Chapter 17

RECENT ADVANCES IN THE CHARACTERIZATION OF COMPOSITE DIELECTRIC STRUCTURES

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Abstract

The central problem in predicting the dielectric behavior of heterogeneous materials (like, e.g., composite or nanostructured systems, powders or mixtures) consists in the evaluation of their effective macroscopic properties, still taking into account the actual microscale material features. This leads to the concept of homogenization, a coarse graining approach addressed to determine the relationship between the microstructure and the effective behavior: the prediction of the effective electromagnetic properties of a composite material from those of its constituent material phases is the major objective of various homogenization models. The resulting effective properties can be observed at the macroscale, where the refined effects of the morphology cannot be directly measured.

Dispersions of particles (inclusions with a given shape and a given volume) in a host homogeneous matrix are the most studied heterogeneous structures. From the historical point of view, early mixture theories generally work well when the volumetric proportion of the inclusion phase is small and when the contrast between the electromagnetic properties of the two material phases is not large. More recently, refined and improved models have been developed in order to yield better predictions, also in these critical situations.

Recent increases in activity in the field are, at least, partially caused by the interest in selective absorbers of solar and infrared radiation, by an increasing number of applications in astronomy and atmospheric physics, by several applications in the design of novel materials in optics and in material science, and by the indications that the electromagnetic behavior of the composite system may be very different from the behavior of individual components.

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These approaches can be applied not only to the static (d.c.) electric and magnetic properties, but also to the case of wave propagation in low frequency (l.f.) or high frequency (h.f.) regime. It is in fact well known that when any form of energy propagates through a medium containing scatterers (particles), the entrained energy will be either redistributed in various directions by scattering or absorbed by intrinsic absorption mechanisms. The standard homogenization theories can be applied also in such cases provided that the wavelength of the propagating field is much larger than the average size of the particles. Recently, these methodologies have been applied to light scattering from coatings, to heat transfer in powder insulators, to chemical and nuclear reactors, to cryogenic insulation and, finally, to microwave or laser coatings.

In all heterogeneous or composite materials, the nonlinear regime and the anisotropic character have not yet been investigated thoroughly. Nevertheless, both the nonlinear and the anisotropic features are relevant in many materials science problems (crystal optics, optical bistability and optical devices). Therefore, we devote this work to the development of some analytical models able to take into account the refined effects of the nonlinearity and the anisotropy of the constituents.

1. Introduction

A widely dealt topic concerning the physical behavior of heterogeneous materials (mixtures) is that of calculating their permittivity starting from the knowledge of the permittivity of each medium composing the mixture as well as of the structural properties of the mixture itself (percentage of each medium, shapes and relative positions of the single parts of the various media). Clearly, it concerns with isotropic linear media, which combine to form linear mixtures. In literature we find a large number of approximate analytical expressions for the effective permittivity of composed media as a function of the permittivity of its homogeneous constituents and some stoichiometric parameter [1-3]. Each of these relationships should yield correct results for a particular kind of microstructure or, in other words, for a well defined morphology of the composite material.

From the historical point of view, we remember some theories describing a mixture composed by two linear isotropic components: one of the most famous is the Maxwell formula developed for a strongly diluted suspension of spheres [4]; a similar methodology has been applied to the case of a mixture of parallel circular cylinders [1,3].

An alternative model is provided by the differential scheme, which derives from the mixture characterization approach used by Bruggeman [5]. In this case the relations should maintain the validity also for less diluted suspensions. This procedure is based on the following considerations: let's suppose that the effective permittivity of a composite medium is known to be ε . Now, if a small additional volume of inclusions is embedded in the matrix, the change in the permittivity is approximated to be that which arise if an infinitesimal volume of inclusions were added to a uniform, homogeneous matrix with permittivity ε . This leads, in the simpler and most studied case, to some differential equations described in the following sections.

The first papers concerning mixtures of ellipsoids were written by Fricke [6,7] dealing with the electrical characterization of inhomogeneous biological tissues containing spheroidal particles: he found out some explicit relationships that simply were an extension of the Maxwell formula to the case with ellipsoidal inclusions.

In current literature Maxwell's relation for spheres and Fricke's expressions for ellipsoids are the so-called Maxwell-Garnett Effective Medium Theory results [8,9]: both theories hold

on under the hypothesis of the very low concentration of the dispersed component. Once more, we observe that the classical approximation for spheres has been derived in different contexts by Maxwell [4], Maxwell-Garnett [10], Wagner [11] and Bottcher [12] as a generalized Clausius-Mossotti-Lorentz-Lorenz relation [2].

In recent literature some applications of the Bruggeman procedure to mixtures of ellipsoids have been shown in connection with the problem of characterizing the dielectric response of water-saturated rocks [13-15]. In these works the authors have shown that the Bruggeman method, applied to this specific problem, leads to results in good agreement with the empirical Archie's law [16], which describes the dependence of the dc conductivity of brine-saturated sedimentary rocks on porosity. A complete discussion about the implementation of the differential schemes to dispersions of aligned or random oriented ellipsoids can be found in Ref. [17].

In general, the electrical (thermal, elastic and so on) properties of composite materials are strongly microstructure dependent. The relationships between microstructure and properties may be used for designing and improving materials, or conversely, for interpreting experimental data in terms of micro-structural features. Ideally, the aim is to construct a theory that employs general micro-structural information to make some accurate property predictions. A simpler goal is the provision of property for different class of microstructures.

A great number of works has been devoted to describe the relationship between microstructure and properties: in [18] a functional unifying approach has been applied to better understand the intrinsic mathematical properties of a general mixing formula. A fundamental result is given by the Hashin-Shtrikman's variational analysis [19,20], which provides an upper and lower bound for composite materials, irrespective of the microstructure. In particular, for a two-phase material, these bounds are given by two expressions of the Maxwell-Fricke type. Finally, a method to find the relation between the spatial correlation function of the dispersed component and the final properties of the material is derived from the Brown [21] and Torquato [22-24] expansions.

Some other types of microstructures have been taken into consideration. For example, the problem of the mixture characterization has been exactly solved in the case of linear and nonlinear random mixtures, that is, materials for which the various components are isotropic, linear and mixed together as an ensemble of particles having random shapes and positions [25,26]. This approach permits to apply the mixture theories to dielectric poly-crystals and random networks [27-29].

One of the most important problems in homogenization theories is that of describing the interactions among the particles in order to consider arbitrary concentrated mixtures. To this aim, a multipole theory describing the interactions of dielectric cylinders in a uniform field has been developed for considering arbitrarily dense dispersions [30]. Such a multipole expansion has been applied to the dielectric characterization of composite materials formed by a regular array of parallel cylinders, obtaining the effective permittivity with a numerically efficient technique. A similar treatment, concerning multipole interactions of spheres, can be found in earlier literature [31,32].

Several works have been devoted to the quantitative evaluation of the local fluctuations of electric fields (or other observables) in the neighborhood of an inhomogeneity. Such fluctuations can easily extend over a spatial domain so large to result out-of-reach for numerical simulations. On the other hand, homogenization theories simply do not take these features into account. This situation is approached by means of the density of state (DOS) concept [33-35]. The use of the DOS as a tool to characterize some relevant quantities has been made both in the electrical and in the mechanical systems, as well as for multi-cracked materials [36,37]. If we subdivide a region containing an inclusion in a large number of very small domains and we count the number of domains in which a given component E of the electric field has values in the interval ($E, E+\Delta E$), then we can effectively define the stress density. This theoretical concept is a valuable tool to quantify the space distribution of any vector or tensor field.

Two important aspects, which have not been taken into account thoroughly in the development of such theories, are the nonlinearity and the anisotropy of the phases of a heterogeneous structure. Therefore, in this work we outline some mathematical procedures able to take into account these specific physical effects. In particular, we describe some generalizations of the Maxwell-Garnett theory obtained by means of the differential scheme and by considering the nonlinear behavior of the materials forming the whole system. Moreover, we describe a complete and detailed approach useful to deal with anisotropic or graded particles embedded in anisotropic matrix. We have solved this problem by adopting a series of mathematical techniques widely used in elasticity theory and in micro- or nano-mechanics.

The structure of the paper is the following: in Section 2 we briefly review the Maxwell-Garnett theory and we present some generalization based on the differential scheme (both for aligned and random oriented ellipsoids). In Section 3 we cope with the problem of homogenizing a dispersion of nonlinear particle embedded in a linear matrix. We obtain the mixing rule for the hypersusceptibility of the material. In Section 4 we describe a new methodology for analyzing anisotropic systems. The study of a single anisotropic particle in anisotropic environment allows us to define the so-called Eshelby tensors, very useful to summarize all the geometrical and physical properties of an arbitrary inhomogeneity. Then, we draw some comparisons between the results obtained with the anisotropic models and those obtained with the standard Maxwell-Garnett approach. Finally, in Section 5 we prove two theorems concerning the case of functionally graded ellipsoidal particles.

It must be underlined that from a merely mathematical standpoint, the problem of calculating the mixture permittivity is identical to a number of others, for instance to that regarding permeability (in a magnetostatic situation), conductivity (in d.c. condition), thermal conductivity (in a steady-state thermal regime) and so on. Therefore, each theoretical formula predicts the effective value of any thermal, magnetic or electrical specific quantities.

2. Maxwell-Garnett Theory and Generalizations

The Italian astronomer Ottaviano Fabrizio Mossotti (1791-1863) developed a model for interstellar dust by considering it as a gas of little dielectric particles; at the same time, the German physicist Rudolf Clausius (1822-1888) obtained similar results in terms of the refraction index [2]. These contributions led to the remarkable Clausius-Mossotti equation, which is the first result in the theory of heterogeneous material. Successively, the Danish mathematician Ludvig Lorenz (1829- 1891) published some works on the effective refractive index in mixtures and the Dutch physicist Hendrik Lorentz (1853-1928) deduced the same results from the electromagnetism Maxwell equations [2]. These four seminal investigations have given the name to the so-called Clausius-Mossotti-Lorentz-Lorenz relation. Finally, we

observe that the classical approximation for spheres has been derived in different contexts by Maxwell [4], Maxwell-Garnett [10], Wagner [11] and Bottcher [12], as a generalized Clausius-Mossotti-Lorentz-Lorenz relation, which is the classical starting point of all these theories [2]. The first improving taking into account arbitrarily dense dispersions is given by the differential scheme or differential effective medium theory [5]. The corresponding result is called Bruggeman asymmetric formula or, equivalently, Bruggeman-Hanai formula [2]. It corresponds to our Eq. (2.8) or Eq. (2.20) with the depolarization factors equal to 1/3 (see below for details). In this section we review the application of the Maxwell-Garnett idea to a dispersion of aligned or random oriented ellipsoids. Moreover, we describe recent results obtained with the differential scheme applied to dispersions with arbitrary microstructure.

2.1. Characterization of Dispersions of Aligned Ellipsoids

The theory for dispersion of aligned ellipsoids is based on the following result, which describes the behavior of a single ellipsoidal particle (ε_2) embedded in a homogeneous medium (ε_1). Let the axes of the ellipsoid be $a_x=a_1$, $a_y=a_2$ and $a_z=a_3$ (aligned with axes x, y, z of the reference frame) and let a uniform electrical field $\vec{E}_0 = (E_{0x}, E_{0y}, E_{0z})$ applied to the structure. Then, according to Stratton [38] or Landau [39] a uniform electrical field appears inside the ellipsoid and it can be computed as follows. We define the function

$$R(s) = \sqrt{(s + a_x^2)(s + a_y^2)(s + a_z^2)}$$
(2.1)

and the depolarization factors along each axis

$$L_{j} = \frac{a_{x}a_{y}a_{z}}{2} \int_{0}^{+\infty} \frac{ds}{\left(s + a_{j}^{2}\right)R(s)}$$
(2.2)

We remark that $L_x+L_y+L_z=1$. Therefore, the electrical field inside the ellipsoid is given, in components, by [38,39]

$$E_{sj} = \frac{E_{0j}}{1 + L_j \frac{\varepsilon_2 - \varepsilon_1}{\varepsilon_1}}$$
(2.3)

This is the main result that plays an essential role in the further development of the theory. Now, we are ready to consider a dispersion of aligned ellipsoids (ε_2) embedded in a homogeneous medium (ε_1), see Fig. 1. Moreover, let *c* be the volume fraction of the embedded ellipsoids. To begin, we consider a diluted dispersion (c <<1) and thus we may evaluate the average value of the electrical field over the mixture volume by means of the following relationship



Figure 1. Structure of a dispersion of aligned ellipsoids. The external surface of the mixture is a greater ellipsoid with the same shape of the inclusions.

This means that we do not take into account the interactions among the inclusions because of the very low concentration: each little ellipsoid behaves as a single one in the whole space. Once more, to derive Eq. (2.4), we approximately take into account a uniform electrical field $\vec{E}_0 = (E_{0x}, E_{0y}, E_{0z})$ in the space outside the inclusions. To define the mixture we are going to characterize, we consider a greater ellipsoid, which contains all the other ones. This ellipsoid represents the external surface of the composite materials. This ellipsoid has, by definition, the same shape of the inclusions and then the axes are given by βa_x , βa_y and βa_z where β is a positive constant (it is aligned to the embedded ellipsoids, see Fig. 1). As one can simply verify, the depolarization factors of this ellipsoid are the very same of each inclusion contained in the mixture. Moreover, we may observe that the overall behavior of the mixture is anisotropic because of the alignment of the ellipsoidal particles. So, if we define the equivalent principal permittivity of the mixture along the axes x, y and z as $\varepsilon_{eff,x}$, $\varepsilon_{eff,y}$ and $\varepsilon_{eff,z}$, we may write down these expressions for the average value of the components of the electrical field inside the whole mixture

$$\left\langle E_{j}\right\rangle = \frac{E_{0j}}{1 + L_{j} \frac{\varepsilon_{eff,j} - \varepsilon_{1}}{\varepsilon_{1}}}$$
(2.5)

These expressions are derived considering the whole mixture as a single inclusion in the space and then we have used the basic result given by Eq. (2.3). Now, by substituting Eq. (2.3) in Eq. (2.4) and by drawing a comparison with Eq. (2.5) we may find expressions for $\varepsilon_{eff,x}$, $\varepsilon_{eff,y}$ and $\varepsilon_{eff,z}$, which are the effective principal permittivities of the whole composite material

$$\varepsilon_{eff,j} = \varepsilon_1 + c(\varepsilon_2 - \varepsilon_1) \frac{1}{1 + (1 - c)L_j \frac{\varepsilon_2 - \varepsilon_1}{\varepsilon_1}} = \varepsilon_1 + c(\varepsilon_2 - \varepsilon_1) \frac{1}{1 + L_j \frac{\varepsilon_2 - \varepsilon_1}{\varepsilon_1}} + O(c^2)$$
(2.6)

Each of the three independent relations, which appears in Eq. (2.6), may be recast in the unified form $\varepsilon = F(\varepsilon_l, \varepsilon_2, c)$ where ε represents $\varepsilon_{eff,x}$, $\varepsilon_{eff,y}$ or $\varepsilon_{eff,z}$. We use this very simple form to review the Bruggeman procedure (or differential scheme) that is the method to find a second mixture relationship considering a first theory describing the composite material (actually the function F). This second theory is usually more efficient than the first one, even if the mixture is not strongly diluted. In Bruggeman scheme the initially low concentration is gradually increased by infinitesimal additions of the dispersed component [5]. We start from $\varepsilon = F(\varepsilon_l, \varepsilon_2, c)$ for a mixture where c is the volume fraction of ellipsoids: we consider a unit volume of the mixture $(1m^3)$ and we add a little volume dc_0 of inclusions. Therefore, we consider another mixture between a medium with permittivity ε (volume equals to 1 m³) and a second medium (ε_2) with volume dc_0 . In these conditions the volume fraction of the mixture we can write: $\varepsilon + d\varepsilon = F(\varepsilon, \varepsilon_2, dc_0)$. In the final composite material, with the little added volume dc_0 , the matrix (ε_l) will have effective volume l-c and the dispersed medium (ε_2) will have effective volume $c+dc_0$.

The original volume fraction of the second medium is c/1 and the final one is $(c + dc_0)/(1 + dc_0)$; so, it follows that the variation of the volume fraction of inclusions obtained by adding the little volume dc_0 is simply given by: $dc = (c + dc_0)/(1 + dc_0) - c/1 = dc_0(1 - c)/(1 + dc_0) \approx dc_0(1 - c)$.

Therefore, we have $\varepsilon + d\varepsilon = F(\varepsilon, \varepsilon_2, dc/(1-c))$. With a first order expansion we simply obtain: $\varepsilon + d\varepsilon = F(\varepsilon, \varepsilon_2, 0) + \frac{\partial F(\varepsilon, \varepsilon_2, c)}{\partial c} \Big|_{c=0} \frac{dc}{1-c}$ and taking into account the obvious

relation $\mathcal{E} = F(\mathcal{E}, \mathcal{E}_2, 0)$ we obtain the differential equation: $\frac{d\mathcal{E}}{dc} = \frac{1}{1-c} \frac{\partial F(\mathcal{E}, \mathcal{E}_2, c)}{\partial c} \Big|_{c=0}$. This equation, when the function *F* is given, defines a new function, which should better describe the mixture when it is not strongly diluted. We may apply the method to the three expressions given in Eq. (2.6) obtaining the following differential equations (*j* = *x*, *y*, *z*)

$$\frac{d\varepsilon_{eff,j}}{dc} = \frac{1}{1-c} \left(\varepsilon_2 - \varepsilon_{eff,j} \right) \frac{1}{1+L_j \frac{\varepsilon_2 - \varepsilon_{eff,j}}{\varepsilon_{eff,j}}} \quad (j = x, y, z)$$
(2.7)

These equations may be easily solved with the auxiliary conditions $\varepsilon_{eff,j}(c=0)=\varepsilon_l$ (for any value j = x, y, z) obtaining the results [17]

$$1 - c = \frac{\varepsilon_2 - \varepsilon_{eff,j}}{\varepsilon_2 - \varepsilon_1} \left(\frac{\varepsilon_1}{\varepsilon_{eff,j}}\right)^L j \quad (j = x, y, z)$$
(2.8)

These are the final expressions, which characterize a dispersion of aligned ellipsoids, obtained by means of the Bruggeman approach. The depolarization factors are given by Eq. (2.2). We may derive some simplified version of this result in some limiting cases. First, we consider a case with $a_z \rightarrow \infty$: the ellipsoids degenerate to parallel elliptic cylinders. We may define the eccentricity of the elliptic base of these cylinders as $e=a_y/a_x$. So, the expressions for the depolarization factors can be evaluated as follows: $L_x = \frac{e}{e+1}$, $L_y = \frac{1}{e+1}$ and $L_z = 0$. Therefore, Eq. (2.8) yields the simplified results [17]

$$\begin{cases} 1-c = \frac{\varepsilon_2 - \varepsilon_{eff,x}}{\varepsilon_2 - \varepsilon_1} \left(\frac{\varepsilon_1}{\varepsilon_{eff,x}}\right)^{\frac{e}{e+1}} \\ 1-c = \frac{\varepsilon_2 - \varepsilon_{eff,y}}{\varepsilon_2 - \varepsilon_1} \left(\frac{\varepsilon_1}{\varepsilon_{eff,y}}\right)^{\frac{1}{e+1}} \\ \varepsilon_{eff,z} = c\varepsilon_2 + (1-c)\varepsilon_1 \end{cases}$$
(2.9)

The first two equations describe the principal permittivities in the directions (axes x and y) orthogonal to the cylinders and the third one defines the principal permittivity along the axes of the cylinders (axes z).

