Numerical identification of effective multipole moments of polarizable particles

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***Abstract*—In electromechanics of particles, the effective moment method relies on the knowledge of the induced multipole moments. A general multipole theory is available in the literature, however, only linear multipole model is usually exploited when determining numerically these effective moments. Since this axial model do not apply to all electrostatic applied field, we examine a more general multipole model.**

I. Introduction

When a dielectric particle is subjected to an electrostatic field, interfacial polarization mechanisms cause a charge accumulation on the surface between the particle and the medium in which it is suspended. This polarization creates forces and torques that are exploited in dielectrophoretic phenomena used for the characterization and the manipulation of biological particles [1]. In the effective moment method the particle under consideration is substituted by a set of multipoles (dipole, quadrupole, octupole,...) producing the same field distortion caused by the presence of the particle. In the conventional dielectrophoresis theory, it is usually assumed that only a dipole is induced [2]. Although this approximation seems to be adequate in many circumstances, exceptions exist and higher-order multipole corrections are required to predict the particle behavior [3]. In particular, non-spherical particles can have significant higher-order components, and in some cases these higher-order terms strongly influence the observable motions in the dielectrophoresis and electrorotation phenomena.

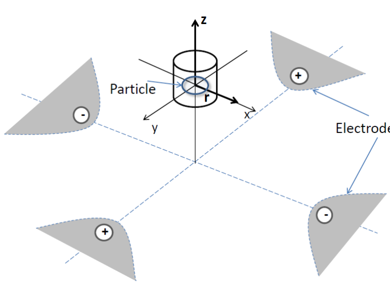

Fig. 1. Example of a 3D system of electrodes and a particle.

Green and Jones proposed to consider linear multipoles to determine the dipole moment and higher-order moments [4] (see also subsection II.B). This axial multipole model cannot be used if the external field is not aligned with the revolution symmetry axis. It is unfortunately the most frequent situation in biological dielectrophoretic applications. For instance, in cylindrically symmetric systems, the radial component of the field is usually higher than the z-component (Fig. 1). Here, we study a more general multipole model to identify the equivalent model of the polarized particle.

In the following, the multipole expansion is first introduced and numerical results are proposed to show the relevance of the proposed approach.

II. Model and method

A. Induced potential

The particle and the surrounding medium are considered to be linear media. The electrostatic potential is obtained by solving Poisson's equation without free charge in the system.

The total potential U_{total} outside the particle is the sum of both applied potential U_{ext} and induced potential U_{ind} caused by the polarization of the particle, *i.e.*

$$\begin{aligned} U_{\text{total}} &= U_{\text{ext}} + U_{\text{ind}} \\ &= \sum_{n,m} A_{n,m} r^n \mathcal{Y}_n^m(\theta,\varphi) + \sum_{n,m} \frac{B_{n,m}}{r^{n+1}} \mathcal{Y}_n^m(\theta,\varphi), \end{aligned} \tag{1}$$

where $\mathcal{Y}_n^m$ are the complex spherical harmonics, with θ and φ the angles of the spherical coordinate system. The magnitudes $A_{n,m}$ and $B_{n,m}$ can be determined numerically or analytically using proper boundary conditions.

The multipole polarization coefficients p_n^m are related to $B_{n,m}$ by [5]

$$p_n^m = \sqrt{\frac{2n+1}{4\pi}} \mathcal{N}_n^m B_{n,m}, \text{ with } \mathcal{N}_n^m = \sqrt{\frac{2n+1}{4\pi} \frac{(n-m)!}{(n+m)!}}. \tag{2}$$

For a spherical particle with radius a and permittivity ε_p suspended in a medium with permittivity ε_m, the $B_{n,m}$ can be expressed in terms of the $A_{m,n}$ [1]:

$$B_{n,m} = \frac{K_n}{(2n+1)} a^{2n+1} A_{n,m}, \tag{3}$$

where

$$K_n = \frac{n(2n+1)(\varepsilon_m - \varepsilon_p)}{(n+1)\varepsilon_p + n\varepsilon_m}, \tag{4}$$

is the generalized Clausius-Mossotti factor.

B. Calculation of the effective multipole moments

Using the orthogonality property of the spherical harmonics the individual moments are determined according to:

$$p_n^m = \sqrt{\frac{2n+1}{4\pi}} \mathcal{N}_n^m R^{n+1} \int_S \mathcal{Y}_n^m(\theta, \varphi)\, U_{\text{ind}}(R, \theta, \varphi) ds, \quad (5)$$

where S is a spherical surface centered on the particle with a radius R larger than the largest dimension of the particle. The linear multipoles correspond to the case $m = 0$ in the expression (5).

