. 7. Oblate ellipsoid with $a = b$.

Fig. 8. Force on an ellipsoid with $a = b = 10\mu$m and $c = 2.5\mu$m moving away from the center of the trap.

the correct behavior of the force.

In this case the particle has a considerable size in comparison with the trap, and produces a higher deformation of the field in its surroundings. Compare figures 4 and 6 to see how the deformation of the field adopts a more complicated shape in this case. This creates the need for higher order multipolar terms to be included in the calculations. Notice how the octupolar term (n=3) produces significant changes in the force values both in figures 5(A) and 5(B).

When positions away from the regions of zero electric field are studied —Fig. 5(C) and 5(D), the agreement between the MST calculation and the dipolar prediction is better. The dipolar approximation shows the correct trends in the force in these positions but, as in the previous case, the values predicted depart significantly from the ones predicted by the MST approach. The inclusion of the quadrupolar and octupolar terms corrects most of the error, and produces very good
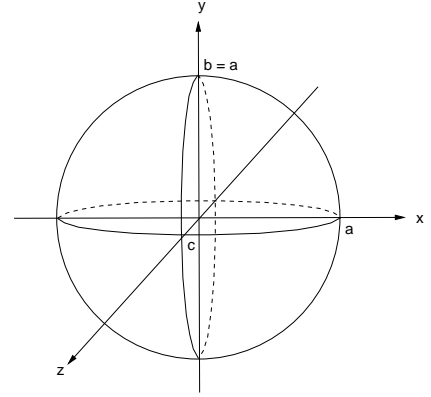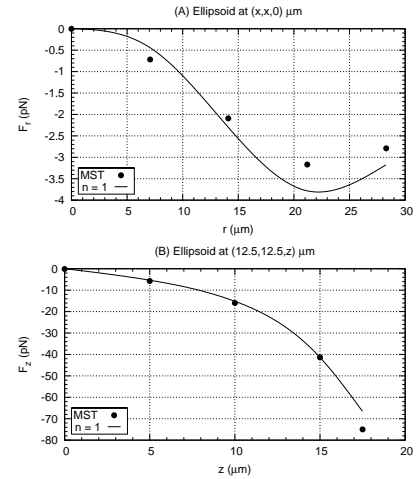
agreement with the full Maxwell stress tensor calculations at a fraction of the computational cost.

B. Influence of the particle shape: Oblate ellipsoid

While a spherical shape can be used to approximate some biological cells, ellipsoidal shapes are far more flexible and allow a much closer representation of cells with irregular shapes. For the present calculations an oblate ellipsoid is used, as shown in Fig. 7. Oblate shapes can be used to approximate lenticular particles and cells such as the biconcave human erythrocytes.

Unfortunately, only a dipolar approximation is available for ellipsoids in the literature [18]. This makes the calculation fail in axis of symmetry of the trap when using the dipolar approximation, since the prediction is of zero force. For positions outside the axis of symmetry the quality of the solution is mediocre on average, and it worsens with proximity to the electrodes, as shown in Fig. 8.

Only for positions very close to the electrodes the error is significant at the chosen position $x = y = 12.5$ μm in Fig. 8(B). However, the average quality of the dipolar approxima-

tion is not very good, as the results of the comparison along the $x = y$ axis show in Fig. 8(A). Errors of up to 40% happen in the positions close to the centre of the trap, and even far away from this symmetry point the error stays between 10% and 20% for most of the positions. Good agreement with the MST calculation of the force is only found in a very small region, where the dipolar solution goes from overestimating the force to underestimating it.

Since the axis $x = y$ is where the best possible results can be obtained when using the dipolar approach —the prediction worsens as the positions close in any symmetry axis of the trap—, a better model than the dipolar one is needed in the case of irregularly shaped particles in single-cell traps.

In view of these results a detailed calculation of the forces on non-spherical particles requires the use of the Maxwell stress tensor method for the calculation of the force.

VI. CONCLUSIONS

After careful comparison of the DEP forces in an eight electrode trap it is clear that very precise calculations of the forces can be done for spherical particles using the equivalent multipole method when higher order terms are included. The dipolar approximation should only be used for rough estimates of the force, and attention should be paid to the fact that it produces zero force predictions at points where the field is zero.

In the case of spherical particles, a multipolar approximation of order 2 or 3, depending on the particle to trap size ratio, produces results of very good quality to be of use in the optimization of the trap design. Since all the trends in the forces are correctly represented by this approximation, a fast design optimization can be done by changing trap parameters and studying the increase or decrease of the holding forces with each change. This will also be of some help to gauge the behavior of non-spherical particles in the trap, although the designer should be aware of the limitations in this later case.

The calculations show that the multipolar approximation currently being used in the literature provides a good approximation for the DEP force on spherical particles. The use of the dipolar approximation for ellipsoids should be done with care, however, since the lack of higher order expressions for this case severely limits its accuracy.

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