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Multipole analysis of a generic system of dielectric cylinders and application to fibrous materials

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Abstract

A multipole theory describing the interactions between dielectric cylinders in a uniform field is developed. We treat the most general case of N parallel cylinders placed in arbitrary positions. The exact theory is obtained by developing the polarisation charge surface density on each cylinder in a Fourier series. The related coefficients, the so-called multipoles, may be obtained from a linear set of equations which is derived and analysed in the paper. For systems of closely spaced cylinders, with high ratio of the dielectric constant of the cylinders compared to that of the homogeneous medium (in the worst case, conductive cylinders in contact with each other) a very large number of multipole terms is required to achieve convergence. In spite of the large number of required terms, the general multipole expansion is rapidly convergent in all other cases and is important from a theoretical point of view. Numerical results are presented for canonical dispositions of cylinders and for more complicated arrangements. Finally, such a multipole expansion has been applied to the dielectric characterisation of composite materials formed by a regular array of parallel cylinders, thereby obtaining the equivalent permittivity using a numerically efficient technique.

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1. Introduction

In this paper, we present a general theory, which describes any geometric disposition of parallel dielectric cylinders embedded in an orthogonal electric field. As it is well known, these results equally apply to magnetisable cylinders in a uniform magnetic field, to conductive cylinders in a uniform current density field or to thermal conductive cylinders in a uniform heat flux. Anyway, throughout all the paper, we will always refer to the dielectric case. In such theoretical derivation the cylinders have, on a given reference plane, the centres in completely arbitrary position (except for the overlapping case which is not taken into consideration). This means that the theory may be used for many purposes ranging from theoretical physics to advanced technology and biology: the disposition may be completely random or strictly regular generating a reticular (crystalline) structure; moreover, the method may be used for few cylinders or for a very large number of cylindrical interacting particles. This topic is of vital importance in a number of theories, e.g., the electrical or magnetic characterisation of mixtures obtained by random or regular immersion of cylindrical particles in some homogeneous media (artificial or biological fibrous materials) [1,2], the study of the interparticle forces in electric and magnetic fields [3,4], the dielectrics breakdown in artificial or metal-loaded dielectrics [5] and some other physical situations. A similar treatment, concerning multipole interactions of spheres, can be found in earlier literature [6,7].

With N aligned cylinders having fixed positions in an orthogonal field, the system of linear equations for the interacting multipole moments of each cylinder is derived. The knowledge of all the multipole moments for a cylinder is equivalent to that of the polarisation charge density on its surface.

The set of equations can be solved either by methods based on successive approximation (iterative relaxation techniques) or by standard inversion methods (Gaussian elimination), obtaining in both cases good results because the system is well conditioned. Moreover, the formulas for the electric potential (or field) are obtained as multipole moments expansions. Some interesting dispositions of the cylindrical particles are theoretically and numerically analysed. The resulting equipotential lines are shown in different cases. Finally, the dielectric characterisation of periodic embeddings of cylinders has been considered approaching the problem with the multipole expansion technique. A method to obtain the equivalent dielectric constant of such an array of cylinders is described and applied with a volume fraction ranging from zero to the case of cylinders in contact. The solution exhibits fast convergence for values of the relative permittivity between cylinders and hosting medium up to some hundreds.

2. Statement of the problem: multipole expansions

We consider N parallel cylinders embedded in a homogeneous media (permittivity ε_1) where a uniform field E_0 is present. The cylinders are considered perpendicular to the x - y plane. The external applied field is aligned to the x -axis of the reference

system (main frame). We deal with a two-dimensional problem analysed in the main reference frame x – y .

Each cylinder has permittivity ϵ_2 , radius R and centre in position \bar{R}_i ($i = 1, \dots, N$) in this main frame (plane x – y). Besides the above-stated main frame we introduce N other reference systems with origin in \bar{R}_i (centre of the i th base of the cylinder) and axes parallel to those of the main frame. In such systems we will use orthogonal coordinates (x_i, y_i) and polar coordinates (r_i, φ_i) (see Fig. 1).

In this section, we want to derive a mathematical model, which represents the multipole description of the system of cylinders. The resulting total electric field is generated by the free charges (ideally placed at infinity) corresponding to the uniform field E_0 and by the polarisation charges induced on the cylindrical surfaces. We introduce the corresponding total electric potential V that takes into account both the applied field E_0 and the perturbation generated by the induced polarisation charge on each cylinder.

A straightforward application of the Gauss law gives the following relations for the polarisation charge density on the i th surface:

$$\sigma_i = \epsilon_0 \left(1 - \frac{\epsilon_2}{\epsilon_1} \right) \frac{dV}{dn} \Big|_{R^-,i} = \epsilon_0 \left(\frac{\epsilon_1}{\epsilon_2} - 1 \right) \frac{dV}{dn} \Big|_{R^+,i} \tag{1}$$

where $dV/dn|_{R^-,i}$ and $dV/dn|_{R^+,i}$ are the normal derivatives of the total electric potential V calculated inside and outside the i th cylindrical surface, respectively. We observe that the charge density σ_i depends only on the variable φ_i on the i th reference frame: therefore $\sigma_i(\varphi_i)$ is a periodic function of its argument, which may be developed in Fourier series. Thus, we introduce the multipole moments, used in this work, as the Fourier coefficients of such polarisation charge density:

$$A_n^i = \frac{1}{2\pi} \int_0^{2\pi} \sigma_i(\varphi_i) \exp(-jn\varphi_i) d\varphi_i, \tag{2}$$

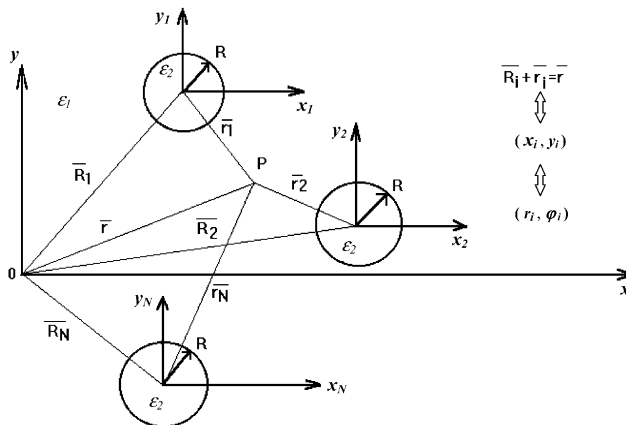


Fig. 1. A two-dimensional representation of an arbitrary system of cylinders: the adopted notations and the reference frames.

where j is the imaginary unit throughout all the paper. Of course, since the total induced polarisation charge on each cylinder is zero, we have $A_0^i = 0$ for any index i . So, the coefficients A_n^i are useful to represent the functions $\sigma_i(\varphi_i)$ in trigonometric series:

$$\sigma_i(\varphi_i) = \sum_{n=-\infty}^{+\infty} A_n^i \exp(jn\varphi_i). \quad (3)$$