A second case deals with a mixture of inclusions shaped as ellipsoids of revolution; we consider $a_x=a_y$ and thus we define the eccentricity as $e=a_z/a_x=a_z/a_y$. The depolarization factors may be computed in closed form as follows and the results depend on the shape of the ellipsoid; it is prolate (of ovary or elongated form) if e>1 and oblate (of planetary or flattened form) if e<1

$$\begin{cases} L_{x} = L_{y} = \frac{e}{2} \int_{0}^{+\infty} \frac{d\xi}{(\xi+1)^{2} (\xi+e^{2})^{1/2}} = \begin{cases} \frac{e}{4p^{3}} \left[2ep + \ln \frac{e-p}{e+p} \right] & \text{if } e > 1 \\ \frac{e}{4q^{3}} \left[\pi - 2eq - 2arctg \frac{e}{q} \right] & \text{if } e < 1 \end{cases} \\ L_{z} = \frac{e}{2} \int_{0}^{+\infty} \frac{d\xi}{(\xi+1) (\xi+e^{2})^{3/2}} = \begin{cases} \frac{1}{2p^{3}} \left[e \ln \frac{e+p}{e-p} - 2p \right] & \text{if } e > 1 \\ \frac{1}{2q^{3}} \left[2q - e\pi + 2earctg \frac{e}{q} \right] & \text{if } e < 1 \end{cases} \end{cases}$$

$$(2.10)$$

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We may verify that $2L_x+L_z=1$ for any value of *e*. For sake of completeness, we show the complete expressions for the depolarization factors in the case of generally shaped ellipsoids. The results have been expressed in terms of the elliptic integrals and have been derived under the assumptions $0 < a_x < a_y < a_z$, $0 < e = a_x/a_y < 1$ and $0 < g = a_y/a_z < 1$. Now, we have $L_x+L_y+L_z=1$. The final expressions follow

$$\begin{aligned}
L_{x} &= \frac{1}{1 - e^{2}} - \frac{e}{(1 - e^{2})\sqrt{1 - e^{2}g^{2}}} E(v, q) \\
L_{y} &= \frac{e(1 - e^{2}g^{2})}{(1 - e^{2})(1 - g^{2})\sqrt{1 - e^{2}g^{2}}} E(v, q) - \frac{eg^{2}}{(1 - g^{2})\sqrt{1 - e^{2}g^{2}}} F(v, q) - \frac{e^{2}}{1 - e^{2}} \\
L_{z} &= \frac{eg^{2}}{(1 - g^{2})\sqrt{1 - e^{2}g^{2}}} [F(v, q) - E(v, q)]
\end{aligned}$$
(2.11)

Here the quantities v and q are defined by $v = \arcsin\sqrt{1 - e^2 g^2}$ and $q = \sqrt{\frac{1 - g^2}{1 - e^2 g^2}}$

and the elliptic integrals are defined below [40,41]

$$\begin{cases} F(v,q) = \int_{0}^{v} \frac{d\alpha}{\sqrt{1 - q^{2} \sin^{2} \alpha}} = \int_{0}^{senv} \frac{dx}{\sqrt{\left(1 - x^{2}\right)\left(1 - q^{2} x^{2}\right)}} \\ E(v,q) = \int_{0}^{v} \sqrt{1 - q^{2} \sin^{2} \alpha} \, d\alpha = \int_{0}^{senv} \frac{\sqrt{1 - q^{2} x^{2}}}{\sqrt{1 - x^{2}}} \, dx \end{cases}$$
(2.12)

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2.2. Characterization of Dispersions of Randomly Oriented Ellipsoids

To begin, we are interested in the electrical behavior of a single ellipsoidal inclusion (ε_2) arbitrarily oriented in the space and embedded in a homogeneous medium (ε_1). We define three unit vectors, which indicate the principal directions of the ellipsoids in the space: they are referred to as \hat{n}_x , \hat{n}_y and \hat{n}_z and they are aligned with the axes a_x , a_y and a_z of the ellipsoid, respectively. By using Eq. (2.3), we may compute the electrical field inside the inclusion, induced by a given external uniform electric field

$$\vec{E}_{s} = \frac{\left(\vec{E}_{0} \cdot \hat{n}_{x}\right)\hat{n}_{x}}{1 + L_{x}\frac{\varepsilon_{2} - \varepsilon_{1}}{\varepsilon_{1}}} + \frac{\left(\vec{E}_{0} \cdot \hat{n}_{y}\right)\hat{n}_{y}}{1 + L_{y}\frac{\varepsilon_{2} - \varepsilon_{1}}{\varepsilon_{1}}} + \frac{\left(\vec{E}_{0} \cdot \hat{n}_{z}\right)\hat{n}_{z}}{1 + L_{z}\frac{\varepsilon_{2} - \varepsilon_{1}}{\varepsilon_{1}}}$$
(2.13)

This result simply derives from the sum of the three contributes to the electrical field along each axes and it may be written in explicit form, as follows

$$E_{s,q} = \sum_{k}^{x,y,z} E_{0,k} \sum_{j}^{x,y,z} \frac{n_{j,k}n_{j,q}}{1 + L_j \frac{\varepsilon_2 - \varepsilon_1}{\varepsilon_1}}$$
(2.14)

where $n_{j,k}$ is the *k*-th component of the unit vector \hat{n}_j (j = x, y, z).

For the following derivation, we are interested in the average value of the electrical field inside the ellipsoid over all the possible orientations of the ellipsoid itself and then we have to compute the average value of the quantity $n_{j,k} n_{j,q}$. Performing the integration over the unit sphere (by means of spherical coordinates) we obtain, after some straightforward computations, $\langle n_{j,k} n_{j,q} \rangle = \frac{1}{3} \delta_{k,q}$. Therefore, the average value of the electrical field (inside the randomly oriented inclusion), may be written as

$$\left\langle E_{s,q} \right\rangle = \frac{E_{0,q}}{3} \sum_{j}^{x,y,z} \frac{1}{1 + L_j \frac{\varepsilon_2 - \varepsilon_1}{\varepsilon_1}}$$
 (2.15)

Now, we are ready to consider a mixture of randomly oriented ellipsoids. In Fig. 2 one can find the structure of the composite material. We may define the volume of the mixture by means of a sphere which contains all the ellipsoidal inclusions and which represents the external surface of the heterogeneous material. Once more, let c be the volume fraction of the embedded ellipsoids. The average value of the electrical field over the mixture (inside the sphere) is approximately computed by using Eq. (2.15)



Figure 2. Structure of a dispersion of randomly oriented ellipsoids.

Then, we define ε as the effective permittivity of the whole mixture (which is isotropic because of the randomness of the orientations) by means of the relation $\langle \vec{D} \rangle = \varepsilon \langle \vec{E} \rangle$; to evaluate ε we may compute the average value of the displacement vector inside the random material. We also define V as the total volume of the mixture, V_e as the total volume of the embedded ellipsoids and V_o as the volume of the remaining space among the inclusions (so that $V=V_e \cup V_o$). The average value of $\vec{D}(\vec{r}) = \varepsilon(\vec{r})\vec{E}(\vec{r})$ is evaluated as follows

$$\left\langle \vec{D} \right\rangle = \frac{1}{V} \int_{V} \mathcal{E}(\vec{r}) \vec{E}(\vec{r}) d\vec{r} = \frac{1}{V} \mathcal{E}_{1} \int_{V} \vec{E}(\vec{r}) d\vec{r} + \frac{1}{V} \mathcal{E}_{2} \int_{V} \vec{E}(\vec{r}) d\vec{r} = = \frac{1}{V} \mathcal{E}_{1} \int_{V} \vec{E}(\vec{r}) d\vec{r} + \frac{1}{V} \mathcal{E}_{1} \int_{V} \vec{E}(\vec{r}) d\vec{r} + \frac{1}{V} \mathcal{E}_{2} \int_{V} \vec{E}(\vec{r}) d\vec{r} - \frac{1}{V} \mathcal{E}_{1} \int_{V} \vec{E}(\vec{r}) d\vec{r} =$$
(2.17)
$$= \mathcal{E}_{1} \left\langle \vec{E} \right\rangle + c (\mathcal{E}_{2} - \mathcal{E}_{1}) \left\langle \vec{E}_{s} \right\rangle$$

Drawing a comparison between Eq. (2.15), (2.16) and (2.17) we may find a complete expression, which allows us to estimate the equivalent permittivity ε and its first order expansion with respect to the volume fraction c

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$$\varepsilon = \varepsilon_{1} + \frac{\frac{1}{3}c(\varepsilon_{2} - \varepsilon_{1})\sum_{j}^{x,y,z} \frac{\varepsilon_{1}}{\varepsilon_{1} + L_{j}(\varepsilon_{2} - \varepsilon_{1})}}{1 + c\left[\frac{1}{3}\sum_{j}^{x,y,z} \frac{\varepsilon_{1}}{\varepsilon_{1} + L_{j}(\varepsilon_{2} - \varepsilon_{1})} - 1\right]} = \varepsilon_{1} + \frac{1}{3}c\varepsilon_{1}(\varepsilon_{2} - \varepsilon_{1})\sum_{j}^{x,y,z} \frac{1}{\varepsilon_{1} + L_{j}(\varepsilon_{2} - \varepsilon_{1})} + O(c^{2})$$

$$(2.18)$$

This result concerns the characterization of a very diluted dispersion of randomly oriented ellipsoids with given shape (i.e. with fixed depolarization factors L_j or eccentricities e and g). As before, to adapt this relationship to arbitrarily diluted composite materials we use the Bruggeman procedure [5], which leads to the following differential equation [17]

$$\frac{d\varepsilon}{dc} = \frac{1}{1-c} \varepsilon \left(\varepsilon_2 - \varepsilon\right) \frac{1}{3} \sum_{j}^{x,y,z} \frac{1}{\varepsilon + L_j \left(\varepsilon_2 - \varepsilon\right)}$$
(2.19)

The solution of this equation depends on the values of the depolarization factors showing the relationship between the overall permittivity and the shape of the ellipsoidal inclusions. We search for the solution in two particular cases: a dispersion of ellipsoids of rotation and a dispersion of generally shaped ellipsoids. In the first case we have $L_x=L_y$ and $2L_x+L_z=1$ and thus only one factor completely defines the shape of the inclusions. The solution of Eq. (2.19) yields the final result [17]

$$1 - c = \frac{\varepsilon_2 - \varepsilon}{\varepsilon_2 - \varepsilon_1} \left(\frac{\varepsilon_1}{\varepsilon}\right)^{\frac{3L(1 - 2L)}{2 - 3L}} \left[\frac{(1 + 3L)\varepsilon_1 + (2 - 3L)\varepsilon_2}{(1 + 3L)\varepsilon_1 + (2 - 3L)\varepsilon_2}\right]^{\frac{2(3L - 1)^2}{(2 - 3L)(1 + 3L)}}$$
(2.20)

where $L=L_x$ is given by Eq. (2.10) and represents the depolarization factor along the directions orthogonal to the principal axes of each inclusion. To complete the study we analyze a mixture of ellipsoids with three independent axes. For such generally shaped ellipsoids the relation $L_x+L_y+L_z=1$ holds true and therefore we may use two factors (L_x and L_y) as parameters which completely define the shape of the inclusions. To simply integrate Eq. (2.19) we define the following quantities depending on these depolarization factors

$$\begin{cases}
A = 3L_x^2 L_y + 3L_x L_y^2 - 3L_x L_y \\
B = L_x + L_y - 6L_x^2 L_y^2 - 8L_x L_y - 4L_x^3 L_y - 4L_x L_y^3 + \\
+ 11L_x^2 L_y + 11L_y^2 L_x - 3L_x^2 - 3L_y^2 + 4L_x^3 + 4L_y^3 - 2L_x^4 - 2L_y^4 \\
C = 4L_x^3 L_y + 4L_x L_y^3 - 2L_x L_y - 2L_x^2 L_y - 2L_y^2 L_x + 6L_x^2 L_y^2 + \\
+ 2L_x^2 + 2L_y^2 - 4L_x^3 - 4L_y^3 + 2L_x^4 + 2L_y^4 \\
D = L_x L_y - L_x - L_y + L_x^2 + L_y^2
\end{cases}$$
(2.21)

By means of a lengthy but straightforward integration we have found the solution as follows [17]

$$1 - c = \frac{\varepsilon_2 - \varepsilon}{\varepsilon_2 - \varepsilon_1} \left(\frac{\varepsilon_1}{\varepsilon}\right)^{\underline{A}} \left[\frac{(D-1)\varepsilon_1^2 - 2(D+1)\varepsilon_1\varepsilon_2 + D\varepsilon_2^2}{(D-1)\varepsilon^2 - 2(D+1)\varepsilon\varepsilon_2 + D\varepsilon_2^2} \right]^{\underline{B}} \frac{B}{2D(D-1)} \cdot \left[\frac{\sqrt{1+3D}}{\sqrt{1+3D}} \frac{\varepsilon_2 + (D-1)\varepsilon - (D+1)\varepsilon_2}{\varepsilon_2 - 2(D+1)\varepsilon_2} \frac{\sqrt{1+3D}}{\sqrt{1+3D}} \frac{\varepsilon_2 - (D-1)\varepsilon_1 + (D+1)\varepsilon_2}{\varepsilon_2 - (D-1)\varepsilon_1 + (D+1)\varepsilon_2} \right]^{\underline{B}(D+1) + C(D-1)} \frac{B(D+1) + C(D-1)}{2D(D-1)\sqrt{1+3D}} \frac{B(D+1) + C(D-1)}{(2.22)}$$

The complete model describes the equivalent permittivity as function of the following parameters: the permittivities of the two involved materials ε_2 and ε_1 , the volume fraction *c* of the embedded ellipsoids and the characteristic eccentricities *e* and *g*. Finally, $\varepsilon = \varepsilon (\varepsilon_1, \varepsilon_2, c, e, g)$.



Figure 3. Results for a mixture of randomly oriented and generally shaped ellipsoids. The surface $\varepsilon / \varepsilon_l$ versus the eccentricities *e* and *g* is shown with the assumptions $\varepsilon_2 / \varepsilon_l = 10$ and c = 1/2.

The irrational equation (Eq. (2.22)) has been numerically solved and a typical result is shown in Fig. 3 where one can deduce the effects of the shape of the inclusions on the effective macroscopic dielectric constant of the material. We have considered $\varepsilon_2/\varepsilon_1=10$, c=1/2

and we have plotted the values of $\varepsilon / \varepsilon_l$ in terms of the eccentricities *e* and *g* of the embedded ellipsoids. The limiting cases of interest have been clearly indicated.

When the above procedure is implemented for evaluating the aforesaid permittivity, a sensible dependence of the results on the shape of the inclusions (actually on the eccentricities) is shown. The closed form analysis of a dispersion of ellipsoids offers a simple but clear example of the dependence of the macroscopic behavior of composite materials on the microstructure or microscopic morphology [17]. The results may suggest a hint for explaining why sometimes there are some inconsistencies between the standard mixture formulae and corresponding experiments: typically, standard formulae are based on the Maxwell relation for a mixture of spheres and do not take into account any different shapes of the inclusions, which may be present in actual heterogeneous media.

3. Nonlinear Dispersions

In recent material science development, considerable attention has been devoted to electromagnetically nonlinear composite structures due to their applications, for instance, to integrated optical devices (such as optical switching and signal processing devices) [42-43]. More specifically, intrinsic optical bistability has been extensively studied theoretically as well as experimentally [44].

Many attempts have been made in order to take into account dielectric nonlinearity in the constitutive equations of the phases of a composite structure. A systematic perturbation expansion method was developed and employed to solve electrostatic and quasi-static boundary values problems of weakly nonlinear media [45]. The results have been verified by means of numerical simulation [46].

A lot of work has also been devoted to the analysis of the huge enhancing, caused by local field effects, of the effective cubic nonlinearity in random structures of poly-crystals [47-51]. Finally, the problems of second and third harmonic generation in random, dielectrically nonlinear composites have been tackled and fully general expressions for the equivalent second- and third-order hypersusceptibilities have been given in terms of the nonlinear behavior of the constituents [52,53].

Recent progress in this field can be ascribed to Goncharenko et al. [54], who dealt with dielectrically linear and nonlinear spheroidal inclusions of geometric factors probabilistically distributed. Then Lakhtakia and Mackay studied the size-dependent Bruggeman theory, which considers the effective particle dimension for non-dilute dispersions [55]. Furthermore, a wide survey of mixture theory applications has been made by Mackay [56], when he analyzed the peculiar properties exhibited by metamaterials. Important results concerning a dispersion of dielectrically nonlinear and graded parallel cylinders have been achieved by Wei and Wu [57].

In all of these cases, a linear medium has been considered containing spherical inclusions randomly located, or at most spheroidal inclusions having fixed orientation. In the following, we consider a dispersion of dielectrically nonlinear ellipsoidal particles randomly oriented in a linear matrix and we describe the results of a mathematical procedure able to perform the needed averages of the electric quantities over all orientations of the inclusions [58].

3.1. Single Nonlinear Ellipsoid

A nonlinear isotropic and homogenous ellipsoid can be described from the electrical point of view by the constitutive equation $\vec{D} = \varepsilon(E)\vec{E}$, where \vec{D} is the electric displacement inside the particle, \vec{E} is the electric field and the function ε depends only on the modulus E of \vec{E} .

We present a general solution to the problem of a nonlinear ellipsoidal particle embedded in a linear material. The theory is based on the following result derived for the linear case, which describes the behavior of one electrically linear ellipsoidal particle of permittivity ε_2 in a linear homogeneous medium of permittivity ε_1 . As before, let the axes of the ellipsoid be a_x , a_y and a_z (aligned with axes x, y, z of ellipsoid reference frame) and let a uniform electric field $\vec{E}_0 = (E_{0x}, E_{0y}, E_{0z})$ be applied to the structure. As above discussed, the electric field $\vec{E}_s = (E_{sx}, E_{sy}, E_{sz})$ inside the ellipsoid is uniform and it can be expressed as follows

$$E_{si} = \frac{E_{0i}}{1 + L_i (\varepsilon_2 / \varepsilon_1 - 1)}$$
(3.1)

The main result follows: the electric field inside the inclusion is uniform even in the nonlinear case and it may be calculated by means of the following system of equations [58]

$$E_{si} = \frac{E_{0i}}{1 + L_i [\varepsilon(E_s)/\varepsilon_1 - 1]}$$
(3.2)

If a solution of (3.2) exists, due to self-consistency, all the boundary conditions are fulfilled and the problem is completely analogous to its linear counterpart, provided that $\varepsilon_2 = \varepsilon(E_s)$.