C. Solution of the problem

The particle of interest in our problem is cylindrically symmetric, immersed in a containing medium with permittivity ε_m. The particle is assumed to be sufficiently small to consider the external electric field constant in its closed region. Consequently, the 3D problem is transformed into two axisymmetric problems, as shown in fig.2. The electric potential in the whole space is obtained using both solutions:

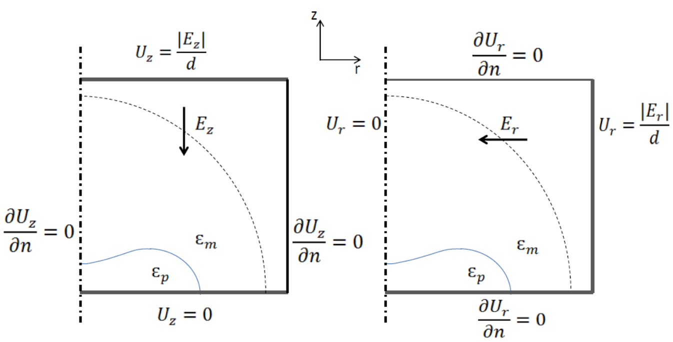

Fig. 2. Boundary conditions for the radial and z-axis potential calculations.

$$U(r, z, \theta) = U_z + U_r \cos(\varphi). \quad (6)$$

Two linear problems for U_z and U_r are then required to be solved:

$$\int_\Omega r \left(\frac{\partial U_r}{\partial r} \frac{\partial v}{\partial r} + \frac{\partial U_r}{\partial z} \frac{\partial v}{\partial z} \right) drdz + \int_\Omega \frac{U_r}{r} v drdz = 0, \quad (7)$$

and

$$\int_\Omega r \left(\frac{\partial U_z}{\partial r} \frac{\partial v}{\partial r} + \frac{\partial U_z}{\partial z} \frac{\partial v}{\partial z} \right) drdz = 0. \quad (8)$$

III. Numerical results

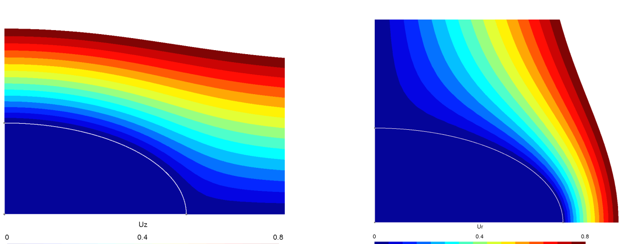

Fig. 3. Details of the solutions U_z (left) and U_r (right). The white line is the boundary of the particle. $\varepsilon_p/\varepsilon_m = 10^4$.

The numerical solution of problems (7) and (8) is performed by using the finite element method and the implementation is based on the `getfem++` finite element library [6] (see Fig. 3). Fig. 4 and Fig. 5 show the example of the numerical results for a spheroidal shaped (prolate) particle with an eccentricity (ratio) of 2:1.

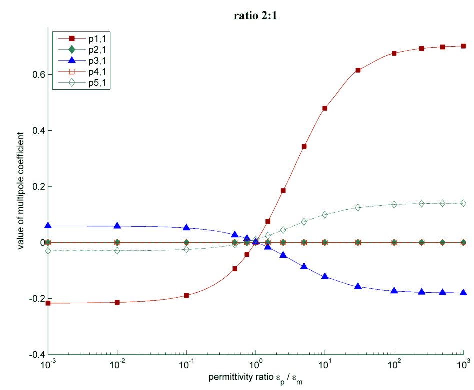

Fig. 4. Polarization coefficients following the radial axis.

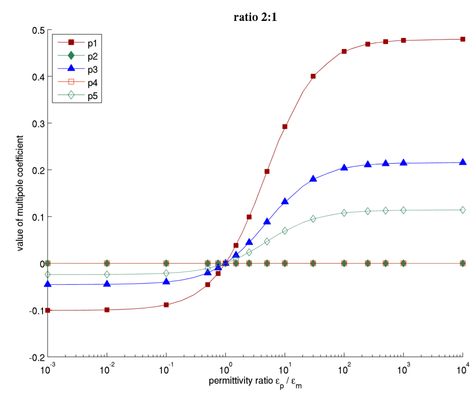

Fig. 5. Polarization coefficients following the z-axis.

This numerical results obtained for the coefficients of polarization, following the z-direction and following the radial direction, show a dominant dipole component with slightly higher values for the radial direction. Accordingly, the effect of this radial polarization has to be taken into consideration in the effective multipole expansion for a more accurate description of the particle behavior.

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