The total electric potential may be written as follows:

$$V(\bar{r}) = \begin{cases} -E_0 x + V_1(\bar{r}) & \text{if } \|\bar{r} - \bar{R}_i\| > R \ \forall i \text{ (outside the cylinders),} \\ -E_0 x + V_2^i(\bar{r}) & \text{if } \|\bar{r} - \bar{R}_i\| < R \text{ (inside the } i\text{th cylinder),} \end{cases} \quad (4)$$

where the potentials $V_1(\bar{r})$ and $V_2^i(\bar{r})$ are the perturbations generated only by the polarisation charges; here $\bar{r} = (x, y)$ is the position vector of a point P in the main frame (see Fig. 1). Now, we search for the functions $V_1(\bar{r})$ and $V_2^i(\bar{r})$ in terms of multipole moments. To do this, we remember that these perturbations to the overall potential must satisfy the two-dimensional Laplace equation, which may be simply solved, in polar coordinates, as follows. We define $\psi_i^{\text{in}}(\bar{r})$ and $\psi_i^{\text{out}}(\bar{r})$ as the electric potential inside and outside the i th cylinder respectively, generated solely by its polarisation; therefore $\psi_i^{\text{in}}(\bar{r})$ and $\psi_i^{\text{out}}(\bar{r})$ depend only on the charge distribution $\sigma_i(\varphi_i)$ on the i th cylinder. It is well known that the general solution of the Laplace equation inside and outside a given circle may be written as follows [8]:

$$\begin{aligned} \psi_i^{\text{in}}(r_i, \varphi_i) &= \sum_{n=-\infty}^{+\infty} r_i^{|n|} k_n^i \exp(jn\varphi_i), \\ \psi_i^{\text{out}}(r_i, \varphi_i) &= \sum_{n=-\infty}^{+\infty} r_i^{-|n|} h_n^i \exp(jn\varphi_i), \end{aligned} \quad (5)$$

where the complex coefficients k_n^i and h_n^i may be written in terms of the multipole A_n^i by introducing the boundary conditions on the lateral surface S_i of the i th cylinders:

$$\begin{aligned} -\varepsilon_0 \frac{d\psi_i^{\text{out}}}{dn} \Big|_R + \varepsilon_0 \frac{d\psi_i^{\text{in}}}{dn} \Big|_R &= \sigma_i(\varphi_i) \quad \text{on } S_i, \\ \psi_i^{\text{out}}|_R &= \psi_i^{\text{in}}|_R \end{aligned} \quad (6)$$

Substituting Eqs. (3) and (5) into Eq. (6), by means of straightforward calculations we may find k_n^i and h_n^i in terms of the multipole A_n^i and these expressions have been used in Eq. (5) obtaining

$$\begin{aligned} \psi_i^{\text{in}}(r_i, \varphi_i) &= \sum_{n=-\infty}^{+\infty} R \left(\frac{r_i}{R}\right)^{|n|} \frac{A_n^i}{2\varepsilon_0|n|} \exp(jn\varphi_i), \\ \psi_i^{\text{out}}(r_i, \varphi_i) &= \sum_{n=-\infty}^{+\infty} R \left(\frac{r_i}{R}\right)^{-|n|} \frac{A_n^i}{2\varepsilon_0|n|} \exp(jn\varphi_i). \end{aligned} \quad (7)$$

Finally, the complete expressions for the electric potential in the overall structure of aligned cylinders may be written by using Eq. (4), as follows:

$$V(\vec{r}) = \begin{cases} -E_0x + V_1 = -E_0x + \sum_{k=1}^N \psi_k^{\text{out}} \\ \qquad = -E_0x + \sum_{k=1}^N \sum_{n=-\infty}^{+\infty} R\left(\frac{r_k}{R}\right)^{-|n|} \frac{A_n^k}{2\epsilon_0|n|} \exp(jn\varphi_k) \\ \qquad \text{if } \|\vec{r} - \vec{R}_i\| > R \forall i \text{ (outside the cylinders)} \\ -E_0x + V_2^i = -E_0x + \psi_i^{\text{in}} + \sum_{\substack{k=1 \\ k \neq i}}^N \psi_k^{\text{out}} \\ \qquad = -E_0x + \sum_{n=-\infty}^{+\infty} R\left(\frac{r_i}{R}\right)^{|n|} \frac{A_n^i}{2\epsilon_0|n|} \exp(jn\varphi_i) \\ \qquad + \sum_{\substack{k=1 \\ k \neq i}}^N \sum_{n=-\infty}^{+\infty} R\left(\frac{r_k}{R}\right)^{-|n|} \frac{A_n^k}{2\epsilon_0|n|} \exp(jn\varphi_k) \\ \qquad \text{if } \|\vec{r} - \vec{R}_i\| < R \text{ (inside the } i\text{th cylinder),} \end{cases} \quad (8)$$

where $\vec{r} = (x, y)$ and by using simple changes of coordinates, we have defined $r_k = \|\vec{r} - \vec{R}_k\|$ and $\varphi_k = \varphi(\vec{r} - \vec{R}_k)$ ($k = 1, \dots, N$), having introduced the single valued function $\varphi(\vec{v})$ which gives the angle corresponding to the plane vector \vec{v} (i.e. the angle that \vec{v} makes with the x -axis). We remember that each cylinder has centre in position \vec{R}_i ($i = 1, \dots, N$). Therefore, we have written the electric potential in the whole system in terms of the above-defined multipole moments. In the next section we show a method to evaluate the multipole coefficients when the geometrical structure of the system is given. Actually, this system will describe the effective interactions among the cylinders.

3. Set of equations for the multipole moments

Still now, we have stated that the coefficients A_n^i contain all the information about the induced polarisation charge and the total electric potential in the system of cylinders. The aim of this section is to build a set of equations for these multipole moments.

To this purpose, we consider the definition given by Eq. (2) and we write the charge density in terms of the potential, see Eq. (1); for convenience, we perform this operation choosing the external potential. Hence, we obtain the following relation:

$$A_n^i = \frac{1}{2\pi} \int_0^{2\pi} \exp(-jn\varphi_i) \epsilon_0 \left(\frac{\epsilon_1}{\epsilon_2} - 1 \right) \frac{dV}{dn} \Big|_{R^+, i} d\varphi_i. \quad (9)$$

Now, we need to calculate the normal derivative, which appears in the integral. To do this, we express the total external potential in the i th system coordinates (as a

function of r_i and φ_i), obtaining (see Eq. (8), first expression)

$$\begin{aligned}
 V &= -E_0x + \sum_{k=1}^N \sum_{n=-\infty}^{+\infty} R\left(\frac{r_k}{R}\right)^{-|n|} \frac{A_n^k}{2\epsilon_0|n|} \exp(jn\varphi_k) \\
 &= -E_0(X_i + r_i \cos \varphi_i) + \sum_{n=-\infty}^{+\infty} R\left(\frac{r_i}{R}\right)^{-|n|} \frac{A_n^i}{2\epsilon_0|n|} \exp(jn\varphi_i) \\
 &\quad + \sum_{\substack{k=1 \\ k \neq i}}^N \sum_{n=-\infty}^{+\infty} R\left(\frac{\|\bar{r}_i + \bar{R}_i - \bar{R}_k\|}{R}\right)^{-|n|} \frac{A_n^k}{2\epsilon_0|n|} \exp[jn\varphi(\bar{r}_i + \bar{R}_i - \bar{R}_k)] \quad (10)
 \end{aligned}$$