3.2. Population of Nonlinear Dielectric Ellipsoids

The aim of this section is to extend the results, holding for a single inclusion, to a mixture of randomly oriented nonlinear ellipsoids in a linear homogeneous matrix. The permittivity of the inclusions is described by the isotropic nonlinear relation $\varepsilon(E) = \varepsilon_2 + \alpha E^2$ and the linear matrix has permittivity ε_1 . The Kerr nonlinearity is termed *focusing* or *defocusing* according to the fact that $\alpha > 0$ or $\alpha < 0$, respectively [59]. The overall permittivity function of the dispersion is expected to be isotropic because of the random orientation of the particles and therefore it can be expanded in series with respect to the field modulus $\varepsilon(E) = \varepsilon_{eff} + \beta E^2 + \delta E^4 + ...$, where the coefficients ε_{eff} , β , and δ depend on various parameters of the mixture such as the eccentricities of the ellipsoids, the volume fraction *c* of the included phase, the permittivities ε_1 , ε_2 and α . The homogenization procedure should provide the coefficients α and β of the first nonlinear term of the expanded constitutive equations for inclusions and mixture, respectively, are often called hyper-susceptibilities.

The result is derived under the assumption of Kerr-like constitutive equation of the composite medium that is of the form $\varepsilon(E) = \varepsilon_{eff} + \beta E^2$, which neglects higher order terms.

To begin the analysis, we substitute $\varepsilon(E) = \varepsilon_2 + \alpha E^2$ holding for a single ellipsoid, in Eq. (3.2) describing the internal field

$$E_{si} = \frac{\varepsilon_1 E_{0i}}{\varepsilon_1 + L_i \left[\varepsilon_2 - \varepsilon_1 + \alpha \left(E_{sx}^2 + E_{sy}^2 + E_{sz}^2 \right) \right]}$$
(3.3)

This is an algebraic system of degree nine with three unknowns, namely E_{sx} , E_{sy} , and E_{sz} . It might be hard, if not impossible, to be solved analytically, but we are interested, for our purposes, in just the first terms of a series expansion for the solution. To obtain it, we may adopt the *ansatz* $E_{si} = \lambda_i E_{0i} + \mu_i E_{0i}^3$ and solve for λ_i and μ_i . For sake of brevity, we omit here the simple but long calculation, which leads to the solution [58]

$$\vec{E}_{s} = \sum_{i} \left[\frac{\varepsilon_{1} \vec{E}_{0} \cdot \hat{n}_{i}}{b_{i}} - \frac{\alpha \varepsilon_{1}^{3} L_{i} \vec{E}_{0} \cdot \hat{n}_{i}}{b_{i}^{2}} \sum_{j} \frac{\left(\vec{E}_{0} \cdot \hat{n}_{j}\right)^{2}}{b_{j}^{2}} \right] \hat{n}_{i}$$
(3.4)

where $b_i = (1 - L_i)\varepsilon_1 + L_i\varepsilon_2$. We observe that the first term represents the classical Lorentz field appearing in a dielectrically linear ellipsoidal inclusion. The second term is the first nonlinear contribution, which is directly proportional to the inclusion hyper-susceptibility α (from now on we will omit the additional higher order terms). The principal directions of each ellipsoid in space are referred to as \hat{n}_x , \hat{n}_y and \hat{n}_z , and they correspond to the axes a_x , a_y and a_z of the ellipsoid.

We shall now average it over all the possible orientations of the particle. The result of the process is the following [58]

$$\left\langle \vec{E}_{s} \right\rangle = \vec{E}_{0} \left(\varepsilon_{1} M - \alpha \varepsilon_{1}^{3} E_{0}^{2} N \right)$$
 (3.5)

where M and N depend on the linear term of the permittivities and on the geometry of the inclusions

$$M = \frac{1}{3} \sum_{i=1,2,3} \frac{1}{b_i} \qquad N = \frac{1}{15} \left[\sum_{i=1,2,3} \sum_{j=1,2,3} \frac{L_i}{b_i^2 b_j^2} + 2 \sum_{i=1,2,3} \frac{L_i}{b_i^4} \right]$$
(3.6)

We note that the average field inside the particle is aligned with the external field and thus the average behavior of the inclusion is isotropic.

If we now consider a mixture with a volume fraction c << l of randomly oriented, dielectrically nonlinear, ellipsoids embedded in a homogeneous matrix with permittivity ε_l ,

we can evaluate a different kind of average, the one of the electric field over all of the space occupied by the mixture. It can be done via the following relationship

$$\left\langle \vec{E} \right\rangle = c \left\langle \vec{E}_s \right\rangle + (1 - c) \vec{E}_0$$
(3.7)

This means that we do not take into account the interactions among the inclusions because of the very low concentration: each ellipsoid behaves as an isolated one.

To evaluate the equivalent constitutive equation, we compute the average value of the displacement vector inside the random material [58]

$$\left\langle \vec{D} \right\rangle = \varepsilon_1 \left\langle \vec{E} \right\rangle + c \varepsilon_1 (\varepsilon_2 - \varepsilon_1) M \vec{E}_0 + c \alpha \varepsilon_1^4 P E_0^2 \vec{E}_0$$
(3.8)

where P is defined as:

$$P = \frac{1}{15} \left[\sum_{i=1,2,3} \sum_{j=1,2,3} \frac{1}{b_i^2 b_j^2} + 2 \sum_{i=1,2,3} \frac{1}{b_i^4} \right]$$
(3.9)

From Eqs. (3.5), (3.7), and (3.8) it follows that all the averaged vector quantities are aligned with \vec{E}_0 , therefore, we can continue our computations with scalar quantities; moreover, from now on, we will leave out the average symbols $\langle \cdot \rangle$. Eqs. (3.5), (3.7), and (3.8) may then be rewritten as

$$\begin{cases} E_s = \varepsilon_1 M E_0 - \alpha \varepsilon_1^3 E_0^3 N \\ E = c E_s + (1 - c) E_0 \\ D = \varepsilon_1 E + c \varepsilon_1 (\varepsilon_2 - \varepsilon_1) M E_0 + c \alpha \varepsilon_1^4 P E_0^3 \end{cases}$$
(3.10)

These are the main equations describing the overall mixture behavior. By solving system (3.10), we search for a relation between D and E: after straightforward calculations, the nonlinear constitutive equation for the composite medium has found in the form $\vec{D} = \varepsilon(E)\vec{E} = (\varepsilon_{eff} + \beta E^2)\vec{E}$, where [58]

$$\varepsilon_{eff} = \varepsilon_1 + \frac{c\varepsilon_1(\varepsilon_2 - \varepsilon_1)M}{(1 - c + c\varepsilon_1 M)} = \varepsilon_1 \frac{1 - c + c\varepsilon_2 M}{1 - c + c\varepsilon_1 M}$$
(3.11)

$$\frac{\beta}{\alpha} = c\varepsilon_1^4 \frac{P + c[(\varepsilon_2 - \varepsilon_1)MN + P(\varepsilon_1M - 1)]}{(1 - c + c\varepsilon_1M)^4}$$
(3.12)

The already mentioned quantities M, N and P, depend only on geometrical factors (ellipsoid eccentricities) and on the linear terms of the permittivities.

Eq. (3.11), giving the linear approximation for the permittivity, coincides with the Maxwell-Garnett formula for a dispersion of ellipsoids, Eq. (2.18). Moreover, Eq. (3.12) represents the mixture to inclusion hyper-susceptibility ratio.



Figure 4. Plots of the surfaces $\varepsilon_{eq} / \varepsilon_l$ and β / α versus the eccentricities which define the shape of the particles with $\varepsilon_l = 1$, $\varepsilon_2 = 10$ and c = 1/5.

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Figure 5. The same plots of Figure 4 with the assumptions $\varepsilon_1=10$, $\varepsilon_2=1$ and c=1/5. The amplification of the hyper-susceptibility assumes the greatest values when $\varepsilon_1 > \varepsilon_2$ and we are dealing with elliptic lamellae.

The methodology was applied to examine the actual effects of particle nonsphericity on mixtures. In Fig. 4 and 5 we show plots of the properties of the overall mixture as a function of the eccentricities of the ellipsoids composing the mixture itself. In Fig. 4 one can see the plots of the quantities $\varepsilon_{eff}/\varepsilon_l$ and β/α versus the aspect ratios $0 < e = a_x/a_y < 1$ and $0 < g = a_y/a_z < 1$ defining the shape of the particles, derived from Eqs. (3.11) and (3.12) with $\varepsilon_l=1$, $\varepsilon_2=10$ and c=1/5. In Fig. 5 the same plots are derived with the following parameter values: $\varepsilon_l=10$, $\varepsilon_2=1$ and c=1/5. In both cases we may observe that the amplification of the hypersusceptibility assumes the greatest values when dealing with planar nonlinear particles

(elliptic lamellae). More surprisingly, hyper-susceptibility ratio tends to assume its highest values (greater than 50) when $\varepsilon_l > \varepsilon_2$.

If we use the depolarization factors for spherical objects $(L_x=L_y=L_z=1/3)$ we obtain the simplified expression

$$\varepsilon(E) = \overbrace{\varepsilon_1 \frac{2\varepsilon_1 + \varepsilon_2 - 2c(\varepsilon_1 - \varepsilon_2)}{2\varepsilon_1 + \varepsilon_2 + c(\varepsilon_1 - \varepsilon_2)}}^{\mathcal{E}_{eff}} + \frac{\beta E^2}{\left[\frac{81c\varepsilon_1^4 \alpha E^2}{2\varepsilon_1 + \varepsilon_2 + c(\varepsilon_1 - \varepsilon_2)}\right]^4}$$
(3.13)

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which corresponds to the following hyper-susceptibility ratio, already derived in recent literature by Stroud et al. [44]

$$\frac{\beta}{\alpha} = \frac{81c\varepsilon_1^4}{\left[2\varepsilon_1 + \varepsilon_2 + c(\varepsilon_1 - \varepsilon_2)\right]^4} = c\left(\frac{\varepsilon_{eff} + 2\varepsilon_1}{\varepsilon_2 + 2\varepsilon_1}\right)^4$$
(3.14)

4. Eigenfield and Inclusion in Electrostatics: Applications to Anisotropic Composite Materials

One of the most important preliminary issues in the homogenization theory for composite materials is the knowledge of the behavior of a single particle embedded in a given matrix. Once this problem is solved, the homogenization procedure continues by means of some ad hoc averaging of the electrical quantities over the whole region occupied by the heterogeneous material [1,2]. Typically, when an averaging process is chosen it generates a particular effective mean field theory [3]. The problem of a single particle, formulated for isotropic ellipsoidal particles embedded in isotropic environment, is well known and largely spread in the applications. The aim of the present section is to introduce a methodology to cope with the completely anisotropic problem and to illustrate the relative outcomes. In particular we have found explicit expressions for the electric field both inside and outside the ellipsoidal particle. We have followed an approach that is widely utilized in similar problems within the elasticity theory. The problem of an inhomogeneity in heterogeneous elastic materials has been completely solved by Eshelby in the case of isotropic environment by means of a very elegant mathematical procedure [60,61]. In this section we follow that line of thought but we apply it to anisotropic dielectric composite systems. The complete development of the Eshelby theory for the elasticity theory can be found in Ref. [62], where all the details are deeply analyzed. As above described for the dielectric case, also for elastic materials the knowledge of the behavior of a single inhomogeneity has opened the way to the characterization of the composite elastic materials from the mechanical point of view (microand nano-mechanics) [63-65]. Anyway, we do not use any results of the elastic Eshelby theory and we present all the detailed proofs within the electrostatic theory: so, the development remains self-contained. Nevertheless, it is interesting to remark the strong analogy between electrostatics and elastostatics: in Tab. 1 we draw a comparison among all the corresponding elastic and electric quantities for the reader interested in such a similarity. The electric equations are written in absence of free charges and the elastostatic relations are written in absence of external forces: the analogy holds on when all the sources are absent or remotely applied. For brevity, we do not discuss here the meaning of all the elastic quantities, which are explained in standard elasticity textbooks [66].

Electric quantities			Elastic quantities		
Electric field	E _i	$E_i = -\frac{\partial V}{\partial x_i}$	Elastic strain	$\mathcal{E}_{s,ij}$	$\varepsilon_{s,ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$
Electric potential	V		Elastic displacement	<i>u</i> _i	
Electric displacement	D_i		Stress tensor	T _{ij}	
Maxwell equation	$\frac{\partial D_i}{\partial x_i} = 0$		Balance of forces	$\frac{\partial T_{ij}}{\partial x_i} = 0$	
Permittivity tensor	\mathcal{E}_{ij}		Stiffness tensor	C_{ijkh}	
Constitutive equation	$D_i = \varepsilon_{ij} E_j$		Constitutive equation	$T_{ij} = C_{ijkh} \varepsilon_{s,kh}$	

 Table 1. Comparison among the most important quantities and basic equations of the electrostatics and the elasticity theory.

This analysis of anisotropic systems has immediate application to the field of the liquid crystals. In fact, our hypotheses on the microstructure describe a material positionally disordered, but orientationally ordered, which corresponds to a nematic phase in liquid crystals [67,68]. The level of ordering is reflected in the macroscopic properties. For example, from an optical point of view, we may observe that the optical axes are given by the directions of orientation of the single crystals.

In this context we remember the important results concerning the internal electric field of anisotropic and bianisotropic spheres [69] and the corresponding effective medium theories in random anisotropic media [70,71].

4.1. Green Function for Anisotropic Media

An important preliminary issue for the following purposes is the determination of the electric Green function for an anisotropic environment. Therefore, we have to solve the basilar

equation of the electrostatics, as described in Tab. 1, with an impulsive source corresponding to a charged point Q. It means that we have to solve the following differential problem

$$\vec{\nabla} \cdot \left[\vec{\varepsilon} \, \vec{\nabla} \, V(\vec{r}) \right] = -Q \,\delta(\vec{r}) \quad \text{or} \quad \varepsilon_{kl} \, \frac{\partial}{\partial x_k} \frac{\partial}{\partial x_l} V(\vec{r}) = -Q \,\delta(\vec{r}) \tag{4.1}$$

with an arbitrary permittivity tensor $\vec{\mathcal{E}}$ having elements \mathcal{E}_{kl} . This problem can be straightforwardly solved by means of the three-dimensional Fourier transform, which converts the vector $\vec{\mathcal{r}}$ to the vector $\vec{\Omega}$. As well known, the differential operators must be transformed via the rule $\partial/\partial x_k \rightarrow i\Omega_k$, simply obtaining this result for the electrical potential in the transformed domain

$$\widetilde{V}\left(\vec{\Omega}\right) = \frac{Q}{\varepsilon_{kl}\Omega_k\Omega_l} = \frac{Q}{\vec{\Omega}^T \vec{\varepsilon} \,\vec{\Omega}}$$
(4.2)

It is worth saying that any kind of anisotropy can be modeled through the procedure here presented, including uniaxial, biaxial and also gyrotropic media, in which the permittivity tensor contains an antisymmetric part. However, in the following, we consider a symmetric permittivity tensor in order to exploit diagonalization by means of a suitable orthogonal matrix \vec{R} ; this is done for sake of simplicity in the exposition and it does not restrict the generality of the presented approach. Therefore, we may assume the diagonalization $\vec{\varepsilon} = \vec{R}^T \vec{\Delta} \vec{R}$ where $\vec{\Delta}$ is a diagonal matrix with the principal permittivities of the medium (positive numbers). The electric potential can be written in the original spatial domain as follows

$$V(\vec{r}) = \frac{1}{(2\pi)^3} \int_{\Re^3} \widetilde{V}(\vec{\Omega}) \exp(i\vec{\Omega}^T \vec{r}) d\vec{\Omega} = \frac{Q}{(2\pi)^3} \int_{\Re^3} \frac{\exp(i\vec{\Omega}^T \vec{r}) d\vec{\Omega}}{\left(\sqrt{\vec{\Delta}}\vec{R}\vec{\Omega}\right)^T \left(\sqrt{\vec{\Delta}}\vec{R}\vec{\Omega}\right)}$$
(4.3)

Here $\sqrt{\Delta}$ represents the diagonal matrix with the three square roots of the principal permittivities. The last integral can be handled with the substitution $\vec{y} = \sqrt{\Delta}\vec{R}\vec{\Omega}$, which leads to the differential relation $d\vec{y} = \sqrt{\det}\vec{\Delta}d\vec{\Omega} = \sqrt{\det}\vec{\varepsilon}d\vec{\Omega}$ (det $\vec{\Delta} = \det\vec{\varepsilon}$ since $\vec{\Delta}$ and $\vec{\varepsilon}$ are equivalent matrices). Thus, we have

$$V(\vec{r}) = \frac{Q}{(2\pi)^3 \sqrt{\det \vec{\varepsilon}}} \int_{\Re^3} \frac{\exp\left(i\vec{r}\,^T \vec{R}^T \sqrt{\vec{\Delta}}^{-1} \vec{y}\right) d\vec{y}}{(\vec{y})^T (\vec{y})}$$
(4.4)

Now, we may remember the well-known transform couple $1/\|\vec{r}\| \to 4\pi/\|\vec{\Omega}\|^2$ (the norm symbol $\|\vec{v}\|$ means $\sqrt{\vec{v}^T \vec{v}}$, as usual), which helps us to solve the integral in Eq. (4.4) as follows

$$V(\vec{r}) = \frac{Q}{4\pi\sqrt{\det\vec{\varepsilon}}} \frac{1}{\left\|\sqrt{\vec{\Delta}}^{-1}\vec{R}\vec{r}\right\|} = \frac{Q}{4\pi\sqrt{\det\vec{\varepsilon}}\left[\vec{r}^{T}\vec{\varepsilon}^{-1}\vec{r}\right]}$$
(4.5)

We have described a complete proof for sake of completeness and because the Green function is the fundamental starting point for this section; Eq. (4.5) can be also verified with other methods, as reported e.g. in [39].

All the electrostatic results concerning a generic potential $V_{TOT}(\vec{r})$ in an anisotropic environment can be obtained with a convolution integral between the above Green function and the total effective spatial charge distribution $\rho_{TOT}(\vec{r})$

$$V_{TOT}(\vec{r}) = \frac{1}{4\pi\sqrt{\det\vec{\varepsilon}}} \int_{\Re^3} \frac{\rho_{TOT}(\vec{x})d\vec{x}}{\sqrt{(\vec{r}-\vec{x})^T \vec{\varepsilon}^{-1}(\vec{r}-\vec{x})}}$$
(4.6)

This is true because of the linearity and of the space invariant property of the original partial differential equation analyzed.