(here $\bar{R}_p = (X_p, Y_p)$ is the centre of the p th cylinder). The first term takes into account the applied field, the second one the perturbation generated by the i th induced charge and the third the potential generated by the other cylinders expressed in terms of the position vector \bar{r}_i in the i th reference frame. The first two terms are expressed as functions of r_i and φ_i as requested, the third term is not in this condition and it will be developed by means of an expansion theorem described in the appendix. If two vectors $\bar{A} = (r_a \cos \varphi_a, r_a \sin \varphi_a)$ and $\bar{B} = (r_b \cos \varphi_b, r_b \sin \varphi_b)$ are given on the plane and the condition $\|\bar{A}\| < \|\bar{B}\|$ is fulfilled, the following off-centered expansion holds true for any integer n , positive or negative:

$$\frac{e^{jn\varphi(\bar{A}-\bar{B})}}{\|\bar{A}-\bar{B}\|^{|n|}} = \sum_{h=0}^{+\infty} \frac{(-1)^n r_a^h}{r_b^{|n|+h}} \binom{|n|+h-1}{h} e^{j[n+h \operatorname{sgn}(n)]\varphi_b} e^{-jh \operatorname{sgn}(n)\varphi_a}. \quad (11)$$

The theorem may be used in the third term of Eq. (10) making the substitutions $\bar{A} = \bar{r}_i$ and $\bar{B} = \bar{R}_k - \bar{R}_i$. The condition $\|\bar{A}\| < \|\bar{B}\|$ is fulfilled when we compute the normal derivative on the i th cylinder.

So, the external potential is written in i th cylindrical coordinates, as follows:

$$\begin{aligned}
 V(r_i, \varphi_i) &= -E_0(X_i + r_i \cos \varphi_i) + \sum_{n=-\infty}^{+\infty} R\left(\frac{r_i}{R}\right)^{-|n|} \frac{A_n^i}{2\epsilon_0|n|} \exp(jn\varphi_i) \\
 &\quad + \sum_{\substack{k=1 \\ k \neq i}}^N \sum_{n=-\infty}^{+\infty} \sum_{h=0}^{+\infty} R^{|n|+1} \frac{A_n^k}{2\epsilon_0|n|} \binom{|n|+h-1}{h} \frac{(-1)^n r_i^h}{\|\bar{R}_k - \bar{R}_i\|^{|n|+h}} \\
 &\quad \times \exp[j(n+h \operatorname{sgn}(n))\varphi(\bar{R}_k - \bar{R}_i)] \exp[-jh \operatorname{sgn}(n)\varphi_i]. \quad (12)
 \end{aligned}$$

Now, we can perform the derivative with respect to r_i , calculated for $r_i = R$. The result is

$$\begin{aligned}
 \left. \frac{dV}{dn} \right|_{R^+, i} &= \left. \frac{\partial V(r_i, \varphi_i)}{\partial r_i} \right|_{r_i=R} \\
 &= -E_0 \cos \varphi_i - \sum_{n=-\infty}^{+\infty} \frac{A_n^i}{2\epsilon_0} \exp(jn\varphi_i) \\
 &\quad + \sum_{\substack{k=1 \\ k \neq i}}^N \sum_{n=-\infty}^{+\infty} \sum_{h=0}^{+\infty} \frac{(-1)^n h A_n^k}{2\epsilon_0|n|} \binom{|n|+h-1}{h} \left(\frac{R}{\|\bar{R}_k - \bar{R}_i\|}\right)^{|n|+h} \\
 &\quad \times \exp[j(n+h \operatorname{sgn}(n))\varphi(\bar{R}_k - \bar{R}_i)] \exp[-jh \operatorname{sgn}(n)\varphi_i]. \quad (13)
 \end{aligned}$$

Finally, substituting (13) in (9), and by using the orthonormality of the imaginary exponential functions, we obtain a first form of the linear system of equations for the multipole moments:

$$\begin{aligned}
 A_n^i = \varepsilon_0 \left(\frac{\varepsilon_1}{\varepsilon_2} - 1 \right) & \left\{ -\frac{E_0}{2} (\delta_{1,n} + \delta_{-1,n}) - \frac{A_n^i}{2\varepsilon_0} \right. \\
 & + \sum_{\substack{k=1 \\ k \neq i}}^N \sum_{q=-\infty}^{+\infty} \sum_{h=0}^{+\infty} \frac{(-1)^q h A_q^k}{2\varepsilon_0 |q|} \binom{|q| + h - 1}{h} \left(\frac{R}{\|\bar{R}_k - \bar{R}_i\|} \right)^{|q|+h} \\
 & \left. \times \exp[j(q + h \operatorname{sgn}(q))\varphi(\bar{R}_k - \bar{R}_i)] \delta_{-h \operatorname{sgn}(q),n} \right\}. \tag{14}
 \end{aligned}$$

Now, it is important to note that, $\sigma_i(\varphi_i)$ being a real valued function, the relation $A_{-n}^i = A_n^{i*}$ (where the symbol * means complex conjugate) holds true; moreover, as said above, since the total induced charge on each cylinder is zero, we have $A_0^i = 0$. Thus, we may build a system for the unknowns A_n^i for $n \geq 1$ and for $1 \leq i \leq N$. Therefore, we simplify Eq. (14) by taking into account the hypothesis $n \geq 1$. With some straightforward calculation we obtain the system in the following final form ($n \geq 1$ and $1 \leq i \leq N$):

$$\begin{aligned}
 A_n^i = -E_0 \varepsilon_0 \frac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 + \varepsilon_2} \delta_{1,n} \\
 + \frac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 + \varepsilon_2} \sum_{\substack{k=1 \\ k \neq i}}^N \sum_{q=1}^{+\infty} (-1)^q A_q^{k*} \binom{q + n - 1}{q} \left(\frac{R}{\bar{R}_k - \bar{R}_i} \right)^{q+n}. \tag{15}
 \end{aligned}$$

having used the simple property

$$\frac{n}{q} \binom{q + n - 1}{n} = \binom{q + n - 1}{q}.$$

Here, recalling the definition $\bar{R}_k = (X_k, Y_k)$ for the centres of the cylinders, we have defined for convenience the corresponding complex numbers $\hat{R}_k = X_k + j Y_k$. Eq. (15) is the most important result achieved in this work and it allows us to calculate the multipoles, which completely define the electric potential and field over the whole structure. These coefficients depend only on the geometrical disposition of the system (centres $\hat{R}_j = X_j + j Y_j$ and radius R) and on the permittivities of the media involved. So, formula (15) solves the general problem of the N dielectric cylinders embedded in a perpendicular field. Some properties of system (15) are the following:

- if the field E_0 is zero all the multipoles are zero because no polarisation charge is induced.
- if $\|\bar{R}_i - \bar{R}_k\| \rightarrow \infty$ for any i and k the cylinders are so far away from each other that they do not interact and the interaction term (second line in Eq. (15)) vanishes: it follows that $A_1^i = -E_0 \varepsilon_0 (\varepsilon_1 - \varepsilon_2) / (\varepsilon_1 + \varepsilon_2)$ for any i and all other multipoles are zero.
- the multipole coupling terms fall off in magnitude with powers of the interparticle separation distance, and, in particular, the coupling of higher-order multipoles to each other falls off with large powers of this distance. So, the use of this coupled

multipole expansion results in a matrix that is highly diagonal dominated, which means that iterative methods converge very rapidly. Also, since the matrix may be considered sparse, very large system of particles can be analysed with this method.