4.2. Eigenfield and Inclusion Concepts

We define a certain region of the space as an *inclusion* when the constitutive equation, in that zone, assumes the form $\vec{D} = \vec{\varepsilon} (\vec{E} - \vec{E}^*)$ where $\vec{E}^* (\vec{r})$ is an assigned vector function of the position \vec{r} , which is named *eigenfield*. We remark that the concept of inclusion is determined by the presence of a given eigenfield, which modifies the constitutive equation as above discussed, but it is not connected with the permittivity tensor $ec{\mathcal{E}}$, which remains homogeneous in the entire space. In this section, in order to indicate spatial variations of the permittivity tensor, we adopt the term inhomogeneity (see next paragraphs). The eigenfield, defined in some region of the space, acts as a sort of source of electric field and its effects can be studied as follows. If the free charge distribution is absent in this region we may use the equation $\vec{\nabla} \cdot \vec{D} = 0$ obtaining $\vec{\nabla} \cdot \left[\vec{\varepsilon} \left(\vec{E} - \vec{E}^* \right) \right] = 0$ or, equivalently, Gauss $\vec{\nabla} \cdot \left[\vec{\varepsilon} \vec{E} \right] = \vec{\nabla} \cdot \left[\vec{\varepsilon} \vec{E}^* \right]$. Now, we can introduce the electric potential in the standard way, by writing the relation $\vec{\nabla} \cdot \left[\vec{\varepsilon} \vec{\nabla} V(\vec{r}) \right] = -\vec{\nabla} \cdot \left[\vec{\varepsilon} \vec{E}^* \right]$ or, similarly, the generalized Poisson equation $\vec{\nabla} \cdot \left[\vec{\varepsilon} \vec{\nabla} V(\vec{r}) \right] = -\rho^*$ where $\rho^* = \vec{\nabla} \cdot \left[\vec{\varepsilon} \vec{E}^* \right]$ is the charge distribution equivalent to the eigenfield. In this context the introduction of the concepts of eigenfield and inclusion has not a given direct physical meaning but it is a physical-mathematical expedient very useful to solve some problems in the electrostatics of the inhomogeneities, as we will show later on. So, we want to analyze the effects of the presence of a given inclusion (described by its eigenfield) on the electrical quantities. To begin, we suppose that the eigenfield is defined in the whole three-dimensional space and, therefore, we may solve the generalized Poisson equation by means of the Green function introduced in the previous paragraph

$$V_{TOT}(\vec{r}) = \frac{1}{4\pi\sqrt{\det\vec{\varepsilon}}} \int_{\Re^3} \frac{\vec{\nabla} \cdot \left[\vec{\varepsilon}\vec{E}^*(\vec{x})\right] d\vec{x}}{\sqrt{(\vec{r}-\vec{x})^T \vec{\varepsilon}^{-1}(\vec{r}-\vec{x})}} = \frac{1}{4\pi\sqrt{\det\vec{\varepsilon}}} \int_{\Re^3} \frac{\frac{\partial}{\partial x_l} \left[\varepsilon_{lk} E_k^*(\vec{x})\right] d\vec{x}}{\sqrt{(\vec{r}-\vec{x})^T \vec{\varepsilon}^{-1}(\vec{r}-\vec{x})}}$$
(4.7)

Now, we can use a sort of integration by part, holding on for multiple integrals, which can be written, in its general formulation, as follows

$$\int_{\Re^3} \mathcal{G}(\vec{x}) \frac{\partial \lambda(\vec{x})}{\partial x_l} d\vec{x} = -\int_{\Re^3} \lambda(\vec{x}) \frac{\partial \mathcal{G}(\vec{x})}{\partial x_l} d\vec{x}$$
(4.8)

where $\vartheta(\vec{x})$ and $\lambda(\vec{x})$ are two given functions with sufficiently regular behavior at infinity (such a property can be simply derived by the divergence Gauss theorem). The application of this relation to Eq. (4.7) leads to

$$V_{TOT}(\vec{r}) = -\frac{1}{4\pi\sqrt{\det\vec{\varepsilon}}} \int_{\Re^3} \varepsilon_{lk} E_k^{*}(\vec{x}) \frac{\partial}{\partial x_l} \left(\frac{1}{\sqrt{(\vec{r}-\vec{x})^T \vec{\varepsilon}^{-1}(\vec{r}-\vec{x})}} \right) d\vec{x}$$
(4.9)

Moreover, it easy to recognize the validity of the expression

$$\frac{\partial}{\partial x_l} \frac{1}{\sqrt{\left(\vec{r} - \vec{x}\right)^T \vec{\varepsilon}^{-1} \left(\vec{r} - \vec{x}\right)}} = -\frac{\partial}{\partial r_l} \frac{1}{\sqrt{\left(\vec{r} - \vec{x}\right)^T \vec{\varepsilon}^{-1} \left(\vec{r} - \vec{x}\right)}}$$
(4.10)

and therefore we can put Eq. (4.9) in the following final form

$$V_{TOT}(\vec{r}) = \frac{1}{4\pi\sqrt{\det\vec{\varepsilon}}} \int_{\Re^3} \varepsilon_{lk} E_k^{*}(\vec{x}) \frac{\partial}{\partial r_l} \left(\frac{1}{\sqrt{(\vec{r}-\vec{x})^T \vec{\varepsilon}^{-1}(\vec{r}-\vec{x})}} \right) d\vec{x}$$
(4.11)

If the eigenfield $E_k^*(\vec{x})$ is constant in a limited region V of the space we can say that we are dealing with a *uniform* or *homogeneous inclusion* V and the relative electric potential over the entire space become

$$V_{TOT}(\vec{r}) = \frac{1}{4\pi\sqrt{\det\vec{\varepsilon}}} \varepsilon_{lk} E_k^* \frac{\partial}{\partial r_l} \int_V \frac{d\vec{x}}{\sqrt{(\vec{r}-\vec{x})^T} \vec{\varepsilon}^{-1}(\vec{r}-\vec{x})}$$
(4.12)

We define the *anisotropic harmonic potential* of an arbitrary region V as

$$\psi_V(\vec{r}) = \int_V \frac{d\vec{x}}{\sqrt{(\vec{r} - \vec{x})^T \vec{\varepsilon}^{-1} (\vec{r} - \vec{x})}}$$
(4.13)

So, Eq. (4.12) can be written as

$$V_{TOT}(\vec{r}) = \frac{1}{4\pi\sqrt{\det\vec{\varepsilon}}} \varepsilon_{lk} E_k^* \frac{\partial\psi_V(\vec{r})}{\partial r_l}$$
(4.14)

Moreover, we define the *isotropic harmonic potential* of a region Ω as

$$\Phi_{\Omega}\left(\vec{q}\right) = \int_{\Omega} \frac{d\,\vec{y}}{\sqrt{\left(\vec{q} - \vec{y}\right)^{T} \left(\vec{q} - \vec{y}\right)}} \tag{4.15}$$

In electrostatics and more generally in physics and mathematics many useful properties are well known for the isotropic harmonic potential: in order to utilize these properties in our context, it could be interesting to obtain a relation between the anisotropic and the isotropic potentials defined in Eqs. (4.13) and (4.15) respectively. To this aim, we undertake the following reasoning starting from Eq. (4.13) and recalling the diagonalization $\vec{\varepsilon} = \vec{R}^T \vec{\Delta} \vec{R}$ for the permittivity tensor

$$\psi_{V}(\vec{r}) = \int_{V} \frac{d\vec{x}}{\sqrt{(\vec{r} - \vec{x})^{T} \vec{R}^{T} \vec{\Delta}^{-1} \vec{R}(\vec{r} - \vec{x})}} = \int_{V} \frac{d\vec{x}}{\sqrt{\left[\vec{\Delta}^{-1/2} \vec{R}(\vec{r} - \vec{x})\right]^{T} \left[\vec{\Delta}^{-1/2} \vec{R}(\vec{r} - \vec{x})\right]}}$$
(4.16)

By using the substitution $\vec{y} = \vec{\Delta}^{-1/2} \vec{R} \vec{x}$, which leads to $d\vec{x} = \sqrt{\det \vec{\varepsilon} d \vec{y}}$, we obtain

$$\psi_V(\vec{r}) = \sqrt{\det \vec{\varepsilon}} \int_{\vec{\Delta}^{-1/2} \vec{R}V} \frac{d \vec{y}}{\left\|\vec{\Delta}^{-1/2} \vec{R} \vec{r} - \vec{y}\right\|} = \sqrt{\det \vec{\varepsilon}} \Phi_{\vec{\Delta}^{-1/2} \vec{R}V} \left(\vec{\Delta}^{-1/2} \vec{R} \vec{r}\right)$$
(4.17)

where the symbol $\vec{\Delta}^{-1/2} \vec{R} V$ represents the deformation of the volume *V* under the effect of the linear operator $\vec{\Delta}^{-1/2} \vec{R}$. A very simple property of the isotropic harmonic potential is the following

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$$\Phi_{\Omega}\left(\vec{R}\vec{q}\right) = \Phi_{\vec{R}^{T}\Omega}\left(\vec{q}\right) \tag{4.18}$$

holding on for any orthogonal rotation matrix \vec{R} . This property can be easily verified as follows

$$\Phi_{\Omega}\left(\vec{R}\vec{q}\right) = \int_{\Omega} \frac{d\vec{y}}{\left\|\vec{R}\vec{q} - \vec{y}\right\|} = \int_{\vec{R}^{T}\Omega} \frac{d\vec{v}}{\left\|\vec{R}\vec{q} - \vec{R}\vec{v}\right\|} = \int_{\vec{R}^{T}\Omega} \frac{d\vec{v}}{\left\|\vec{q} - \vec{v}\right\|} = \Phi_{\vec{R}^{T}\Omega}\left(\vec{q}\right)$$
(4.19)

where we have used the substitution $\vec{y} = \vec{R}\vec{v}$ which leads to $d\vec{y} = d\vec{v}$ since the determinant of a rotation matrix is unitary (we have also considered $\|\vec{R}\vec{q} - \vec{R}\vec{v}\| = \|\vec{q} - \vec{v}\|$: a rotation matrix does not alter the length of a vector). Now, we can apply the property given in Eq. (4.18) to Eq. (4.17) obtaining

$$\psi_{V}(\vec{r}) = \sqrt{\det \vec{\varepsilon}} \Phi_{\vec{\Delta}^{-1/2}\vec{R}V}\left(\vec{\Delta}^{-1/2}\vec{R}\vec{r}\right) = \sqrt{\det \vec{\varepsilon}} \Phi_{\vec{\Delta}^{-1/2}\vec{R}V}\left(\underline{\vec{R}}\vec{R}^{T}\vec{\Delta}^{-1/2}\vec{R}\vec{r}\right) = \sqrt{\det \vec{\varepsilon}} \Phi_{\vec{\lambda}^{-1/2}\vec{R}V}\left(\vec{R}^{T}\vec{\Delta}^{-1/2}\vec{R}\vec{r}\right) = \sqrt{\det \vec{\varepsilon}} \Phi_{\sqrt{\vec{\varepsilon}}^{-1}V}\left(\sqrt{\vec{\varepsilon}}^{-1}\vec{r}\right)$$

$$(4.20)$$

where we have used the diagonalization $\vec{\varepsilon} = \vec{R}^T \vec{\Delta} \vec{R}$ for the symmetric permittivity tensor. The operation $\sqrt{\vec{\varepsilon}}$ assumes a precise meaning by writing $\sqrt{\vec{\varepsilon}} = \vec{R}^T \sqrt{\vec{\Delta}} \vec{R}$ where $\sqrt{\vec{\Delta}}$ is simply the tensor with the square roots of the diagonal elements of $\vec{\Delta}$ (of the principal permittivities); in fact, the product $\sqrt{\vec{\varepsilon}} \sqrt{\vec{\varepsilon}}$ can be simply calculated obtaining, as result, the permittivity tensor $\vec{\varepsilon}$ itself. Similar considerations can be also applied to the square root of the inverse tensor $\vec{\varepsilon}^{-1}$, which can be written as $\sqrt{\vec{\varepsilon}}^{-1} = \vec{R}^T \sqrt{\vec{\Delta}}^{-1} \vec{R}$. However, Eq. (4.20) is the researched relationship between the anisotropic and the isotropic potentials.

Finally, by composing Eqs. (4.14) and (4.20), we obtain the following general relation for the electric potential generated, in the whole anisotropic space, by a uniform eigenfield

$$V_{TOT}(\vec{r}) = \frac{1}{4\pi} \varepsilon_{lk} E_k^* \frac{\partial}{\partial r_l} \Phi_{\sqrt{\vec{\varepsilon}}^{-1} V} \left(\sqrt{\vec{\varepsilon}}^{-1} \vec{r}\right)$$
(4.21)

written in terms of the isotropic harmonic potential defined in Eq. (4.15) (but related to the region $\sqrt{\vec{\varepsilon}}^{-1}V$ and calculated in the argument $\sqrt{\vec{\varepsilon}}^{-1}\vec{r}$).

4.3. Ellipsoidal Uniform Inclusion

We wish to specialize the result given in Eq. (4.21) for an inclusion with an ellipsoidal shape. So, we assume that the region V is described by

$$V: \sum_{i=1}^{3} \frac{r_i^2}{a_i^2} \le 1 \quad \text{or} \quad V: \ \vec{r}^T \vec{a}^{-2} \vec{r} \le 1$$
(4.22)

where a_1 , a_2 and a_3 are the semi-axes of the ellipsoid aligned with the reference frame and we have defined a diagonal matrix \vec{a} with the diagonal elements equal to a_1 , a_2 and a_3 . In order to develop the integral in Eq. (4.21) we may better characterize the region $\sqrt{\vec{\varepsilon}}^{-1}V$. If a point \vec{y} belongs to $\sqrt{\vec{\varepsilon}}^{-1}V$ we can write $\vec{y} = \sqrt{\vec{\varepsilon}}^{-1}\vec{r}$ where $\vec{r} \in V$; so, by considering the inverse relation $\vec{r} = \sqrt{\vec{\varepsilon}}\vec{y}$, and substituting it in Eq. (4.22), we obtain a useful description for the ellipsoidal set $\sqrt{\vec{\varepsilon}}^{-1}V$

$$\sqrt{\vec{\varepsilon}}^{-1}V : \quad \vec{y}^T \left(\sqrt{\vec{\varepsilon}}\,\vec{a}^{-2}\sqrt{\vec{\varepsilon}}\,\right) \vec{y} \le 1 \tag{4.23}$$

So, the region $\sqrt{\vec{\varepsilon}}^{-1}V$ is again ellipsoidal but the ellipsoid is not aligned to the axes of the reference frame and it is described by the tensor $\sqrt{\vec{\varepsilon}}\vec{a}^{-2}\sqrt{\vec{\varepsilon}}$. Therefore, it is not diagonal but symmetric and positive definite and always diagonalizable by means of suitable rotation matrix \vec{P}

$$\sqrt{\vec{\varepsilon}}\,\vec{a}^{-2}\sqrt{\vec{\varepsilon}} = \vec{P}^T \vec{b}^{-2} \vec{P} \tag{4.24}$$

where \vec{b} is a diagonal matrix containing the three semi-axis b_1 , b_2 and b_3 of the rotated ellipsoid $\sqrt{\vec{\varepsilon}}^{-1}V$; of course, these three values are the eigenvalues of the tensor $\sqrt{\vec{\varepsilon}}\vec{a}^{-2}\sqrt{\vec{\varepsilon}}$. Moreover, it is important to observe that the rotation matrix \vec{P} , which diagonalizes $\sqrt{\vec{\varepsilon}}\vec{a}^{-2}\sqrt{\vec{\varepsilon}}$, is different from the previously introduced rotation matrix \vec{R} , which instead diagonalizes the permittivity tensor $\vec{\varepsilon}$. Anyway, a point \vec{y} belongs to $\sqrt{\vec{\varepsilon}}^{-1}V$ if $\vec{y}^T (\vec{P}^T \vec{b}^{-2} \vec{P}) \vec{y} \le 1$ or, similarly, if $(\vec{P}\vec{y})^T \vec{b}^{-2} (\vec{P}\vec{y}) \le 1$; hence, we define a point $\vec{z} = \vec{P}\vec{y}$ belonging to the domain $V' = \vec{P}\sqrt{\vec{\varepsilon}}^{-1}V$. So, the point \vec{z} belongs to V' if and only if $\vec{z}^T \vec{b}^{-2} \vec{z} \le 1$. Therefore, since $V' = \vec{P}\sqrt{\vec{\varepsilon}}^{-1}V$, we can write $\sqrt{\vec{\varepsilon}}^{-1}V = \vec{P}^T V'$ where V' is the ellipsoid $\vec{z}^T \vec{b}^{-2} \vec{z} \le 1$ aligned with the reference frame under consideration. At the end of these considerations we may transform the isotropic potential appearing in Eq. (4.21) as follows

$$\Phi_{\sqrt{\vec{\varepsilon}}^{-1}V}\left(\sqrt{\vec{\varepsilon}}^{-1}\vec{r}\right) = \Phi_{\vec{p}^{T}V'}\left(\sqrt{\vec{\varepsilon}}^{-1}\vec{r}\right) = \Phi_{V'}\left(\vec{P}\sqrt{\vec{\varepsilon}}^{-1}\vec{r}\right)$$
(4.25)

In the second equality we have used the property given in Eq. (4.18) and described in the previous paragraph. Finally the electric potential generated, in the whole anisotropic space, by a uniform ellipsoidal eigenfield is given by

$$V_{TOT}(\vec{r}) = \frac{1}{4\pi} \varepsilon_{lk} E_k^* \frac{\partial}{\partial r_l} \Phi_{V'} \left(\vec{P} \sqrt{\vec{\varepsilon}}^{-1} \vec{r} \right)$$
(4.26)

We remember that \vec{P} and \vec{b} are defined by the diagonalization $\sqrt{\vec{\varepsilon}}\vec{a}^{-2}\sqrt{\vec{\varepsilon}} = \vec{P}^T\vec{b}^{-2}\vec{P}$ and the region V' is defined by all the points \vec{z} satisfying $\vec{z}^T\vec{b}^{-2}\vec{z} \leq 1$. The final result given in Eq. (4.26) is the most important result in order to write the electric potential $V_{TOT}(\vec{r})$ in closed form: in fact, now, the isotropic electric potential $\Phi_{V'}$ is written in terms of an ellipsoidal region aligned to the reference frame. In the following sections, we find out simple analytical expressions for the electric field both inside $(\vec{r} \in V)$ and outside $(\vec{r} \in \Re^3 \setminus V)$ the ellipsoidal inclusion.

4.4. Electric Field Inside the Inclusion

The aim of this section is to find an explicit expression for the electric field generated inside the inclusion in terms of the uniform eigenfield above defined. We need to develop Eq. (4.26) with a well-known important property of the isotropic harmonic potential, described below. The isotropic harmonic potential generated by a unitary density in a given volume V' is defined by

$$\Phi_{V'}(\vec{z}) = \int_{V'} \frac{d\,\vec{p}}{\|\vec{z} - \vec{p}\|}$$
(4.27)

where V' represents the region $\vec{z}^T \vec{b}^{-2} \vec{z} \le 1$ and it can be represented by means of the following integral [37,62]

$$\Phi_{V'}(\vec{z}) = \pi b_1 b_2 b_3 \int_0^{+\infty} \frac{1 - f(\vec{z}, s)}{R(s)} ds$$
(4.28)

Here the functions $f(\vec{z},s)$ and R(s) are defined as follows [37,62]

$$f(\vec{z},s) = \sum_{i=1}^{3} \frac{z_i^2}{b_i^2 + s}; \qquad R(s) = \sqrt{(b_1^2 + s)(b_2^2 + s)(b_3^2 + s)}$$
(4.29)

Such an integral representation can be utilized in Eq. (4.26) as follows

$$V_{TOT}(\vec{r}) = \frac{1}{4\pi} \varepsilon_{lk} E_k^* \frac{\partial}{\partial r_l} \left[\pi b_1 b_2 b_3 \int_0^{+\infty} \frac{1 - f(\vec{z}, s)}{R(s)} ds \right]_{\vec{z} = \vec{P} \sqrt{\vec{z}}^{-1} \vec{r}}$$
(4.30)

The electric field can be calculated differentiating the previous relation with respect to the position vector \vec{r} . In components we obtain

$$E_{j}(\vec{r}) = \frac{\varepsilon_{lk}E_{k}^{*}}{4}b_{1}b_{2}b_{3}\frac{\partial}{\partial r_{j}}\frac{\partial}{\partial r_{l}}\left[\int_{0}^{+\infty}\frac{f(\vec{z},s)}{R(s)}ds\right]_{\vec{z}=\vec{P}\sqrt{\vec{z}}^{-1}\vec{r}} =$$

$$= \frac{\varepsilon_{lk}E_{k}^{*}}{4}b_{1}b_{2}b_{3}\int_{0}^{+\infty}\sum_{i=1}^{3}\frac{1}{b_{i}^{2}+s}\left[\frac{\partial}{\partial r_{j}}\frac{\partial}{\partial r_{l}}\left(z_{i}^{2}\right)_{\vec{z}=\vec{P}\sqrt{\vec{z}}^{-1}\vec{r}}\right]\frac{ds}{R(s)}$$

$$(4.31)$$

The term in brackets can be developed in this way (the index *i* is not summed)

$$\frac{\partial}{\partial r_{j}} \frac{\partial}{\partial r_{l}} \left(z_{i}^{2}\right)_{\vec{z}=\vec{P}\sqrt{\vec{\varepsilon}}^{-1}\vec{r}} = \frac{\partial}{\partial r_{j}} \frac{\partial}{\partial r_{l}} \left[P_{iq} \left(\sqrt{\vec{\varepsilon}}^{-1}\right)_{qs} r_{s} \right] \left[P_{ip} \left(\sqrt{\vec{\varepsilon}}^{-1}\right)_{pr} r_{r} \right] = \\
= P_{iq} P_{ip} \left(\sqrt{\vec{\varepsilon}}^{-1}\right)_{qs} \left(\sqrt{\vec{\varepsilon}}^{-1}\right)_{pr} \left(\delta_{jr} \delta_{ls} + \delta_{rl} \delta_{js}\right) = \\
= P_{iq} P_{ip} \left(\sqrt{\vec{\varepsilon}}^{-1}\right)_{ql} \left(\sqrt{\vec{\varepsilon}}^{-1}\right)_{pj} + P_{iq} P_{ip} \left(\sqrt{\vec{\varepsilon}}^{-1}\right)_{ql} \left(\sqrt{\vec{\varepsilon}}^{-1}\right)_{pl} \left(\sqrt{\vec{\varepsilon}}^{-1}\right)_{pl} \right] \quad (4.32)$$

For convenience, we define the tensor \vec{F} , appearing in Eq. (4.31), as follows

$$F_{jl} = \sum_{i=1}^{3} \frac{1}{b_i^2 + s} \left[\frac{\partial}{\partial r_j} \frac{\partial}{\partial r_l} \left(z_i^2 \right)_{\vec{z} = \vec{P} \sqrt{\vec{z}}^{-1} \vec{r}} \right]$$
(4.33)

It can be easily handled in tensor notation

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$$\ddot{F} = 2\sqrt{\ddot{\varepsilon}}^{-1}\ddot{P}^{T}\left(\ddot{b}^{2} + s\ddot{I}\right)^{-1}\ddot{P}\sqrt{\ddot{\varepsilon}}^{-1} = 2\sqrt{\ddot{\varepsilon}}^{-1}\left(\ddot{P}^{T}\ddot{b}^{2}\ddot{P} + s\ddot{I}\right)^{-1}\sqrt{\ddot{\varepsilon}}^{-1}$$
(4.34)

Previously, we have stated that $\sqrt{\vec{\varepsilon}}\vec{a}^{-2}\sqrt{\vec{\varepsilon}} = \vec{P}^T\vec{b}^{-2}\vec{P}$ and, therefore, we also have $\sqrt{\vec{\varepsilon}}^{-1}\vec{a}^2\sqrt{\vec{\varepsilon}}^{-1} = \vec{P}^T\vec{b}^2\vec{P}$. This latter relation placed in Eq. (4.34) leads to the following simple expression

$$\vec{F} = 2\sqrt{\vec{\varepsilon}}^{-1} \left(\sqrt{\vec{\varepsilon}}^{-1} \vec{a}^2 \sqrt{\vec{\varepsilon}}^{-1} + s\vec{I}\right)^{-1} \sqrt{\vec{\varepsilon}}^{-1} = 2\left(\vec{a}^2 + s\vec{\varepsilon}\right)^{-1}$$
(4.35)

It is interesting to observe that, proceeding with the calculations, the auxiliary quantities \vec{P} and \vec{b} , defined in Eq. (4.24), gradually disappear, obtaining the final results only in terms of $\vec{\varepsilon}$ and \vec{a} , which are the quantities with a direct physical and geometrical meaning. Moreover, since the tensor \vec{F} does not depend on the position \vec{r} we have obtained an important achievement: the electric field generated inside the ellipsoidal inclusion is uniform. Returning to Eq. (4.31) for this electric field and recalling the definition given in Eq. (33), we obtain

$$E_{j} = \frac{\varepsilon_{lk} E_{k}^{*}}{4} b_{1} b_{2} b_{3} \int_{0}^{+\infty} F_{jl} \frac{ds}{R(s)}$$
(4.36)

or, in tensor notation

$$\vec{E} = \frac{1}{4} \int_{0}^{+\infty} \vec{F} \vec{\varepsilon} \frac{\det(\vec{b})}{R(s)} ds \vec{E}^{*} = \frac{1}{4} \int_{0}^{+\infty} 2(\vec{a}^{2} + s\vec{\varepsilon})^{-1} \vec{\varepsilon} \frac{\det(\vec{b})}{R(s)} ds \vec{E}^{*}$$
(4.37)

From the above-discussed relation $\sqrt{\vec{\varepsilon}}^{-1}\vec{a}^2\sqrt{\vec{\varepsilon}}^{-1} = \vec{P}^T\vec{b}^2\vec{P}$ we easily obtain $\vec{P}\sqrt{\vec{\varepsilon}}^{-1}\vec{a}^2\sqrt{\vec{\varepsilon}}^{-1}\vec{P}^T = \vec{b}^2$ and consequently the term $\det(\vec{b})/R(s)$ can be further expanded as

$$\frac{\det(\vec{b})}{R(s)} = \frac{\sqrt{\det(\vec{b}^2)}}{\sqrt{\det(\vec{b}^2 + s\vec{I})}} = \frac{\sqrt{\det(\vec{P}\sqrt{\vec{\varepsilon}}^{-1}\vec{a}^2\sqrt{\vec{\varepsilon}}^{-1}\vec{P}^T)}}{\sqrt{\det(\vec{P}\sqrt{\vec{\varepsilon}}^{-1}\vec{a}^2\sqrt{\vec{\varepsilon}}^{-1}\vec{P}^T + s\vec{I})}} = \frac{\det(\vec{a})}{\sqrt{\det(\vec{a}^2 + s\vec{\varepsilon})}} \quad (4.38)$$

where we have repeatedly utilized the Binet theorem for the product of two determinants (which can be stated in the form $\det(\vec{a})\det(\vec{b}) = \det(\vec{a}\vec{b})$ for two arbitrary tensors \vec{a} and \vec{b}). The final result, derived from Eqs. (4.37) and (4.38), is

$$\vec{E} = \left\{ \frac{\det(\vec{a})}{2} \int_{0}^{+\infty} \frac{\left(\vec{a}^{2} + s\vec{\varepsilon}\right)^{-1}\vec{\varepsilon}}{\sqrt{\det(\vec{a}^{2} + s\vec{\varepsilon})}} ds \right\} \vec{E}^{*}$$
(4.39)

We have find the uniform electric field \vec{E} generated inside a uniform ellipsoidal inclusion (\vec{a}) in an anisotropic environment ($\vec{\varepsilon}$) in terms of the eigenfield \vec{E}^* .

4.5. Electric Field Outside the Inclusion

The aim of this section is to find an explicit expression for the electric field generated outside the inclusion in terms of the uniform eigenfield. Again, we need to develop Eq. (4.26) with another important property of the isotropic harmonic potential. It is defined in Eq. (4.27) and it can be represented by means of the following integral, in the region outside V'[37,62]

$$\Phi_{V'}(\vec{z}) = \pi b_1 b_2 b_3 \int_{\eta(\vec{z})}^{+\infty} \frac{1 - f(\vec{z}, s)}{R(s)} ds$$
(4.40)

where the functions $f(\vec{z},s)$ and R(s) are defined in Eq. (4.29) and the quantity $\eta(\vec{z})$ satisfies the relation $f(\vec{z},\eta(\vec{z})) = 1$ [37,62]. The resulting electric field for $\vec{r} \in \Re^3 \setminus V$ is given by (see Eq. (4.26))

$$E_{j}(\vec{r}) = -\frac{\varepsilon_{lk}E_{k}}{4\pi} \frac{\partial}{\partial r_{j}} \frac{\partial}{\partial r_{l}} \left[\Phi_{V'}(\vec{z})\right]_{\vec{z}=\vec{P}\sqrt{\vec{z}}}$$
(4.41)

The substitution $\vec{z} = \vec{P}\sqrt{\vec{\varepsilon}}^{-1}\vec{r}$ immediately leads to the formula

$$\frac{\partial}{\partial r_{j}}\frac{\partial}{\partial r_{l}}\left[\Phi_{V'}(\vec{z})\right]_{\vec{z}=\vec{P}\sqrt{\vec{z}}^{-1}\vec{r}} = \left(\sqrt{\vec{z}}^{-1}\right)_{jq}P^{T}_{qs}\frac{\partial^{2}\Phi_{V'}(\vec{z})}{\partial z_{s}\partial z_{i}}P_{in}\left(\sqrt{\vec{z}}^{-1}\right)_{nl}$$
(4.42)

Now, for differentiating the harmonic potential $\Phi_{V'}(\vec{z})$ with respect to z_s and z_i we may use the generalized Leibnitz rule because the argument \vec{z} appears both in the lower limit and in the integrand of Eq. (40). The result is

$$\frac{\partial^2 \Phi_{V'}(\vec{z})}{\partial z_s \partial z_i} = \pi b_1 b_2 b_3 \left[\frac{\partial f(\vec{z},\eta)}{\partial z_i} \frac{1}{R(\eta)} \frac{\partial \eta(\vec{z})}{\partial z_s} - \int_{\eta(\vec{z})}^{+\infty} \frac{\partial^2 f(\vec{z},s)}{\partial z_s \partial z_i} \frac{ds}{R(s)} \right]$$
(4.43)

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The derivative $\partial \eta(\vec{z})/\partial z_s$ can be calculated by recalling the definition of the function $\eta(\vec{z})$ (which satisfies the relation $f(\vec{z},\eta(\vec{z}))=1$) and by using the Dini theorem for differentiating the implicit functions. So, from $f(\vec{z},\eta(\vec{z}))=1$ and from the definition of the function f given in Eq. (4.29), we obtain

$$\frac{\partial f}{\partial z_s} + \frac{\partial f}{\partial \eta} \frac{\partial \eta}{\partial z_s} = 0 \quad \Rightarrow \quad \frac{\partial \eta}{\partial z_s} = -\frac{\frac{\partial f}{\partial z_s}}{\frac{\partial f}{\partial \eta}} = 2 \frac{z_s}{b_s^2 + \eta} \left(\sum_{k=1}^3 \frac{z_k^2}{\left(b_k^2 + \eta\right)^2} \right)^{-1}$$
(4.44)

These derivatives are also useful to simplify Eq. (4.43)

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$$\frac{\partial f}{\partial z_i} = 2 \frac{z_i}{b_i^2 + s} \implies \frac{\partial^2 f}{\partial z_s \partial z_i} = \frac{2\delta_{si}}{b_i^2 + s}$$
(4.45)

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Summing up, we may use Eqs. (4.44) and (4.45) in Eq. (4.43), we insert Eq. (4.43) in Eq. (4.42) and we obtain an expanded version of Eq. (4.41) for the external electric field

$$E_{j}(\vec{r}) = \frac{b_{l}b_{2}b_{3}}{2}\sqrt{\vec{\varepsilon}}^{-1}{}_{jq}P^{T}{}_{qs}\left[\frac{-2z_{s}z_{i}}{R(\eta)(b_{s}^{2}+\eta)(b_{i}^{2}+\eta)}\frac{1}{\sum_{k=1}^{3}\frac{z_{k}^{2}}{(b_{k}^{2}+\eta)^{2}}} + \int_{\eta(\vec{\varepsilon})}^{+\infty}\frac{\delta_{si}ds}{R(s)(b_{i}^{2}+s)}\right]P_{in}\sqrt{\vec{\varepsilon}}^{-1}{}_{nl}\varepsilon_{lk}E_{k}^{*}$$
(4.46)

where the bracket must be calculated for $\vec{z} = \vec{P}\sqrt{\vec{\varepsilon}}^{-1}\vec{r}$. As before, we wish to eliminate the auxiliary quantities \vec{P} and \vec{b} , defined in Eq. (4.24) obtaining the final result only in terms of $\vec{\varepsilon}$ and \vec{a} , which are the quantities with a direct meaning in our problem. We start from the definition of the quantity $\eta(\vec{z})$, which satisfies the relation $f(\vec{z},\eta(\vec{z}))=1$. Returning to the spatial variable \vec{r} , we have to obtain an implicit equation for $\eta\left(\vec{P}\sqrt{\vec{\varepsilon}}^{-1}\vec{r}\right)$; we may proceed in this way: the relation $f(\vec{z},\eta(\vec{z}))=1$ implies that $\vec{z}^T(\vec{b}^2 + \eta \vec{I})^{-1}\vec{z} = 1$ and then we obtain the sequence of expressions

$$\left(\vec{P}\sqrt{\vec{\varepsilon}}^{-1}\vec{r}\right)^{T} \left(\vec{b}^{2}+\eta\vec{I}\right)^{-1} \vec{P}\sqrt{\vec{\varepsilon}}^{-1}\vec{r}=1 \implies \vec{r}^{T}\sqrt{\vec{\varepsilon}}^{-1} \left(\vec{P}^{T}\vec{b}^{2}\vec{P}+\eta\vec{I}\right)^{-1}\sqrt{\vec{\varepsilon}}^{-1}\vec{r}=1 \implies \vec{r}^{T}\sqrt{\vec{\varepsilon}}^{-1} \left(\sqrt{\vec{\varepsilon}}^{-1}\vec{a}^{2}\sqrt{\vec{\varepsilon}}^{-1}+\eta\vec{I}\right)^{-1}\sqrt{\vec{\varepsilon}}^{-1}\vec{r}=1 \implies \vec{r}^{T} \left(\vec{a}^{2}+\eta\vec{\varepsilon}\right)^{-1}\vec{r}=1$$

$$(4.47)$$

Hence, the function η directly depends on the main tensors $\ddot{\varepsilon}$ and \ddot{a} , as expected. Now, we can begin the conversion of Eq. (4.46). The following term, which appears in Eq. (4.46), can be converted with these calculations

$$\sum_{k=1}^{3} \frac{z_{k}^{2}}{\left(b_{k}^{2} + \eta\right)^{2}} = \left[\left(\vec{P}\sqrt{\vec{\varepsilon}}^{-1}\vec{r}\right)^{T} \left(\vec{b}^{2} + \eta\vec{I}\right)^{-2} \vec{P}\sqrt{\vec{\varepsilon}}^{-1}\vec{r} = \vec{r}^{T}\sqrt{\vec{\varepsilon}}^{-1}\vec{P}^{T} \left(\vec{b}^{2} + \eta\vec{I}\right)^{-1} \vec{P}\vec{P}^{T} \left(\vec{b}^{2} + \eta\vec{I}\right)^{-1} \vec{P}\sqrt{\vec{\varepsilon}}^{-1}\vec{r} = \vec{r}^{T}\sqrt{\vec{\varepsilon}}^{-1} \left(\sqrt{\vec{\varepsilon}}^{-1}\vec{a}^{2}\sqrt{\vec{\varepsilon}}^{-1} + \eta\vec{I}\right)^{-1} \left(\sqrt{\vec{\varepsilon}}^{-1}\vec{a}^{2}\sqrt{\vec{\varepsilon}}^{-1} + \eta\vec{I}\right)^{-1} \sqrt{\vec{\varepsilon}}^{-1}\vec{r} = \vec{r}^{T} \left(\sqrt{\vec{\varepsilon}}^{-1}\vec{a}^{2} + \eta\sqrt{\vec{\varepsilon}}\right)^{-1} \left(\vec{a}^{2}\sqrt{\vec{\varepsilon}}^{-1} + \eta\sqrt{\vec{\varepsilon}}\right)^{-1}\vec{r} = \vec{r}^{T} \left(\sqrt{\vec{\varepsilon}}^{-1}\vec{a}^{2} + \eta\sqrt{\vec{\varepsilon}}\right)^{-1} \left(\vec{a}^{2}\sqrt{\vec{\varepsilon}}^{-1} + \eta\sqrt{\vec{\varepsilon}}\right)^{-1}\vec{r} = \vec{r}^{T} \left(\vec{a}^{2} + \eta\vec{\varepsilon}\right)^{-1} \vec{\varepsilon} \left(\vec{a}^{2} + \eta\vec{\varepsilon}\right)^{-1} \vec{r}$$

$$(4.48)$$

So, Eq. (46) can be converted in tensor notation as follows

$$\vec{E}(\vec{r}) = \frac{1}{2} \det(\vec{b}) \sqrt{\vec{\varepsilon}}^{-1} \vec{P}^{T} \left[\frac{-2(\vec{b}^{2} + \eta\vec{I})^{-1} \vec{z} \vec{z}^{T} (\vec{b}^{2} + \eta\vec{I})^{-1}}{\vec{r}^{T} (\vec{a}^{2} + \eta\vec{\varepsilon})^{-1} \vec{\varepsilon} (\vec{a}^{2} + \eta\vec{\varepsilon})^{-1} \vec{r}} \frac{1}{R(\eta)} + \int_{\eta}^{+\infty} \frac{(\vec{b}^{2} + s\vec{I})^{-1} ds}{R(s)} \right] \vec{P} \sqrt{\vec{\varepsilon}}^{-1} \vec{\varepsilon} \vec{E}^{*}$$
(4.49)

We remember that the product $\vec{z} \vec{z}^T$ in the previous expression represents the external product of vectors giving, as result, a tensor $\vec{z} \vec{z}^T$ whose components are given by $(\vec{z} \vec{z}^T)_{ij} = z_i z_j$. With a series of considerations similar to the previous ones we may state that

$$\sqrt{\vec{\varepsilon}}^{-1}\vec{P}^{T}\left(\vec{b}^{2}+\eta\vec{I}\right)^{-1}\vec{z}\,\vec{z}^{T}\left(\vec{b}^{2}+\eta\vec{I}\right)^{-1}\vec{P}\sqrt{\vec{\varepsilon}}^{-1} = \left(\vec{a}^{2}+\eta\vec{\varepsilon}\right)^{-1}\vec{r}\vec{r}^{T}\left(\vec{a}^{2}+\eta\vec{\varepsilon}\right)^{-1}$$
(4.50)

$$\sqrt{\overline{\varepsilon}}^{-1}\overline{P}^{T}\left(\overline{b}^{2}+s\overline{I}\right)^{-1}\overline{P}\sqrt{\overline{\varepsilon}}^{-1}=\left(\overline{a}^{2}+\eta\overline{\varepsilon}\right)^{-1}$$
(4.51)

and therefore, the final equation for the external electric field is the following (we have also used Eq. (4.38))

$$\vec{E}(\vec{r}) = \left\{ \frac{1}{2} \det(\vec{a}) \int_{\eta}^{+\infty} \frac{\left(\vec{a}^{2} + s\vec{\varepsilon}\right)^{-1} \vec{\varepsilon}}{\sqrt{\det(\vec{a}^{2} + s\vec{\varepsilon})}} \, ds - \frac{\det(\vec{a})}{\sqrt{\det(\vec{a}^{2} + \eta\vec{\varepsilon})}} \frac{\left[\left(\vec{a}^{2} + \eta\vec{\varepsilon}\right)^{-1} \vec{r}\right] \left[\vec{\varepsilon} \left(\vec{a}^{2} + \eta\vec{\varepsilon}\right)^{-1} \vec{r}\right]^{T}}{\left[\left(\vec{a}^{2} + \eta\vec{\varepsilon}\right)^{-1} \vec{r}\right]^{T} \left[\vec{\varepsilon} \left(\vec{a}^{2} + \eta\vec{\varepsilon}\right)^{-1} \vec{r}\right]} \right\}} \vec{E}^{*}$$

$$(4.52)$$

where the function η is implicitly defined by $\vec{r}^T (\vec{a}^2 + \eta \vec{\varepsilon})^{-1} \vec{r} = 1$ (see Eq. (4.47)) and the overall behavior of the electric field is simply governed by the main tensors $\vec{\varepsilon}$ and \vec{a} , as expected.