Independently of the numerical technique used to solve the set of equations, the most critical cases appear when the cylinders are in contact ($\|\bar{R}_i - \bar{R}_j\| = 2R$ for some i and j) and when, at the same time, the ratio $\varepsilon_2/\varepsilon_1$ assumes the extreme values zero or infinity. Correspondingly, the characteristic fraction $(\varepsilon_1 - \varepsilon_2)/(\varepsilon_1 + \varepsilon_2)$ takes the limit values 1 and -1 , respectively. Some examples of representation of the equipotential lines for such extreme cases can be found in Figs. 2 and 3 where we have used Eq. (8) to represent the whole electric potential. In Fig. 2 the case of two cylinders aligned with the external electrical field is considered for $\varepsilon_2/\varepsilon_1 \rightarrow \infty$ (Fig. 2a) and $\varepsilon_2/\varepsilon_1 \rightarrow 0$ (Fig. 2b). In Fig. 3 the case of two cylinders perpendicularly aligned with the external electrical field is taken into consideration for $\varepsilon_2/\varepsilon_1 \rightarrow \infty$ (Fig. 3a) and $\varepsilon_2/\varepsilon_1 \rightarrow 0$ (Fig. 3b). In all these cases the value $E_0 = 1$ is taken for the uniform field and 100 multipoles for the cylinders have been used in the main system given by Eq. (15).

Some comments about the distribution of the equipotential lines in these plots follow. In all plots many closely spaced equipotential lines appear in the medium around the cylindrical particles. These lines correspond to the bulk value of the applied and fixed electrical field ($E_0 = 1$, perpendicular to the lines).

When the particles are embedded in the matrix, they modify the equipotential lines both inside and outside the particles. To better understand the behaviour inside the particles we may think to a single cylinder in the matrix: the field E_d inside the cylinder is uniform and given by $E_d = 2E_0/(1 + \varepsilon_2/\varepsilon_1)$. So, if $\varepsilon_2/\varepsilon_1 \rightarrow \infty$ we have $E_d = 0$ and if $\varepsilon_2/\varepsilon_1 \rightarrow 0$ we have $E_d = 2E_0$. This behaviour is qualitatively in agreement with Figs. 2 and 3. In fact, in Figs. 2a and 3a we have $\varepsilon_2/\varepsilon_1 \rightarrow \infty$ and no equipotential lines appear inside the cylinders (the field inside the particles is zero); in Figs. 2b and 3b we have $\varepsilon_2/\varepsilon_1 \rightarrow 0$ and we may observe an internal field greater than the external one, as expected. Moreover, in this case with $\varepsilon_2/\varepsilon_1 \rightarrow 0$, an additional conclusion may be drawn: with a single cylinder we have the uniform internal field $E_d = 2E_0$, with two cylinders aligned with the field the internal electrical field is not uniform in each particle and it has modulus E_d such that $E_0 < E_d < 2E_0$, with two cylinders perpendicularly aligned with the field the internal one is not uniform and we have $E_d > 2E_0$. So, we conclude that the perpendicular configuration generates the greater amplification of the field inside the particles (if $\varepsilon_2/\varepsilon_1 \rightarrow 0$).

4. Induced multipole strengths on a linear chain of parallel cylinders

In this section, we perform the analysis of a simple arrangement of cylinders: we consider a series of parallel cylinders aligned along a straight line that form a given angle ϑ with the applied electric field. This means that the centres of the cylinders may be described by the succession of complex numbers given by: $\hat{R}_k = kd e^{i\vartheta}$ where $k = -\infty \rightarrow +\infty$ and d is the distance between the centres of two adjacent cylinders.

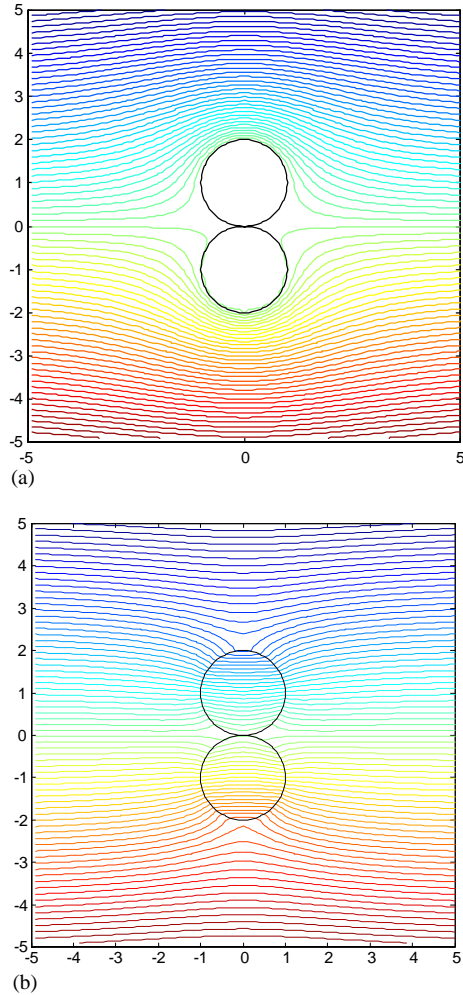


Fig. 2. Equipotential lines for a couple of touching cylinders aligned with the applied electrical field for $\epsilon_2/\epsilon_1 \rightarrow \infty$ (a) and $\epsilon_2/\epsilon_1 \rightarrow 0$ (b).

As before, the applied electric field is directed along the x -axis of the main frame. In these conditions all the cylinders are influenced in the same way by the external field and thus: $A_n^i = A_n$ for each cylinder. This means that the charge distribution is the same on all the cylinders. So, Eq. (15) may be used as follows:

$$\begin{aligned}
 A_n = & -E_0 \epsilon_0 \frac{\epsilon_1 - \epsilon_2}{\epsilon_1 + \epsilon_2} \delta_{1,n} \\
 & + \frac{\epsilon_1 - \epsilon_2}{\epsilon_1 + \epsilon_2} \sum_{k=-\infty}^{+\infty} \sum_{q=1}^{+\infty} (-1)^q A_q^* \binom{q+n-1}{q} \left(\frac{R}{kde^{j\vartheta} - ide^{j\vartheta}} \right)^{q+n}
 \end{aligned} \tag{16}$$

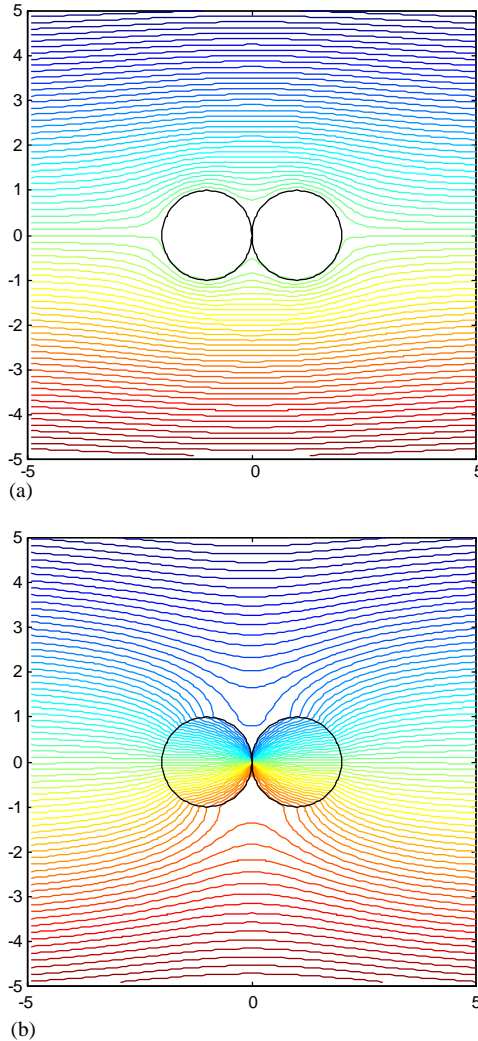


Fig. 3. Equipotential lines for a couple of touching cylinders perpendicularly aligned with the applied electrical field for $\epsilon_2/\epsilon_1 \rightarrow \infty$ (a) and $\epsilon_2/\epsilon_1 \rightarrow 0$ (b).

where the summation on k may be rearranged in the following way:

$$\begin{aligned} \sum_{\substack{k=-\infty \\ k \neq i}}^{+\infty} \left(\frac{R}{kde^{j\theta} - ide^{j\theta}} \right)^{q+n} &= \left(\frac{R}{de^{j\theta}} \right)^{q+n} \sum_{\substack{k=-\infty \\ k \neq i}}^{+\infty} \left(\frac{1}{k-i} \right)^{q+n} \\ &= \left(\frac{R}{de^{j\theta}} \right)^{q+n} \left[\sum_{p=-\infty}^{-1} \left(\frac{1}{p} \right)^{q+n} + \sum_{p=1}^{+\infty} \left(\frac{1}{p} \right)^{q+n} \right] \end{aligned}$$

$$\begin{aligned}
 &= \left(\frac{R}{d e^{j\vartheta}}\right)^{q+n} \sum_{p=1}^{+\infty} \left[\frac{(-1)^{q+n} + 1}{p^{q+n}}\right] \\
 &= \left(\frac{R}{d e^{j\vartheta}}\right)^{q+n} [(-1)^{q+n} + 1] \zeta(q+n)
 \end{aligned} \tag{17}$$

having introduced the Riemann Zeta function $\zeta(z)$ [9]. Therefore, Eq. (16) may be written in the simplified form:

$$\begin{aligned}
 A_n = & -E_0 \varepsilon_0 \frac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 + \varepsilon_2} \delta_{1,n} \\
 & + \frac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 + \varepsilon_2} \sum_{q=1}^{+\infty} \left(\frac{R}{d e^{j\vartheta}}\right)^{q+n} [(-1)^q + (-1)^n] \zeta(q+n) A_q^* \binom{q+n-1}{q}.
 \end{aligned} \tag{18}$$

Now, it is interesting to note that, because of the term $(-1)^q + (-1)^n$, which appears in the system, all the multipoles with $n = 2k$ are zero and therefore only the odd multipoles remain to describe the system. Defining $X_n = A_{2n-1}$ for any $n \geq 1$, we obtain:

$$\begin{aligned}
 X_n = & -E_0 \varepsilon_0 \frac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 + \varepsilon_2} \delta_{1,n} \\
 & - 2 \frac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 + \varepsilon_2} \sum_{q=1}^{+\infty} \left(\frac{R}{d e^{j\vartheta}}\right)^{2q+2n-2} \zeta(2q+2n-2) X_q^* \binom{2q+2n-3}{2q-1}.
 \end{aligned} \tag{19}$$

Finally, recalling the famous connection between the Riemann Zeta function $\zeta(z)$, calculated on even integers, and Bernoulli numbers B_k [9,10], $\zeta(2n) = 2^{2n-1} \pi^{2n} B_{2n} (-1)^{n+1} / (2n)!$, we obtain the final system for the odd multipoles:

$$\begin{aligned}
 X_n = & -E_0 \varepsilon_0 \frac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 + \varepsilon_2} \delta_{1,n} \\
 & - \frac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 + \varepsilon_2} \sum_{q=1}^{+\infty} \left(\frac{2\pi R}{d e^{j\vartheta}}\right)^{2q+2n-2} \frac{(-1)^{q+n} B_{2q+2n-2}}{(2q+2n-2)!} X_q^* \binom{2q+2n-3}{2q-1}.
 \end{aligned} \tag{20}$$

Such particular disposition of cylinders has been taken into account as a simple example and because it is interesting to note that for such a linear chain of cylinders the multipole coupling terms are related to the Bernoulli numbers. However two examples of simulations have been shown in Fig. 4 where the equipotential lines are represented for $E_0 = 1, R = 1, d = 2.5, \vartheta = 45^\circ, \varepsilon_1 = 1, \varepsilon_2 = 10$ (Fig. 4a) and $\varepsilon_2 = \frac{1}{10}$ (Fig. 4b).

5. Characterisation of a regular array of cylinders

A material composed of a mixture of distinct homogeneous media can be considered as a homogeneous one at a sufficiently large observation scale. In literature, the problem of mixture characterisation has been solved in many cases of linear and non-linear mixtures by applying several different methods [1,11]. In the