4.6. The electric Eshelby Tensors

At this stage of the work we have completely solved the problem of a homogeneous ellipsoidal inclusion in an anisotropic environment. This solution can be summarized as follows. Both the Eq. (4.39) for the internal field and the Eq. (4.52) for the external one define a tensor (in brackets) which acts on the eigenfield to give the effective electric field in the corresponding region. By adopting a terminology taken from the elasticity theory, we name such tensors the internal electric Eshelby tensor \vec{S} and the external electric Eshelby tensor $\vec{S}^{\infty}(\vec{r})$ [60-62]. Their complete expressions follow

$$\vec{S} = \frac{\det(\vec{a})}{2} \int_{0}^{+\infty} \frac{\left(\vec{a}^2 + s\vec{\varepsilon}\right)^{-1}\vec{\varepsilon}}{\sqrt{\det(\vec{a}^2 + s\vec{\varepsilon})}} ds$$
(4.53)

$$\vec{S}^{\infty}(\vec{r}) = \frac{\det(\vec{a})}{2} \int_{\eta}^{+\infty} \frac{\left(\vec{a}^{2} + s\vec{\varepsilon}\right)^{-1}\vec{\varepsilon}}{\sqrt{\det\left(\vec{a}^{2} + s\vec{\varepsilon}\right)}} ds - \frac{\det(\vec{a})}{\sqrt{\det\left(\vec{a}^{2} + \eta\vec{\varepsilon}\right)}} \frac{\left[\left(\vec{a}^{2} + \eta\vec{\varepsilon}\right)^{-1}\vec{r}\right]\left[\vec{\varepsilon}\left(\vec{a}^{2} + \eta\vec{\varepsilon}\right)^{-1}\vec{r}\right]}{\left[\left(\vec{a}^{2} + \eta\vec{\varepsilon}\right)^{-1}\vec{r}\right]^{T} \left[\vec{\varepsilon}\left(\vec{a}^{2} + \eta\vec{\varepsilon}\right)^{-1}\vec{r}\right]}$$
(4.54)



Figure 6. Scheme of an inclusion V with eigenfield \vec{E}^* defined by $\vec{D} = \vec{\varepsilon} \left(\vec{E} - \vec{E}^* \right)$ embedded in an anisotropic environment described by $\vec{D} = \vec{\varepsilon} \vec{E}$. The results in terms of the interior points and exterior point Eshelby tensors are also shown.

Such definitions allow us to put the final equations for the electric field (see Eqs. (4.39) and (4.52)) in the very simple form

$$\begin{cases} \vec{E} = \vec{S}\vec{E}^* & \text{if } \vec{r} \in V \\ \vec{E}(\vec{r}) = \vec{S}^{\infty}(\vec{r})\vec{E}^* & \text{if } \vec{r} \in \Re^3 \setminus V \end{cases}$$

$$(4.55)$$

A summarizing scheme of the problem of an inclusion in an anisotropic environment can be found in Fig. 6, where the constitutive equations and the results in terms of the electric Eshelby tensors are reported in both the internal and external regions.

4.7. Equivalence Principle

In this paragraph we show that the problem of an electrostatic inclusion, as previously defined, is very useful to solve the problem of a given anisotropic inhomogeneity placed in an anisotropic matrix. We will show an equivalence principle that reduces the analysis of the behavior of a inhomogeneity to that of an inclusion. Let's start by considering an ellipsoidal inhomogeneity with permittivity tensor $\vec{\varepsilon}_i$ embedded in a anisotropic environment with permittivity $\ddot{\varepsilon}$. We suppose that the whole structure is subjected to an external uniform electric field (remotely applied) \vec{E}^{∞} (of course we have $\vec{D}^{\infty} = \vec{\varepsilon}\vec{E}^{\infty}$). We are searching for the perturbation to this uniform field induced by the presence of the inhomogeneity. The equivalence principle, which we are going to illustrate, has been summarized in Fig. 7. The actual presence of an inhomogeneity can be described by the superimposition of the effects generated by two different situations A and B. The first situation is very simple since it considers the effects of the remote field \vec{E}^{∞} in an homogeneous matrix without the inhomogeneity. In such a case, we simply observe that the displacement vector $\vec{D}^{\infty} = \vec{\varepsilon} \vec{E}^{\infty}$ remains uniform in the entire space. The situation B corresponds to an inclusion scheme where the eigenfield \vec{E}^* is still unknown and it can be determined by imposing the equivalence between the original problem and the superimposition A+B. We define as \vec{D}_{tar} and \vec{E}_{tot} the electric quantities in the initial inhomogeneity problem; as above said the fields \vec{D}^{∞} and \vec{E}^{∞} correspond to the remote applied field and completely describe the situation A; finally, the problem B is described by the electric variables \vec{D} and \vec{E} . Therefore, in any points of the space we have the superimposition $\vec{D}_{tot} = \vec{D}^{\infty} + \vec{D}$ and $\vec{E}_{tot} = \vec{E}^{\infty} + \vec{E}$. Hence, inside the ellipsoid we obtain

$$\vec{\varepsilon}_i \vec{E}_{tot} = \vec{\varepsilon} \vec{E}^{\infty} + \vec{\varepsilon} \left(\vec{E} - \vec{E}^* \right) \text{ and } \vec{E}_{tot} = \vec{E}^{\infty} + \vec{E}$$
(4.56)

These relationships, which must be verified in the internal region, allow us to calculate the exact value of the eigenfield \vec{E}^* that assure the equivalence between the initial problem and the model A+B. Since $\vec{E} = \vec{S}\vec{E}^*$ for $\vec{r} \in V$, we may write



Figure 7. Scheme of the equivalence principle between the inhomogeneity problem and the problem A (homogeneous medium) superimposed to the problem B (inclusion as reported in Fig. 6).

$$\vec{\varepsilon}_{i}\vec{E}_{tot} = \vec{\varepsilon}\vec{E}^{\infty} + \vec{\varepsilon}\left(\vec{S} - \vec{I}\right)\vec{E}^{*} \quad \text{and} \quad \vec{E}_{tot} = \vec{E}^{\infty} + \vec{S}\vec{E}^{*}$$
(4.57)

By substituting the second relation in the first one we have

$$\vec{\varepsilon}_{i}\left(\vec{E}^{\infty}+\vec{S}\vec{E}^{*}\right)=\vec{\varepsilon}\vec{E}^{\infty}+\vec{\varepsilon}\left(\vec{S}-\vec{I}\right)\vec{E}^{*}$$
(4.58)

This is an equation in the eigenfield \vec{E}^* that can be easily solved by obtaining

$$\vec{E}^* = \left[\left(\vec{I} - \vec{\varepsilon}^{-1} \vec{\varepsilon}_i \right)^{-1} - \vec{S} \right]^{-1} \vec{E}^{\infty}$$
(4.59)

This is the value of the eigenfield that ensures the validity of the equivalence principle. Moreover, it is important to calculate the total electric field \vec{E}_{tot} induced inside the inhomogeneity. From the second relation given in Eq. (4.57) we derive $\vec{E}^* = \vec{S}^{-1} \left(\vec{E}_{tot} - \vec{E}^{\infty} \right)$ and therefore, from the first one, we have

$$\vec{\varepsilon}_{i}\vec{E}_{tot} = \vec{\varepsilon}\vec{E}^{\infty} + \vec{\varepsilon}\left(\vec{S} - \vec{I}\right)\vec{S}^{-1}\left(\vec{E}_{tot} - \vec{E}^{\infty}\right)$$
(4.60)

This equation in the unknown \vec{E}_{tot} can be solved with straightforward algebraic calculations, arriving at the solution

$$\vec{E}_{tot} = \left[\vec{I} - \vec{S}\left(\vec{I} - \vec{\varepsilon}^{-1}\vec{\varepsilon}_i\right)\right]^{-1}\vec{E}^{\infty} \quad \left(\vec{r} \in V\right)$$
(4.61)

This is the internal electric field induced in the ellipsoid: this is a uniform vector field since all the quantities involved in Eq. (61) are constants.

Now, we can consider the external region: here the superimposition $\vec{E}_{tot} = \vec{E}^{\infty} + \vec{E}$ simply leads to the relation $\vec{E}_{tot}(\vec{r}) = \vec{E}^{\infty} + \vec{S}^{\infty}(\vec{r})\vec{E}^*$, which, by considering the eigenfield obtained in Eq. (4.59), leads immediately to the final result

$$\vec{E}_{tot}(\vec{r}) = \left\{ \vec{I} + \vec{S}^{\infty}(\vec{r}) \Big[\left(\vec{I} - \vec{\varepsilon}^{-1} \vec{\varepsilon}_i \right)^{-1} - \vec{S} \Big]^{-1} \right\} \vec{E}^{\infty} \quad \left(\vec{r} \in \Re^3 \setminus V \right)$$
(4.62)

The solutions given in Eqs. (4.61) and (4.62), concerning the internal field and the external field respectively, become at last operative when they are coupled with the definitions of the Eshelby tensors, summarized in Eqs. (4.53) and (4.54). Furthermore, we point out that these results have been written in terms of the matrix permittivity tensor $\vec{\varepsilon}$, the inhomogeneity permittivity tensor $\vec{\varepsilon}_i$, the ellipsoid's tensor \vec{a} (contained in the Eshelby tensors) and the externally applied field \vec{E}^{∞} .

4.8. Generalization to Non-linear Inhomogeneities

A non-linear anisotropic (but homogenous) ellipsoid can be described from the electrical point of view by the constitutive equation

$$\vec{D} = \vec{\varepsilon}_i \left(\vec{E}\right) \vec{E} \tag{4.63}$$

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where, \vec{D} is the electric displacement inside the particle, \vec{E} is the electric field and the dielectric tensor function $\vec{\varepsilon}_i(\vec{E})$ depends on the electric field \vec{E} . This functional relationship takes into account all the anisotropic and non-linear possibilities for the electric behavior of the embedded particle. Let's now place this inhomogeneity in a linear (anisotropic) matrix characterized by the tensor permittivity $\vec{\varepsilon}$ and let's calculate the field inside the ellipsoidal inclusion when a uniform external field \vec{E}^{∞} is applied to the system. If the particle were linear, in the dielectric sense, with constant permittivity $\vec{\varepsilon}_i$, we would have, inside the ellipsoid, a uniform electric field \vec{E}_{tot} given by Eqs. (4.61) and (4.53), which lead to

$$\vec{E}_{tot} = \left[\vec{I} - \frac{\det(\vec{a})}{2} \int_{0}^{+\infty} \frac{\left(\vec{a}^2 + s\vec{\varepsilon}\right)^{-1}}{\sqrt{\det(\vec{a}^2 + s\vec{\varepsilon})}} ds \left(\vec{\varepsilon} - \vec{\varepsilon}_i\right)\right]^{-1} \vec{E}^{\infty} \quad (\vec{r} \in V)$$
(4.64)

Conversely, if the sphere were electrically non-linear, it is easy to prove that the internal field would satisfy the implicit equation

$$\vec{E}_{tot} = \left[\vec{I} - \frac{\det(\vec{a})}{2} \int_{0}^{+\infty} \frac{\left(\vec{a}^{2} + s\vec{\varepsilon}\right)^{-1}}{\sqrt{\det(\vec{a}^{2} + s\vec{\varepsilon})}} ds \left[\vec{\varepsilon} - \vec{\varepsilon}_{i}\left(\vec{E}_{tot}\right)\right]\right]^{-1} \vec{E}^{\infty} \quad \left(\vec{r} \in V\right)$$
(4.65)

This is true since the electric field \vec{E}_{tot} , fulfilling Eq. (4.65), satisfies both the Maxwell laws and the boundary conditions at the inclusion surface, as its linear counterpart Eq. (4.64) does when $\vec{\varepsilon}_i = \vec{\varepsilon}_i (\vec{E}_{tot})$. In other words, if a solution of Eq. (4.65) exists, due to selfconsistency, the problem is completely analogous to the linear one, provided that $\vec{\varepsilon}_i = \vec{\varepsilon}_i (\vec{E}_{tot})$. Once Eq. (4.65) is solved for the internal field \vec{E}_{tot} , the external field can be simply determined by Eq. (4.62), which continues to be valid also in this non-linear case (since the non-linearity is limited to the inhomogeneity).

4.9. Computational Aspects of the External Field

Both in the linear and in the non-linear case the external field is given by Eq. (4.62) where the external Eshelby tensor $\vec{S}^{\infty}(\vec{r})$ should be calculated from Eq. (4.54). In this relation appears the function η , which is implicitly defined by $\vec{r}^T (\vec{a}^2 + \eta \vec{\varepsilon})^{-1} \vec{r} = 1$ (see Eq. (4.47)). Hence, when an arbitrary position vector \vec{r} is given, we have to find the corresponding value of η that satisfies $\vec{r}^T (\vec{a}^2 + \eta \vec{\varepsilon})^{-1} \vec{r} = 1$. This can be done with several computational approaches: here we present a simple iterative technique, which yields a simple implementation and a fast convergence. We start from Eq. (4.47), which can be easily rewritten in the form

 $\vec{r}^T \vec{a}^{-2} (\vec{I} + \eta \vec{\epsilon} \vec{a}^{-2})^{-1} \vec{r} = 1$; now we can use the following general property holding on for any tensor \vec{A} and for any scalar quantity η

$$\left(\ddot{I} + \eta \ddot{A}\right)^{-1} = \ddot{I} - \eta \left(\ddot{A}^{-1} + \eta \ddot{I}\right)^{-1}$$
 (4.66)

This tensor relation can be simply verified by direct computation of the product $(\vec{I} + \eta \vec{A})(\vec{I} + \eta \vec{A})^{-1}$ obtaining, after some straightforward calculations, the identity tensor \vec{I} . Anyway, our implicit equation for η can be written as

$$\vec{r}^{T}\vec{a}^{-2}\left\{\vec{I}-\eta\left[\left(\vec{\varepsilon}\vec{a}^{-2}\right)^{-1}+\eta\vec{I}\right]^{-1}\right\}\vec{r}=1$$
(4.67)

With some rearrangements such a relation can be cast in the useful form

$$\eta = \frac{\vec{r}^{T} \vec{a}^{-2} \vec{r} - 1}{\vec{r}^{T} \vec{a}^{-2} \left[\vec{a}^{2} \vec{\varepsilon}^{-1} + \eta \vec{I} \right]^{-1} \vec{r}}$$
(4.68)

This equation is always in implicit form but it can be used to define a recursive scheme as follows

$$\begin{cases} \eta_0(\vec{r}) = 0\\ \eta_{k+1}(\vec{r}) = \frac{\vec{r}^T \vec{a}^{-2} \vec{r} - 1}{\vec{r}^T \vec{a}^{-2} \left[\vec{a}^2 \vec{\varepsilon}^{-1} + \eta_k(\vec{r}) \vec{I} \right]^{-1} \vec{r}} \end{cases}$$
(4.69)

The initial value introduced in Eq. (4.69) corresponds to the value of η for \vec{r} belonging to the ellipsoidal surface. An example of the behavior of this recursive scheme has been shown in Fig. 8 where we have assumed the following tensors in arbitrary units

$$\vec{a} = \begin{bmatrix} 11 & 5 & 9 \\ 5 & 17 & 8 \\ 9 & 8 & 19 \end{bmatrix}; \qquad \vec{\varepsilon} = \begin{bmatrix} 7 & 2 & 3 \\ 2 & 11 & 8 \\ 3 & 8 & 9 \end{bmatrix}$$
(4.70)

As one can verify, both such tensors are symmetric and positive definite, as requested by their physical meaning. We have plotted the iterations for ten different values of \vec{r} described by the simple law $\vec{r} = 20h(1,1,1)$, i.e. the vector \vec{r} has modulus $20h\sqrt{3}$ and direction (1,1,1) for *h* ranging from 1 to 10. We have performed the iterations for 1200 steps and we have represented their behavior for each value of \vec{r} . We may observe that the convergence is

slower for the points with a greater distance from the origin of the reference frame. Nevertheless, the algorithm is always convergent in a practically acceptable number of iterations. Moreover, at the end of the procedure the relation $\vec{r}^T (\vec{a}^2 + \eta(\vec{r})\vec{\varepsilon})^{-1}\vec{r} = 1$ is satisfied with a great accuracy for any values of \vec{r} . Therefore, this simple method can be profitably utilized in the software implementation of the theory described in this section.



Figure 8. Convergence of the iterative algorithm defined in Eq.(4.69) for different values of the position vector \vec{r} (*h*=1..10) and for several steps (*k*=1..1200). We have used the tensors defined in Eq.(4.70).