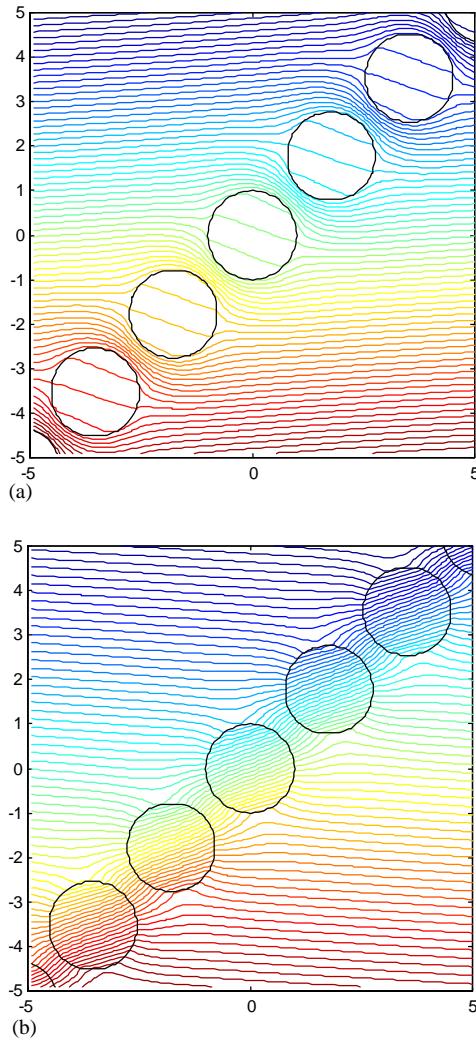


Fig. 4. Equipotential lines for a linear chain of parallel cylinders oriented with an angle $\vartheta = 45^\circ$ with the external applied field. Two examples are reported, having used the following data: $E_0 = 1$, $R = 1$, $d = 2.5$, $\varepsilon_1 = 1$, $\varepsilon_2 = 10$ (a) and $\varepsilon_2 = \frac{1}{10}$ (b).

present section an application of the multipole expansions is presented to obtain the characterisation of a composite material formed by a regular array of cylinders embedded in a given homogeneous matrix. This means that the centres of the cylinders, in a given reference plane, may be described by the regular succession of complex numbers given by: $\hat{R}_{i,k} = (i + jk)d$ where $i = -\infty \rightarrow +\infty$, $k = -\infty \rightarrow +\infty$ and d is the distance between the centres of two adjacent cylinders (as before j is the imaginary unit). Therefore, the couple of index i and k identify a given cylinder of

the array. Once again, the applied electric field is directed along the x -axis of the main frame. In these conditions all the cylinders are influenced in the same way by the external field; so: $A_n^{i,k} = A_n$ for each cylinder. Therefore, Eq. (15) may be used as follows:

$$A_n = -E_0 \varepsilon_0 \frac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 + \varepsilon_2} \delta_{1,n} + \frac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 + \varepsilon_2} \sum_{\substack{i,k \\ (i,k) \neq (s,t)}}^{Z^2} \sum_{q=1}^{+\infty} (-1)^q A_q^* \binom{q+n-1}{q} \left(\frac{R}{(i+jk)d - (s+jt)d} \right)^{q+n}. \quad (21)$$

As before, the lattice summation on k and i may be rearranged in the following way:

$$\begin{aligned} \sum_{\substack{i,k \\ (i,k) \neq (s,t)}}^{Z^2} \left(\frac{R}{(i+jk)d - (s+jt)d} \right)^{q+n} &= \left(\frac{R}{d} \right)^{q+n} \sum_{\substack{i,k \\ (i,k) \neq (s,t)}}^{Z^2} \left(\frac{1}{i-s + j(k-t)} \right)^{q+n} \\ &= \left(\frac{R}{d} \right)^{q+n} \sum_{\substack{n,m \\ (n,m) \neq (0,0)}}^{Z^2} \left(\frac{1}{n+jm} \right)^{q+n}. \end{aligned} \quad (22)$$

The last double sum over all the integer points of the complex plane can be split on four sums corresponding of the four quadrants of the plane itself, obtaining:

$$\begin{aligned} \sum_{\substack{i,k \\ (i,k) \neq (s,t)}}^{Z^2} \left(\frac{R}{(i+jk)d - (s+jt)d} \right)^{q+n} &= \left(\frac{R}{d} \right)^{q+n} [1 + (-1)^{q+n} + j^{q+n} + (-j)^{q+n}] \sum_{n=0}^{+\infty} \sum_{m=1}^{+\infty} \left(\frac{1}{n+jm} \right)^{q+n} \\ &= \left(\frac{R}{d} \right)^{q+n} [1 + (-1)^{q+n} + j^{q+n} + (-j)^{q+n}] \sum_{m=1}^{+\infty} \zeta(q+n, jm) \end{aligned} \quad (23)$$

having introduced the Hurwitz (or generalised) Zeta function $\zeta(z, s)$ [10]. We observe that the expression in Eq. (23) is not zero only if $q+n=4k$, that means $q+n=4, 8, 12 \dots$; in all these case the series is convergent to a real number. Therefore, in such array of cylinders all the multipoles are real numbers ($X_q^* = X_q$). Finally, defining the dimensionless normalised multipoles $X_n = A_n / (E_0 \varepsilon_0)$, we can write Eq. (21) in the following definitive form:

$$X_n = -\frac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 + \varepsilon_2} \delta_{1,n} + \frac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 + \varepsilon_2} \sum_{q=1}^{+\infty} (-1)^q X_q \binom{q+n-1}{q} \left(\frac{R}{d} \right)^{q+n} I_{q+n}, \quad (24)$$

where I_M is this lattice sum ($\neq 0$ if and only if $M = 4, 8, 12, \dots$):

$$I_M = [1 + (-1)^M + j^M + (-j)^M] \sum_{m=1}^{+\infty} \zeta(M, jm). \quad (25)$$

Eqs. (24) and (25) completely define the problem of calculating the multipoles induced on a given cylinder of the array. To approach the problem of the mixture characterisation, first of all, we take into account a given finite number of parallel cylinders with bases arbitrarily distributed on the reference plane (of course not overlapping). Moreover, we imagine that all these cylinders are contained in a greater one (with radius $\mathfrak{R} \gg R$ and centre is the origin of the axes), which represents the external surface of the mixture we are going to characterise. In other words we are searching for an ad hoc value of the permittivity, which should be attributed to the whole system (the greatest cylinder) in order to have the same macroscopic behaviour of the composite materials. Such macroscopic behaviour can be observed only at a sufficiently large observation scale, which means at a sufficiently large distance from the mixture itself. If the mixture (cylinder of radius \mathfrak{R}) is exposed to a uniform electric field E_0 along the x -axis and it is considered homogeneous with equivalent permittivity ε_{eq} , outside it, we find an electrical potential given by the standard relation:

$$V(r, \varphi) = -E_0 r \cos \varphi \left(1 + \frac{\mathfrak{R}^2}{r^2} \frac{\varepsilon_1 - \varepsilon_{\text{eq}}}{\varepsilon_1 + \varepsilon_{\text{eq}}} \right), \quad (26)$$

where r and φ represent polar coordinates of the reference frame. On the other hand, if we take into consideration the microstructure of the composite material we may write the electrical potential outside the mixture, at a sufficiently large distance, by using Eq. (8) and by neglecting all the multipoles except for the first one (the dipole moment). So, we simply obtain

$$V(r, \varphi) = -E_0 r \cos \varphi + \sum_{k=1}^N \frac{R^2}{r \varepsilon_0} \operatorname{Re}\{A_1^k e^{j\varphi}\}. \quad (27)$$

If the coefficients A_1^k are real (as in our case), defining $X_1^k = A_1^k / (E_0 \varepsilon_0)$ and $\langle X_1 \rangle = \sum_k X_1^k / N$, we finally obtain

$$V(r, \varphi) = -E_0 r \cos \varphi \left(1 - \frac{R^2}{r^2} N \langle X_1 \rangle \right). \quad (28)$$

Drawing a comparison between Eq. (26) and Eq. (28) we derive, after some straightforward calculations, the following result:

$$\varepsilon_{\text{eq}} = \varepsilon_1 \frac{1 + c \langle X_1 \rangle}{1 - c \langle X_1 \rangle}, \quad (29)$$

where $c = NR^2/\mathfrak{R}^2$ is the volume fraction of the cylinders embedded in the homogeneous media.