4.10. Applications to Anisotropic Composite Materials

The Maxwell-Garnett approximation is one of the most widely used methods for calculating the equivalent dielectric properties of linear isotropic inhomogeneous materials (see Section 2). Here, the effective dielectric tensor of a dispersion of anisotropic inclusions embedded in an anisotropic host is calculated using a generalization of the Maxwell-Garnett approximation. The procedure involves an exact evaluation of the uniform electric field induced inside a single ellipsoidal inclusion and the evaluation of the electrical quantities, averaged over the mixture volume. This approach has been extensively used for studying the properties of two-component mixtures in which both the host and the inclusions are isotropic. So, in order to generalize these situations we consider a population of anisotropic parallel ellipsoids ($\vec{\varepsilon}_i$) randomly embedded in an anisotropic matrix ($\vec{\varepsilon}$). The random character of the system is limited to the positions of the inhomogeneities and not to their orientations. We define the volume fraction of the embedded phase as *c*. The dilute limit is assumed (*c*<<1), so that each inclusion basically "feels" only the uniform, externally applied, electric field. Therefore, the average value of the electric field over the whole structure is given by

$$\left\langle \vec{E} \right\rangle = c \underbrace{\left[\vec{I} - \vec{S} \left(\vec{I} - \vec{\varepsilon}^{-1} \vec{\varepsilon}_i \right) \right]^{-1} \vec{E}^{\infty}}_{\text{see Eq.}(4.61)} + (1 - c) \vec{E}^{\infty} = \left\{ c \begin{bmatrix} \vec{I} - \vec{S} \left(\vec{I} - \vec{\varepsilon}^{-1} \vec{\varepsilon}_i \right) \right]^{-1} + (1 - c) \vec{I} \right\} \vec{E}^{\infty}$$
(4.71)

where we have used Eq. (4.61) for the internal uniform field induced in each ellipsoid. The relation between the average electric field in the heterogeneous system and the external applied one is therefore

$$\vec{E}^{\infty} = \left\{ c \left[\vec{I} - \vec{S} \left(\vec{I} - \vec{\varepsilon}^{-1} \vec{\varepsilon}_i \right) \right]^{-1} + (1 - c) \vec{I} \right\}^{-1} \left\langle \vec{E} \right\rangle$$
(4.72)

At this point we may evaluate the average value of the electric displacement in the dispersion of ellipsoids; we define V as the total volume of the mixture, V_e as the total volume of the embedded ellipsoids and V_o as the volume of the remaining space among the inclusions (so that $V=V_e \cup V_o$ and $c=V_e/V=V_e/(V_e+V_o)$). Then, the average value of $\vec{D}(\vec{r})=\vec{\varepsilon}(\vec{r})\vec{E}(\vec{r})$ follows (see also Eq. (2.17))

$$\left\langle \vec{D} \right\rangle = \vec{\varepsilon} \left\langle \vec{E} \right\rangle + c \left(\vec{\varepsilon}_{i} - \vec{\varepsilon} \right) \left\langle \vec{E}_{tot} \right\rangle = \vec{\varepsilon} \left\langle \vec{E} \right\rangle + c \left(\vec{\varepsilon}_{i} - \vec{\varepsilon} \right) \left[\vec{I} - \vec{S} \left(\vec{I} - \vec{\varepsilon}^{-1} \vec{\varepsilon}_{i} \right) \right]^{-1} \vec{E}^{\infty}$$
(4.73)

where $\langle \vec{E}_{tot} \rangle$ is the average value of the electric field induced inside the ellipsoids; it can be considered uniform and, therefore, we obtain the final result given in Eq. (4.73) by taking into account Eq. (4.61). Now, by substituting Eq. (4.72) in Eq. (4.73) we simply obtain

$$\left\langle \vec{D} \right\rangle = \vec{\varepsilon} \left\langle \vec{E} \right\rangle + c(\vec{\varepsilon}_i - \vec{\varepsilon}) \left[\vec{I} - \vec{S} \left(\vec{I} - \vec{\varepsilon}^{-1} \vec{\varepsilon}_i \right) \right]^{-1} \left\{ c \left[\vec{I} - \vec{S} \left(\vec{I} - \vec{\varepsilon}^{-1} \vec{\varepsilon}_i \right) \right]^{-1} + (1 - c) \vec{I} \right\}^{-1} \left\langle \vec{E} \right\rangle$$

$$= \vec{\varepsilon} \left\langle \vec{E} \right\rangle + c(\vec{\varepsilon}_i - \vec{\varepsilon}) \left\{ c \vec{I} + (1 - c) \left[\vec{I} - \vec{S} \left(\vec{I} - \vec{\varepsilon}^{-1} \vec{\varepsilon}_i \right) \right] \right\}^{-1} \left\langle \vec{E} \right\rangle$$

$$(4.74)$$

Then, we define $\vec{\varepsilon}_{eff}$ as the effective permittivity tensor of the whole mixture by means of the relation $\langle \vec{D} \rangle = \vec{\varepsilon}_{eff} \langle \vec{E} \rangle$. Drawing a comparison between this definition and Eq. (4.74) we may find a complete expression, which allows us to estimate the effective permittivity tensor

$$\vec{\varepsilon}_{eff} = \vec{\varepsilon} + c(\vec{\varepsilon}_i - \vec{\varepsilon}) \left\{ \vec{I} + (1 - c) \vec{S} \vec{\varepsilon}^{-1} (\vec{\varepsilon}_i - \vec{\varepsilon}) \right\}^{-1}$$
(4.75)

By recalling the definition of the internal electric Eshelby tensor we obtain the final result as

$$\vec{\varepsilon}_{eff} = \vec{\varepsilon} + c(\vec{\varepsilon}_i - \vec{\varepsilon}) \left\{ \vec{I} + (1 - c) \frac{\det(\vec{a})}{2} \int_{0}^{+\infty} \frac{(\vec{a}^2 + s\vec{\varepsilon})^{-1}}{\sqrt{\det(\vec{a}^2 + s\vec{\varepsilon})}} ds(\vec{\varepsilon}_i - \vec{\varepsilon}) \right\}^{-1}$$
(4.76)

This relation is valid for low values of the volume fraction c (is exact for c=0). Nevertheless, quite surprisingly, it furnishes exact results also for the extreme case c=1. Anyway, the results cannot be considered correct for large values of the volume fraction. In order to generalize this approach to higher values of the volume fraction we may adopt the differential scheme [5,72]. We indicate with $\vec{\mathcal{E}}_{diff}$ the estimate of the dielectric tensor obtained with this method. As described in previous sections, the incremental procedure leads to the following differential equation for the effective properties

$$\begin{cases} \frac{d\vec{\varepsilon}_{diff}}{dc} = \frac{1}{1-c} \frac{\partial \vec{\varepsilon}_{eff}}{\partial c} \\ \vec{\varepsilon}_{diff} (c=0) = \vec{\varepsilon} \end{cases} c=0, \ \vec{\varepsilon} = \vec{\varepsilon}_{diff} \end{cases}$$
(4.77)

where $\vec{\varepsilon}_{eff}$ is given by dilute result shown in Eq. (4.76). Performing the operations indicated in Eq. (4.77) we simply find the explicit form of the effective differential method

$$\begin{cases} \frac{d\vec{\varepsilon}_{diff}}{dc} = \frac{1}{1-c} \left(\vec{\varepsilon}_{i} - \vec{\varepsilon}_{diff}\right) \left\{ \vec{I} + \frac{\det(\vec{a})}{2} \int_{0}^{+\infty} \frac{\left(\vec{a}^{2} + s\vec{\varepsilon}_{diff}\right)^{-1}}{\sqrt{\det(\vec{a}^{2} + s\vec{\varepsilon}_{diff})}} ds \left(\vec{\varepsilon}_{i} - \vec{\varepsilon}_{diff}\right) \right\}^{-1} \\ \vec{\varepsilon}_{diff} \left(c = 0\right) = \vec{\varepsilon} \end{cases}$$
(4.78)

We summarize the various quantities involved in the previous equations: $\vec{\varepsilon}$ is the tensor permittivity of the matrix, $\vec{\varepsilon}_i$ is the tensor permittivity of the parallel ellipsoids, \vec{a} its tensor of the semi-axes of the ellipsoid and the solution $\vec{\varepsilon}_{diff}$ is the effective dielectric tensor. It is interesting to note that the components of the effective tensor are strongly analytically coupled in the system of differential equations appearing in Eq. (4.78). In order to show a simple example we consider the case with the tensors $\vec{\varepsilon}$, $\vec{\varepsilon}_i$, \vec{a} and $\vec{\varepsilon}_{diff}$ contemporaneously diagonal in the same reference frame. This means that the geometrical principal axes of the ellipsoids are parallel to the optical principal axes of the ellipsoids and of the matrix. Moreover, we assume an isotropic material for the inhomogeneities, i.e. $\vec{\varepsilon}_i = \varepsilon_i \vec{I}$ (ε_i takes the role of scalar permittivity for the ellipsoids). The external medium ($\vec{\varepsilon}$) is instead

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considered anisotropic with three different principal permittivities ($\varepsilon_{10}, \varepsilon_{20}, \varepsilon_{30}$). Similarly, the effective dielectric tensor $\vec{\varepsilon}_{diff}$ has the three principal permittivities $\varepsilon_1, \varepsilon_2$ and ε_3 . Summing up, Eq. (4.78) corresponds to the following system

$$\begin{cases} \frac{d\varepsilon_{k}}{dc} = \frac{1}{1-c} (\varepsilon_{i} - \varepsilon_{k}) \left\{ 1 + \frac{a_{1}a_{2}a_{3}}{2} \int_{0}^{+\infty} \frac{ds(\varepsilon_{i} - \varepsilon_{k})}{(a_{k}^{2} + s\varepsilon_{k})\sqrt{(a_{1}^{2} + s\varepsilon_{1})(a_{2}^{2} + s\varepsilon_{2})(a_{3}^{2} + s\varepsilon_{3})}} \right\}^{-1} \forall k = 1, 2, 3 \\ \varepsilon_{k}(c=0) = \varepsilon_{k0} \end{cases}$$

$$(4.79)$$

Now, in order to obtain a simple model, we consider, as particular case, elliptic cylinders aligned with the x_3 -axis; it means that we perform the limit $a_3 \rightarrow \infty$ in Eq. (4.79). The result is the following

$$\begin{cases} \frac{d\varepsilon_{1}}{dc} = \frac{1}{1-c} (\varepsilon_{i} - \varepsilon_{1}) \left\{ 1 + \frac{a_{1}a_{2}}{2} \int_{0}^{+\infty} \frac{ds(\varepsilon_{i} - \varepsilon_{1})}{(a_{1}^{2} + s\varepsilon_{1})^{3/2} (a_{2}^{2} + s\varepsilon_{2})^{1/2}} \right\}^{-1} \\ \frac{d\varepsilon_{2}}{dc} = \frac{1}{1-c} (\varepsilon_{i} - \varepsilon_{2}) \left\{ 1 + \frac{a_{1}a_{2}}{2} \int_{0}^{+\infty} \frac{ds(\varepsilon_{i} - \varepsilon_{2})}{(a_{1}^{2} + s\varepsilon_{1})^{1/2} (a_{2}^{2} + s\varepsilon_{2})^{3/2}} \right\}^{-1} \\ \frac{d\varepsilon_{3}}{dc} = \frac{1}{1-c} (\varepsilon_{i} - \varepsilon_{3}) \\ \varepsilon_{1}(c = 0) = \varepsilon_{10}, \quad \varepsilon_{2}(c = 0) = \varepsilon_{20}, \quad \varepsilon_{3}(c = 0) = \varepsilon_{30} \end{cases}$$
(4.80)

The integrals appearing in Eq. (4.80) can be solved in closed form by using the following result (that can be simply verified by means of the substitution $x = \sqrt{(a+bs)/(c+ds)}$)

$$\frac{1}{2} \int_{0}^{+\infty} \frac{ds}{(a+bs)^{3/2} (c+ds)^{1/2}} = \frac{1}{\sqrt{ab} \left(\sqrt{ad} + \sqrt{bc}\right)}$$
(4.81)

which is correct for arbitrary positive numbers a, b, c and d. So, by assuming $\varepsilon_{10} = \varepsilon_{20} = \varepsilon_{30} = \varepsilon_m$ (scalar permittivity of the matrix) and by defining the aspect ratio $e=a_2/a_1$, we finally obtain

$$\begin{cases}
\frac{d\varepsilon_1}{dc} = \frac{\varepsilon_i - \varepsilon_1}{1 - c} \frac{\varepsilon_1 e + \sqrt{\varepsilon_1 \varepsilon_2}}{\varepsilon_i e + \sqrt{\varepsilon_1 \varepsilon_2}} \\
\frac{d\varepsilon_2}{dc} = \frac{\varepsilon_i - \varepsilon_2}{1 - c} \frac{\varepsilon_2 + e\sqrt{\varepsilon_1 \varepsilon_2}}{\varepsilon_i + e\sqrt{\varepsilon_1 \varepsilon_2}} \\
\frac{d\varepsilon_3}{dc} = \frac{\varepsilon_i - \varepsilon_3}{1 - c} \\
\varepsilon_1(c = 0) = \varepsilon_2(c = 0) = \varepsilon_3(c = 0) = \varepsilon_m
\end{cases}$$
(4.82)

The solution of such a differential system can be compared with the standard solution obtained by means of the differential method applied without taking into account the anisotropic character of the system. These simpler solutions can be found in Eq. (2.9) and they are reported below for completeness

$$\begin{cases} 1 - c = \frac{\varepsilon_i - \varepsilon_1}{\varepsilon_i - \varepsilon_m} \left(\frac{\varepsilon_i}{\varepsilon_1}\right)^{\frac{e}{e+1}} \\ 1 - c = \frac{\varepsilon_i - \varepsilon_2}{\varepsilon_i - \varepsilon_m} \left(\frac{\varepsilon_i}{\varepsilon_2}\right)^{\frac{1}{e+1}} \\ \varepsilon_3 = c\varepsilon_i + (1 - c)\varepsilon_m \end{cases}$$
(4.83)

The solutions concerning the x_3 direction are perfectly coincident between the two approaches and, therefore, we do not draw further comparison. Indeed, this relation is an exact result describing a parallel connection of capacitors (the interfaces are aligned with the electrical field).

On the other hands, the first two relations in Eq. (4.82) and Eq. (4.83) require more refined checks. We have numerically solved the differential system formed by the first two equations in Eq. (4.82) and the corresponding irrational equations in Eq. (4.83). In Figs. 9 and 10 we have shown the results in terms of the volume fraction *c*, by assuming $\varepsilon_i = 100$ and $\varepsilon_m = 1$, respectively (in arbitrary units). We have drawn a comparison for different values of the aspect ratio of the elliptic cylinders (*e*=0.01, 0.2, 0.5 and 0.8). Being *e*<1, we have explored the situation wherein the axis along x_2 is shorter than the axis along x_1 . Firstly, it is interesting to observe that the estimation of ε_1 with the improved (anisotropic) differential method (Eq. (4.82)); on the other hand, the estimation of ε_2 with the anisotropic differential



Figure 9. Comparison among the results for \mathcal{E}_1 obtained with the anisotropic differential system (Eq.(4.82)) and the standard differential method (Eq.(4.83)). The solutions of Eq.(4.82) (red) are placed under the corresponding solutions of Eq.(4.83) (black).



Figure 10. Comparison among the results for \mathcal{E}_2 obtained with the anisotropic differential system (Eq.(4.82)) and the standard differential method (Eq.(4.83)). The solutions of Eq.(4.82) (red) are placed above the corresponding solutions of Eq.(4.83) (black).

method (Eq. (4.82)) is greater than the estimation obtained with the standard differential method (Eq. (4.83)). This fact can be easily seen in Fig. 9 for the permittivity \mathcal{E}_1 , where the solutions of Eq. (4.82) are placed under the corresponding solutions of Eq. (4.83), and also in

Fig. 10 for \mathcal{E}_2 , where the solutions of Eq. (4.82) are placed above the corresponding solutions of Eq. (4.83). The extent of the differences between the two approaches can be found in Fig. 11 where the variations $\Delta \mathcal{E}$ (values obtained with Eq. (4.82) minus values obtained with Eq. (4.83)) are plotted versus the volume fraction *c* of the composite material. One can see that the relative error can assume values up to 20%. This result proves that the anisotropic character of heterogeneous dielectric systems should be considered with great accuracy since it may modify the behavior of the overall macroscopic properties.



Figure 11. The variations $\Delta \mathcal{E}$ (values obtained with Eq.(4.82) minus values obtained with Eq.(4.83)) are plotted versus the volume fraction *c* of the composite material. One can see that the relative error can assume values up to 20%.

5. Functionally Graded Ellipsoidal Particles

The physical response of materials with spatial gradients in composition and structure is of considerable interest in disciplines as diverse as tribology, geology, microelectronics, optoelectronics, biomechanics, fracture mechanics, and nanotechnology. The damage and failure resistance of surfaces to normal and sliding contact or impact can be changed substantially through such gradients. Also in dielectric structures, graded composites and metamaterials have attracted much attention because their effective properties have advantages over traditional homogeneous composite materials [73-75].

Gradations in microstructure and/or porosity are commonly seen in biological structures such as bamboo, plant stems, and bone, where the strongest elements are located in regions that experience the highest stresses. Gradual changes in the elastic properties of sands, soils, and rocks beneath Earth's surface influence the settlement and stability of structural foundations, plate tectonics, and the ease of drilling into the ground.

Graded transitions in composition, either continuous or in fine, discrete steps, across an interface between two dissimilar materials (such as a metal and a ceramic), can be used to

redistribute thermal stresses or electric fields, to reduce stress concentrations at the intersection between an interface and a free surface and to improve interfacial bonding between dissimilar material.

The typical experiment utilized to define the response of a graded material is the indentation [76] (or also micro- and nano-indentation), which defines the force-penetration curve for an indenter applied on the free surface of the medium. The shape of the gradation inside the material may strongly influence the force-penetration curve and, therefore, the mechanical behavior of the complex material.

With currently available materials synthesis and processing capabilities, engineered gradations in properties, over nanometer to macroscopic length scales, offer appealing prospects for the design of damage-, fracture-, and wear-resistant surfaces in applications as diverse as magnetic storage media, microelectronics, bioimplants for humans, load-bearing engineering structures, protective coatings, and nano- and micro-electromechanical systems.

Moreover, a basic understanding of the propagation of mechanical waves in a continuum having features like functionally graded materials, opens up a wide field of potential engineering applications like design of high frequency signal filters, spectrum analyzers, frequency selective acoustic isolation layers and many others [77].

In the field of dielectric composites there have been a number of attempts, both analytical and experimental, to study the responses of functionally graded materials under specific electric loads and for different microstructures. Moreover, the responses of composites made of functionalized inclusions can be useful and interesting. Various different attempts have been made to treat the composite materials of graded inclusions [78-80]. In this section we present a complete theory for dealing with graded ellipsoidal particles: in particular we prove an equivalence theorem between a graded dielectric ellipsoid (with gradation along a family of internal confocal ellipsoids) and an anisotropic homogeneous ellipsoid. In particular we describe a procedure to obtain the three principal permittivities of the effective ellipsoid when the gradation profile is given.