Eq. (29) allows us to characterise a given mixture with N cylinders when the average value of the normalised dipole moment is computed by means of the multipoles interaction theory described in previous sections. If we consider a finite (N limited) regular array of cylinders with N increasing, we may observe that the average value of the dipole moment converges to the value obtained from Eqs. (24) and (25) concerning an infinite array of cylinders. So, we may use the

system formed by Eqs. (24), (25) and (29) to completely characterise the whole regular composite material. In this case $\langle X_1 \rangle = X_1$ and $c = \pi R^2/d^2$ is the volume fraction subjected to the restriction $0 < c < \pi/4$ (not overlapping cylinders).

The description of some computer simulations follows. In Figs. 5 and 6 the plots of the equivalent permittivity $\varepsilon_{\text{eq}}/\varepsilon_1$ are shown versus the volume fraction c of the composite material. Fig. 5 deals with some cases with $\varepsilon_2/\varepsilon_1 < 1$ and Fig. 6 with different ratios $\varepsilon_2/\varepsilon_1 > 1$. We have numerically verified that the convergence, in such cases, is obtained by using 100 multipoles in the interaction system.

In Fig. 7 one can find the plot of the equivalent permittivity $\varepsilon_{\text{eq}}/\varepsilon_1$ as a function of the ratio $\varepsilon_2/\varepsilon_1$ for the extreme case of cylinders in contact, i.e. $c = \pi/4$, the most critical situation. The computation has been carried out by using two hundred multipoles for any value of the ratio $\varepsilon_2/\varepsilon_1$ in the range $1/300 \rightarrow 300$. The plot is represented in bi-logarithmic scale. The result is compared with two classical theories in the field of the characterisation of mixtures. The first one is the Maxwell theory, which is valid only for very diluted dispersions of cylinders [1,2]. The following Maxwell formula may be obtained starting from Eq. (29) and by using the dipole moment of an isolated cylinder:

$$c \frac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 + \varepsilon_2} = \frac{\varepsilon_1 - \varepsilon_{\text{eq}}}{\varepsilon_1 + \varepsilon_{\text{eq}}}. \quad (30)$$

The second formula, used in the comparison, is the Bruggeman one [12,13] obtained by means of differential schemes and valid also for greater values of the volume

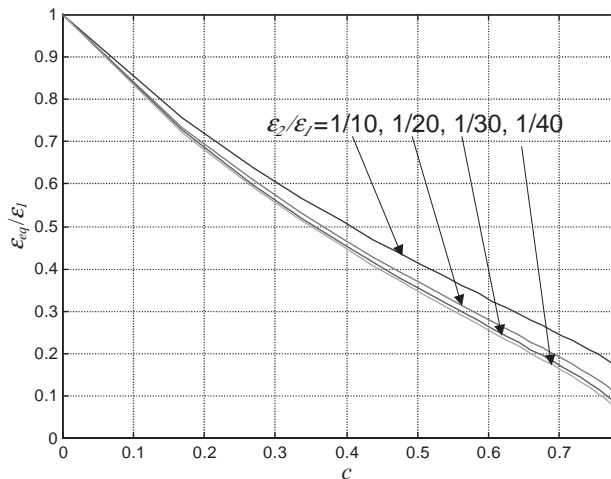


Fig. 5. The plot of the equivalent permittivity $\varepsilon_{\text{eq}}/\varepsilon_1$ is shown versus the volume fraction c of the composite material. Some cases with $\varepsilon_2/\varepsilon_1 < 1$ have been taken into consideration: $\varepsilon_2/\varepsilon_1 = \frac{1}{10}, \frac{1}{20}, \frac{1}{30}, \frac{1}{40}$. The convergence is obtained by using 100 multipoles in the interaction system.

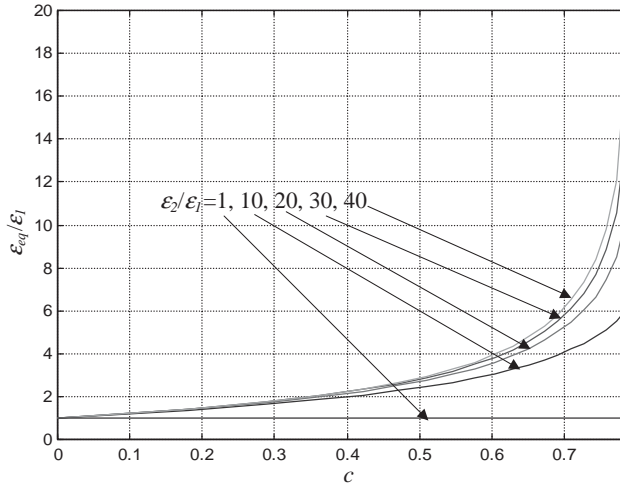


Fig. 6. The plot of the equivalent permittivity ϵ_{eq}/ϵ_1 is shown versus the volume fraction c of the composite material. Some cases with $\epsilon_2/\epsilon_1 > 1$ have been taken into consideration: $\epsilon_2/\epsilon_1 = 1, 10, 20, 30, 40$. The convergence is obtained by using 100 multipoles in the interaction system.

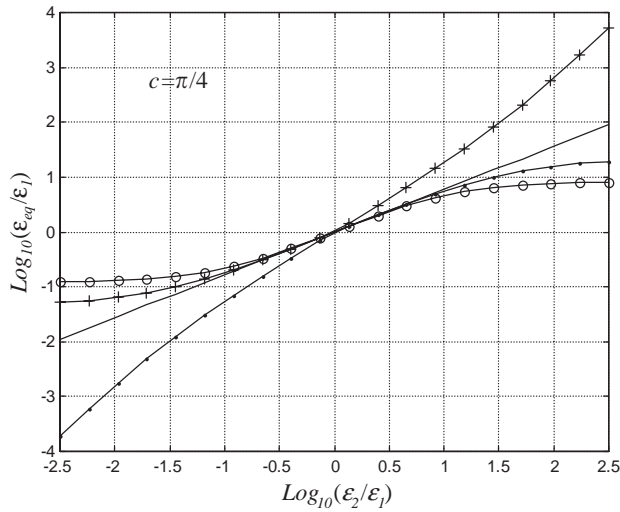


Fig. 7. Plot of the equivalent permittivity ϵ_{eq}/ϵ_1 as function of the ratio ϵ_2/ϵ_1 for the case of touching cylinders: $c = \pi/4$. The computation has been carried out by using 200 multipoles. Continuous line with circles: Maxwell relation. Continuous dotted line and continuous line with plus: solutions of the Bruggeman expression. Continuous line: exact multipole solution (straight line in bi-logarithmic scale perfectly fitted by the empirical expression $\epsilon_{eq}/\epsilon_1 = (\epsilon_2/\epsilon_1)^{\pi/4}$).