5.1. Coated Dielectric Ellipsoidal Particle

The analysis of a coated particle is the most important preliminary issue in order to deal with functionally graded inclusions. We consider the structure represented in Fig. 12 where a dielectric coated particle is taken into consideration. The core is made of an anisotropic material with principal directions of the permittivity tensor aligned with the geometrical principal directions of the internal ellipsoid (semi-axes a_{c1} , a_{c2} , a_{c3}): the principal permittivities are ε_{3k} for k=1,2,3. The shell is occupied by an isotropic material with permittivity ε_2 (semi-axes a_{s1} , a_{s2} , a_{s3}). Finally, the external homogeneous media is isotropic with permittivity ε_1 . The two ellipsoids are confocal (i.e. they have the same foci). The following family of confocal ellipsoids is very useful

$$\frac{x_1^2}{a_{s1}^2 + \xi} + \frac{x_2^2}{a_{s2}^2 + \xi} + \frac{x_3^2}{a_{s3}^2 + \xi} = 1$$
(5.1)



Figure 12. Coated dielectric ellipsoidal particle with external shell (s) and with internal core (c) in a given matrix (m).

If $\xi=0$ Eq. (5.1) describes the external shell (semi-axes a_{s1} , a_{s2} , a_{s3}); if $\xi=\xi_c$ it describes the surface of the internal core (semi-axes a_{c1} , a_{c2} , a_{c3}). Therefore, we have $a_{si}^2+\xi_c = a_{ci}^2$, which is a relationship among the internal semi-axes and the external ones. We assume that the external semi-axes are ordered as follows: $0 < a_{s3} < a_{s2} < a_{s1}$. So, inside the particle we always have $-a_{s3}^2 < \xi < 0$. A given value of ξ in this range represents an ellipsoid placed inside the composite particle. It is also useful to introduce the volume fraction of the core into the whole inclusion, $c=(a_{c1}a_{c2}a_{c3})/(a_{s1}a_{s2}a_{s3})$. We prove the following property.

<u>Theorem 1:</u> under the effects of a uniform field, the inclusion composed by an anisotropic core of permittivities ε_{3k} (for k=1,2,3) with volume fraction c and by an isotropic confocal shell of permittivity ε_2 (see Fig. 12) is exactly equivalent to an anisotropic homogeneous ellipsoid with principal permittivities

$$\mathcal{E}_{eff,k} = \mathcal{E}_2 \frac{\left[\left(\mathcal{E}_{3k} - \mathcal{E}_2 \right) L_{ck} + \mathcal{E}_2 \right] + c \left(\mathcal{E}_{3k} - \mathcal{E}_2 \right) \left(1 - L_{sk} \right)}{\left[\left(\mathcal{E}_{3k} - \mathcal{E}_2 \right) L_{ck} + \mathcal{E}_2 \right] - c \left(\mathcal{E}_{3k} - \mathcal{E}_2 \right) L_{sk}}$$
(5.2)

where L_{ck} and L_{sk} are the depolarization factors of the core and of the shell, respectively (they can be calculated by means of Eqs. (2.2) or (2.11)).

<u>Proof:</u> we consider the structure represented in Fig. 12 under the effect of an externally applied uniform electric field $\vec{E}_o = E_{ok}\vec{e}_k$. We suppose that the solution for the electric potential in the three zones of the space (core, shell and matrix) can be represented as

$$\begin{split} \phi_{c} &= C_{k} x_{k} & \text{if } -a_{s3}^{2} < \xi < \xi_{c} \\ \phi_{s} &= S_{k} x_{k} + T_{k} x_{k} \int_{\xi}^{+\infty} \frac{dt}{R(t) (a_{sk}^{2} + t)} & \text{if } \xi_{c} < \xi < 0 \\ \phi_{m} &= -E_{ok} x_{k} + Q_{k} x_{k} \int_{\xi}^{+\infty} \frac{dt}{R(t) (a_{sk}^{2} + t)} & \text{if } \xi > 0 \end{split}$$
(5.3)

where the sum over k is implied, $R(t)=(a_{s1}^2+t)^{1/2}(a_{s2}^2+t)^{1/2}(a_{s3}^2+t)^{1/2}$ and the variable ξ is defined by Eq. (5.1). The coefficients C_k , S_k , T_k and Q_k can be found with the boundary conditions for the electric potential, which are

$$\phi_{c} = \phi_{s} \quad if \quad \xi = \xi_{c}$$

$$\phi_{s} = \phi_{m} \quad if \quad \xi = 0$$

$$\varepsilon_{3k} \frac{\partial \phi_{c}}{\partial x_{k}} n_{k} = \varepsilon_{2} \frac{\partial \phi_{s}}{\partial n} \quad if \quad \xi = \xi_{c}$$

$$\varepsilon_{2} \frac{\partial \phi_{s}}{\partial n} = \varepsilon_{1} \frac{\partial \phi_{m}}{\partial n} \quad if \quad \xi = 0$$
(5.4)

The long development of such conditions leads to the system

$$\begin{cases} C_{k} = S_{k} + \frac{2}{a_{c1}a_{c2}a_{c3}}L_{ck}T_{k} \\ S_{k} + \frac{2}{a_{s1}a_{s2}a_{s3}}L_{sk}T_{k} = -E_{ok} + \frac{2}{a_{s1}a_{s2}a_{s3}}L_{sk}Q_{k} \\ \varepsilon_{3k}C_{k} = \varepsilon_{2}\left[S_{k} + \frac{2}{a_{c1}a_{c2}a_{c3}}(L_{ck} - 1)T_{k}\right] \\ \varepsilon_{2}\left[S_{k} + \frac{2}{a_{s1}a_{s2}a_{s3}}(L_{sk} - 1)T_{k}\right] = \varepsilon_{1}\left[-E_{ok} + \frac{2}{a_{s1}a_{s2}a_{s3}}(L_{sk} - 1)Q_{k}\right] \end{cases}$$
(5.5)

The solutions follow after straightforward algebra

$$\begin{cases} C_{k} = \frac{\varepsilon_{1}\varepsilon_{2}a_{s1}a_{s2}a_{s3}}{a_{c1}a_{c2}a_{c3}(\varepsilon_{3k} - \varepsilon_{2})(\varepsilon_{2} - \varepsilon_{1})L_{sk}(L_{sk} - 1) - a_{s1}a_{s2}a_{s3}[(\varepsilon_{2} - \varepsilon_{1})L_{sk} + \varepsilon_{1}][(\varepsilon_{3k} - \varepsilon_{2})L_{ck} + \varepsilon_{2}]} E_{ok} \\ S_{k} = \frac{\varepsilon_{1}a_{s1}a_{s2}a_{s3}[(\varepsilon_{3k} - \varepsilon_{2})L_{ck} + \varepsilon_{2}]}{a_{c1}a_{c2}a_{c3}(\varepsilon_{3k} - \varepsilon_{2})(\varepsilon_{2} - \varepsilon_{1})L_{sk}(L_{sk} - 1) - a_{s1}a_{s2}a_{s3}[(\varepsilon_{2} - \varepsilon_{1})L_{sk} + \varepsilon_{1}][(\varepsilon_{3k} - \varepsilon_{2})L_{ck} + \varepsilon_{2}]} E_{ok} \\ T_{k} = -\frac{1}{2}\frac{\varepsilon_{1}a_{s1}a_{s2}a_{c3}(\varepsilon_{3k} - \varepsilon_{2})(\varepsilon_{2} - \varepsilon_{1})L_{sk}(L_{sk} - 1) - a_{s1}a_{s2}a_{s3}[(\varepsilon_{2} - \varepsilon_{1})L_{sk} + \varepsilon_{1}][(\varepsilon_{3k} - \varepsilon_{2})L_{ck} + \varepsilon_{2}]} E_{ok} \\ Q_{k} = \frac{a_{s1}a_{s2}a_{s3}}{2}\frac{a_{c1}a_{c2}a_{c3}(\varepsilon_{3k} - \varepsilon_{2})[(\varepsilon_{2} - \varepsilon_{1})L_{sk} - \varepsilon_{2}] - a_{s1}a_{s2}a_{s3}[(\varepsilon_{2} - \varepsilon_{1})L_{sk} + \varepsilon_{1}][(\varepsilon_{3k} - \varepsilon_{2})L_{ck} + \varepsilon_{2}]}{a_{c1}a_{c2}a_{c3}(\varepsilon_{3k} - \varepsilon_{2})(\varepsilon_{2} - \varepsilon_{1})L_{sk}(L_{sk} - 1) - a_{s1}a_{s2}a_{s3}[(\varepsilon_{2} - \varepsilon_{1})L_{sk} + \varepsilon_{1}][(\varepsilon_{3k} - \varepsilon_{2})L_{ck} + \varepsilon_{2}]} E_{ok} \\ (5.6)$$

It is important to observe that the external field is completely controlled by the coefficients Q_k . In order to analyze the special case of an anisotropic ellipsoid without

external shell, in Eq. (5.6) for Q_k , we consider the following substitutions: $\varepsilon_{3k} \rightarrow \varepsilon_{eff,k}$, $a_{ci}=a_{si}$ for i=1,2,3, $L_{cj}=L_{sj}$ for j=1,2,3. In this case the shell disappears and the result is

$$Q_{k} = \frac{a_{s1}a_{s2}a_{s3}}{2} \frac{\varepsilon_{eff,k} - \varepsilon_{1}}{\left(\varepsilon_{eff,k} - \varepsilon_{1}\right) L_{sk} + \varepsilon_{1}} E_{ok}$$
(5.7)

These coefficients describe the external field for an anisotropic ellipsoid of semi-axes a_{si} and permittivities $\varepsilon_{eff,k}$ placed in a matrix with dielectric constant ε_1 . By drawing a comparison between Q_k given in Eq. (5.6) and Q_k given in Eq. (5.7) we obtain an equation for the effective permittivities of the composite inclusion

$$\frac{c(\varepsilon_{3k}-\varepsilon_2)[(\varepsilon_2-\varepsilon_1)L_{sk}-\varepsilon_2]-(\varepsilon_2-\varepsilon_1)[(\varepsilon_{3k}-\varepsilon_2)L_{ck}+\varepsilon_2]}{c(\varepsilon_{3k}-\varepsilon_2)(\varepsilon_2-\varepsilon_1)L_{sk}(L_{sk}-1)-[(\varepsilon_2-\varepsilon_1)L_{sk}+\varepsilon_1][(\varepsilon_{3k}-\varepsilon_2)L_{ck}+\varepsilon_2]} = \frac{\varepsilon_{eff,k}-\varepsilon_1}{(\varepsilon_{eff,k}-\varepsilon_1)L_{sk}+\varepsilon_1}$$
(5.8)

Finally, by solving the above equation for $\varepsilon_{eff,k}$ we obtain the expression shown in Eq. (5.2). We remark that the result given in Eq. (5.2) does not depend on ε_1 and depends only on the internal properties of the particle. QED.

5.2. Graded Ellipsoidal Inclusion

The previous theorem allows us to consider functionally graded particle with arbitrary permittivity profile $\epsilon(\xi)$ for $-a_{s3}^2 < \xi < 0$. The following result solves the problem of homogenizing graded dielectric inclusions.

<u>Theorem 2:</u> under the effects of a uniform field, the functionally graded ellipsoidal particle with permittivity profile $\varepsilon(\xi)$ (in the entire range $-a_{s3}^2 < \xi < 0$, the variable ξ being defined in Eq. (5.1)) is exactly equivalent to an homogeneous anisotropic ellipsoid with principal permittivities defined by $\varepsilon_k(0)$ where the functions $\varepsilon_k(\xi)$ are solutions of the following differential Riccati equations (k=1,2,3)

$$\begin{cases} \frac{d\varepsilon_{k}(\xi)}{d\xi} = -\frac{[\varepsilon_{k}(\xi) - \varepsilon(\xi)]^{2}}{2\varepsilon(\xi)(a_{sk}^{2} + \xi)} - \frac{1}{R(\xi)}\frac{dR(\xi)}{d\xi}[\varepsilon_{k}(\xi) - \varepsilon(\xi)]\\ \varepsilon_{k}(-a_{s3}^{2}) = \varepsilon(-a_{s3}^{2}) \end{cases}$$
(5.9)

We recall that $R(\xi) = (a_{s1}^2 + \xi)^{1/2} (a_{s2}^2 + \xi)^{1/2} (a_{s3}^2 + \xi)^{1/2}$. The values $\varepsilon_k(s)$ (for a given s in the entire range $-a_{s3}^2 < s < 0$) represent the effective principal permittivities of the ellipsoid defined by the bounds $-a_{s3}^2 < \xi < s$.



Figure 13. Functionally graded inclusion. An infinitesimal ellipsoidal layer $(\xi, \xi + d\xi)$ is considered.

<u>Proof:</u> we take into consideration Fig. 13 where an infinitesimal ellipsoidal layer $(\xi, \xi+d\xi)$ is represented. We suppose that the region $(-a_{s3}^2, \xi)$ has been homogenized by obtaining the effective principal permittivities $\varepsilon_k(\xi)$ (anisotropic core). The infinitesimal ellipsoidal layer $(\xi, \xi+d\xi)$ is characterized by the actual permittivity $\varepsilon(\xi)$ (isotropic shell). Now, we obtain the effective principal permittivities $\varepsilon_k(\xi+d\xi)$ of the larger region $(-a_{s3}^2, \xi+d\xi)$ by utilizing the theorem 1

$$\varepsilon_{k}(\xi + d\xi) = \varepsilon(\xi) \frac{\left(\varepsilon_{k}(\xi) - \varepsilon(\xi)\right)L_{k}(\xi) + \varepsilon(\xi) + c\left(\varepsilon_{k}(\xi) - \varepsilon(\xi)\right)\left(1 - L_{k}(\xi + d\xi)\right)}{\left(\varepsilon_{k}(\xi) - \varepsilon(\xi)\right)L_{k}(\xi) + \varepsilon(\xi) - c\left(\varepsilon_{k}(\xi) - \varepsilon(\xi)\right)L_{k}(\xi + d\xi)}$$
(5.10)

where the volume fraction c is given (up to the first order in $d\xi$) by

$$c = \frac{R(\xi)}{R(\xi + d\xi)} = \frac{R(\xi)}{R(\xi) + \frac{dR(\xi)}{d\xi}d\xi} = \frac{1}{1 + \frac{1}{R(\xi)}\frac{dR(\xi)}{d\xi}d\xi} = 1 - \frac{1}{R(\xi)}\frac{dR(\xi)}{d\xi}d\xi$$
(5.11)

and the depolarization factors of the ellipsoid defined by ξ are

$$L_{k}(\xi) = \frac{R(\xi)}{2} \int_{0}^{+\infty} \frac{ds}{R(\xi+s)(a_{sk}^{2}+\xi+s)}$$
(5.12)

From Eq. (5.11) we may build the difference quotient for the variable $\varepsilon_k(\xi)$

$$\frac{\varepsilon_{k}(\xi+d\xi)-\varepsilon_{k}(\xi)}{d\xi} = \frac{\varepsilon(\xi)}{d\xi} \frac{\left(\varepsilon_{k}(\xi)-\varepsilon(\xi)\right)L_{k}(\xi)+\varepsilon(\xi)+\varepsilon(\xi)-\varepsilon(\xi)\right)\left(1-L_{k}(\xi+d\xi)\right)}{\left(\varepsilon_{k}(\xi)-\varepsilon(\xi)\right)L_{k}(\xi)+\varepsilon(\xi)-\varepsilon(\xi)-\varepsilon(\xi)\right)L_{k}(\xi+d\xi)} - \frac{\varepsilon_{k}(\xi)}{d\xi}$$
(5.13)

By performing the limit for $d\xi \rightarrow 0$ and by using Eq. (5.11) we obtain the first form of the differential equation

$$\frac{d\varepsilon_{k}}{d\xi} = \frac{(\varepsilon_{k} - \varepsilon) \left[(\varepsilon_{k} - \varepsilon) \frac{dL_{k}}{d\xi} - \frac{1}{R} \frac{dR}{d\xi} ((\varepsilon_{k} - \varepsilon)L_{k} + \varepsilon) \right]}{\varepsilon}$$
(5.14)

Now, the derivative of L_k , given in Eq. (5.12), can be found as

$$\frac{dL_k(\xi)}{d\xi} = \frac{1}{R(\xi)} \frac{dR(\xi)}{d\xi} L_k(\xi) - \frac{1}{2(a_{sk}^2 + \xi)}$$
(5.15)

Finally, the substitution of Eq. (5.15) in Eq. (5.14) allows us to obtain the final result shown in Eq. (5.9). QED.



Figure 14. Example of application of the Riccati differential equations: semi-axes $a_{s1}=3$, $a_{s2}=2.2$, $a_{s3}=2$; permittivity profile $\epsilon(\xi)=10+10\sin[8\pi(a_{s3}^2+\xi)/a_{s3}^2]$ in arbitrary units (blue continuous line: $\epsilon_1(\xi)$, red dashed-dotted line: $\epsilon_2(\xi)$, green dashed line: $\epsilon_3(\xi)$).

This theorem, being proved for an arbitrarily shaped ellipsoid, can be also applied to specific geometries like spheres or cylinders (with applications to simple dispersions and to fibrous materials). We show in Fig. 14 an example of solution of the Riccati differential equations for a periodic profile of the permittivity $\varepsilon(\xi)$. Adopted parameters: semi-axes $a_{s1}=3$, $a_{s2}=2.2$, $a_{s3}=2$; permittivity profile $\varepsilon(\xi)=10+10\sin[8\pi(a_{s3}^2+\xi)/a_{s3}^2]$ in arbitrary units.

We move now to the case of a population of functionally graded ellipsoidal particles. We assume that each particle has a given permittivity profile $\varepsilon(\xi)$. We consider that all the particles are embedded in a given matrix. Each of these particles can be substituted by an homogeneous anisotropic inclusion with principal permittivities given by the Riccati equations. These values can be obtained with the first part of the homogenization procedure, i.e. with the integration of Eq.(5.9). The second part of the homogenizing theory consists in finding the effective dielectric constant of the entire dispersion. The generalization of the

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Maxwell-Garnett theory exposed in Section 4 may be used in order to take into account the anisotropic character of the particles

This idea is commonly referred to as multiscale approach: a paradigm effectively coupling different methods and thus providing a unique theoretical device able to pass physical information across different scales. In our case the multiscale two-steps homogenization first solves the problem inside each graded particle and then copes with the overall dispersion of inclusions.

In such a discussion, for simplicity, we have considered only static permittivities but we point out that our methodology can be also applied to the case of frequency dependent permittivities. For example it is possible to consider Drude-like dielectric constant with ξ -dependent plasma frequency and/or ξ -dependent damping coefficient. The graded Drude dielectric function is very useful to analyze the properties of metal-dielectric composites.

6. Conclusion

We have described some homogenizing procedures with several applications to different microstructures, geometries and electric behaviors. We remark that all the approaches and the final formulas can be applied to dielectric permittivity, magnetic permeability, electric and thermal conductivity. In particular we have analyzed the following physical situations:

- the generalization of the Maxwell-Garnett theory through the differential scheme having reference to dispersions of aligned or random oriented ellipsoids.
- nonlinear dispersions of random oriented ellipsoids characterized by a Kerr nonlinear constitutive equation.
- anisotropic behavior of a single inhomogeneity and of a dispersion of anisotropic particles; we have defined the concepts of eigenfield and inclusion by obtaining the dielectric internal and external Eshelby tensors.
- finally we have proved two theorems concerning the electric behavior of functionally graded inhomogeneity; we have outlined a homogenizing procedure based on a system of Riccati differential equations.

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