fraction of the cylinders:

$$1 - c = \frac{\varepsilon_2 - \varepsilon_{\text{eq}}}{\varepsilon_2 - \varepsilon_1} \left(\frac{\varepsilon_1}{\varepsilon_{\text{eq}}} \right)^{1/2}. \quad (31)$$

The formula given in Eq. (31) is a second degree algebraic equation with two positive real solutions: usually the smaller solution is taken when $\varepsilon_2/\varepsilon_1 > 1$ and the greatest one is considered when $\varepsilon_2/\varepsilon_1 < 1$. In Fig. 7 we have reported both the solutions to draw a complete comparison. One can observe the large differences between the exact result obtained with the multipoles interaction method and the previously described earlier theories. It is curious to note that the exact multipole solution of the problem is perfectly fitted by the very simple semi-empirical law $\varepsilon_{\text{eq}}/\varepsilon_1 = (\varepsilon_2/\varepsilon_1)^{\pi/4}$ (straight line in bi-logarithmic scale with angular coefficient equal to $\pi/4$), at least in the range of $\varepsilon_2/\varepsilon_1$ considered in Fig. 7. Anyway, this is only a conjecture very difficult to verify for higher values of the ratio $\varepsilon_2/\varepsilon_1$. To the author's knowledge this question is an open problem. Indeed, a very high number of multipoles should be used to achieve convergence in this extreme case. For instance, it should be underlined that this conjecture is in complete agreement with a theoretical expansion obtained by Mityushev [14]. From Eq. (3.3) of his paper is easily derived the following formula for the case of touching cylinders ($c = \pi/4$):

$$\frac{\varepsilon_{\text{eq}}}{\varepsilon_1} = 1 + \frac{\pi}{2} \rho + \frac{\pi^2}{8} \rho^2 + \mathcal{O}(\rho^2), \quad (32)$$

where the parameter is defined as follows:

$$\rho = \frac{\varepsilon_2/\varepsilon_1 - 1}{\varepsilon_2/\varepsilon_1 + 1}. \quad (33)$$

By using this definition, our conjecture may be simply recast in the form

$$\frac{\varepsilon_{\text{eq}}}{\varepsilon_1} = \left(\frac{1 + \rho}{1 - \rho} \right)^{\pi/4}. \quad (34)$$

At this point it is not difficult to verify that Eq. (32) is exactly the Mc-Laurin expansion of Eq. (34), which contains only the first two terms. Anyway, a complete proof of Eq. (34) is not available at the present stage of the research.

Another interesting result is given in Ref. [15] dealing with perfectly conducting cylinders with volume fraction near its maximum value $c = \pi/4$.

6. Conclusions

The present work describes the derivation of a multipole theory for an arbitrary system of parallel cylinders (two-dimensional problem) obtaining a closed set of equations for the multipole moments induced by an external uniform field. An example is shown dealing with a linear chain of cylinders: the multipole coupling terms are related to the Bernoulli numbers. Finally, the characterisation of a

two-dimensional regular array of cylinders is taken into consideration: the equivalent permittivity has been computed as a function of the stoichiometric coefficient and of the relative dielectric constant between cylinders and hosting medium. In the limiting case of touching cylinders a very simple behaviour is observed for the effective permittivity and it is fitted very well by the simple relation: $\varepsilon_{\text{eq}}/\varepsilon_1 = (\varepsilon_2/\varepsilon_1)^{\pi/4}$. However, further research on this topic will be performed to better understand the actual behaviour of such systems for higher values of the ratio $\varepsilon_2/\varepsilon_1$.

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Appendix A

Here, we give a proof of the off-centered expansion theorem stated in the main text by Eq. (11). We consider two vectors $\vec{A} = (r_a \cos \varphi_a, r_a \sin \varphi_a)$ and $\vec{B} = (r_b \cos \varphi_b, r_b \sin \varphi_b)$ given on the plane and the condition $\|\vec{A}\| < \|\vec{B}\|$ fulfilled; first of all, we take into account the following implications:

$$\begin{aligned} \frac{e^{jn\varphi(\vec{A}-\vec{B})}}{\|\vec{A}-\vec{B}\|^{|n|}} &= \frac{1}{\|\vec{A}-\vec{B}\|^{|n|} e^{-jn\varphi(\vec{A}-\vec{B})}} = \frac{1}{[\|\vec{A}-\vec{B}\| e^{-j \operatorname{sgn}(n)\varphi(\vec{A}-\vec{B})}]^{|n|}} \\ &= \frac{1}{[r_a e^{-j \operatorname{sgn}(n)\varphi_a} - r_b e^{-j \operatorname{sgn}(n)\varphi_b}]^{|n|}} \\ &= \frac{(-1)^n}{r_b^{|n|} e^{-jn\varphi_b} [1 - \frac{r_a}{r_b} e^{j \operatorname{sgn}(n)(\varphi_b - \varphi_a)}]^{|n|}} \end{aligned} \quad (\text{A.1})$$

where $\operatorname{sgn}(n)$ represents the *signum* function which assumes the value +1 if $n > 0$ and the value -1 when $n < 0$. To complete the proof we use the binomial series applied to the brackets in Eq. (A.1):

$$\begin{aligned} (1+z)^m &= \sum_{k=0}^{+\infty} \binom{m}{k} z^k \quad \text{if } |z| < 1, m \in \mathfrak{R}, \\ \binom{m}{k} &= \frac{m(m-1)(m-2)\cdots(m-k+1)}{k!}. \end{aligned} \quad (\text{A.2})$$

Therefore, we let $z = -(r_a/r_b) e^{j \operatorname{sgn}(n)(\varphi_b - \varphi_a)}$ and $m = -|n|$ and we immediately obtain Eq. (11) by using the simple property:

$$\binom{-|n|}{k} = (-1)^k \binom{|n| + k - 1}{k}.$$

This is an elementary method to verify this formula; it may be also derived by taking the leading term in the limit $k \rightarrow 0$ in the identity:

$$e^{jn\varphi(\bar{A}-\bar{B})} N_n(k\|\bar{A}-\bar{B}\|) = \sum_{h=-\infty}^{+\infty} (-1)^n J_h(kr_a) N_{n+h}(kr_b) e^{jh(\varphi_b-\varphi_a)} e^{jn\varphi_b} \quad (\text{A.3})$$

which is easily derived from Eq. 8.53.2 in Ref. [9]. Here the functions $J_m(x)$ are the Bessel functions of the first kind and $N_n(x)$ are the Bessel functions of the second kind. This limiting approach is commonly used in the three-dimensional case dealing with spherical Bessel functions and spherical harmonics [6].

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