Homogenization model of two eccentric spheres

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Abstract

In this paper, we consider the interaction of an electromagnetic field with two eccentric spheres. We propose a quasi-static approach in order to calculate the external electric field, the polarizability and the effective permittivity of the eccentric spheres. We analyze the behavior of the scattering parameters as a function of the dimension and position of the spherical inclusions. Moreover, we consider the case of plasmonic spheres and study the behavior of the plasmon resonances.

1. Introduction

The analysis of the scattering by spherical objects with conducting or dielectric inclusions is a classical topic in the electromagnetic research. The first result, after the works by Mie and Lorentz on the electromagnetic scattering by a spherical object, can be considered the work on the scattering by two concentric spheres [1], and that on the scattering by a perfectly conducting sphere embedded in a dielectric one [2]. A problem of this type is characterized by the large number of applications, for example, many applications have been proposed in order to study the electric interaction with the human brain and heart [3, 4]. Another important field of application of the eccentric-sphere scattering problem is related to the nano-particle fabrication and application. The anisotropic nano-structures, in recent years, have attracted increasing attention, because they have shown superior characteristics with respect to the isotropic structures [5].

In Section 2, we present the quasi-static model of an eccentric spherical inclusion embedded in a dielectric sphere and we obtain an analytical expression for the polarizability and for the effective permittivity of the spheres. In Section 3, we validate the quasi-static results through comparisons with a Finite-Element Method. Moreover, we present a parametric study to clarify the role of the inclusion position and dimension on the polarizability. Furthermore, we present an analysis of the plasmon resonances of the structure. Finally, in Section 4, the conclusions are drawn.

2. Quasi-static Interaction

We start our study by considering a dielectric sphere with an eccentric spherical dielectric inclusion, see Fig. 1. We consider the center of the host sphere on the origin $O$ of a Cartesian coordinate system and the center of the internal sphere on the origin $O’$, we call $R_1$ the radius of the external sphere and $R_2$ the radius of the internal sphere, the last one is situated at a distance $d$ from the center of the host sphere. The centers of the two spheres are located on the $z$ axis. Since the system is in azimuthal symmetry, the potential function will be independent of $\varphi$.

The medium where the external sphere is posed will be considered as a vacuum, i.e., characterized by $\varepsilon_0$, $\mu_0$ and $\sigma_0 = 0$. On the other hand, the properties of the material of the external sphere are the following: $\varepsilon_s$, $\mu_s$, $\sigma_s$ and those of the internal sphere are $\varepsilon_c$, $\mu_c$ and $\sigma_c$. We suppose that the external electric field is directed in the $z$-direction in order to obtain an axial-symmetric problem.

![Fig. 1. Geometry of the problem: a dielectric sphere in a vacuum with an eccentric spherical inclusion.](image-url)
The electric potentials for the free space, host sphere and internal sphere are [6]:

\[
\phi_0(r) = \sum_{n=0}^{\infty} \left(-E_0 r^n + \frac{b_n}{r^{n+1}}\right) P_n(\cos \theta)
\]

\[
\phi_s(r) = \sum_{n=0}^{\infty} \left(a_n^s r^n + \frac{b_n^s}{r^{n+1}}\right) P_n(\cos \theta)
\]

\[
\phi_e(r') = \sum_{n=0}^{\infty} a_n^e r^n P_n(\cos \theta')
\]

respectively, where \(P_n(x)\) is the Legendre polynomial of order \(n\). Note that the potential \(\phi_e\) includes negative-power terms which bring forth singularities at the origin, moreover we can note that the potential \(\phi_e\) is centered in the origin \(O'\). Instead in the expression of this potential there are not the irregular harmonics, because the origin is contained in its domain. This problem is avoided by translating the origin of this potential from \(O\) to \(O'\). In fact, as we will see, after these transformation the discontinuity disappears. The coefficients \(b_n, a_n^s, b_n^s,\) and \(a_n^e\) are the unknowns of our problem. In order to determine these coefficients, we have to impose the boundary conditions on each surface:

\[
\phi_0(r) = \phi_s(r) \quad \text{for} \quad r = R_s
\]

\[
\varepsilon_0 \frac{\partial \phi_0(r)}{\partial r} = \varepsilon_s \frac{\partial \phi_s(r)}{\partial r} \quad \text{for} \quad r = R_s
\]

\[
\phi_s(r') = \phi_e(r') \quad \text{for} \quad r' = R_c
\]

\[
\varepsilon_s \frac{\partial \phi_s(r')}{\partial r} = \varepsilon_e \frac{\partial \phi_e(r')}{\partial r} \quad \text{for} \quad r' = R_c
\]

We can note that the conditions (6, 7) are imposed on the surface of the internal sphere, so the potential \(\phi_e\) is centered in the origin \(O'\), in order to impose the condition on \(r' = R_c\). Moreover we can note that if we had considered a Perfect Electric Conductor (PEC) inclusion, the potential \(\phi_e\) would have been zero, therefore the boundary conditions would be reduced to the equations (4)-(6). To operate the translation of the potential \(\phi_s\) in (7), we apply the Morse-Feshbach formulas [7, 8]. Using these formulas for the potential \(\phi_s\), we obtain [6, 26, 27]:

\[
\phi_s(r') = \sum_{n=0}^{\infty} P_n(\cos \theta') \left(\frac{r'}{a}\right)^n \sum_{y=0}^{\infty} a_y^{n} d^y \gamma_{vn} + \left(\frac{d}{r'}\right)^{n+1} \sum_{y=0}^{\infty} \frac{b_y^{n}}{(d)^{n+1}} \lambda_{vn}
\]

with \(y_{vn} = \frac{(-1)^{y} - n}{(y - n)!}\) and \(\lambda_{vn} = \frac{n!}{(n - y)!y!}\).

The Eq. (8) is the expression of the electric potential inside the external sphere centered in the origin \(O'\). By inserting expressions (1)-(3), and (8) in the boundary conditions (4)-(7), and by using the orthogonality relation for the Legendre polynomials [8], we can write the following equations:

\[
\frac{b_n}{R_c^{n+1}} - a_n^s - \frac{b_n^s}{R_c^{n+1}} = E_0 \delta_{1n}
\]

\[
- \frac{\pi + 1}{n} \frac{b_n}{R_c^{n+1}} - \frac{\varepsilon_s}{\varepsilon_0} a_n^s + \frac{\pi + 1 \varepsilon_s}{n} \frac{b_n^s}{R_c^{n+1}} = E_0 \delta_{1n}
\]

\[
\sum_{y=1}^{\infty} a_y^{n} d^y \gamma_{vn} (-d)^{y-n} + \sum_{y=1}^{\infty} \frac{b_y^{n}}{(d)^{n+1}} \lambda_{vn} = a_n^e = 0
\]

\[
\frac{\varepsilon_s}{\varepsilon_e} \sum_{y=1}^{\infty} \frac{a_y^{n} d^y \gamma_{vn} (-d)^{y-n}}{a_n^e} + \frac{\varepsilon_s}{\varepsilon_e} \sum_{y=1}^{\infty} \frac{b_y^{n}}{(d)^{n+1}} \lambda_{vn} = a_n^e = 0
\]

and for the PEC case we can write equations like the previous ones, but without the (12) and the coefficient \(a_n^e\). The solution of this system of equations gives the unknowns of the problem, \(b_n, a_n^s, b_n^s,\) and \(a_n^e\). In our case, because of the axial symmetry, the electric field \(E_0\) generates a dipole perturbation in the sphere's surroundings; therefore the polarizability can be written as [9]: \(\alpha = 4 \pi \varepsilon_0 b_1 / E_0\). From the polarizability, we can calculate the effective permittivity of the two eccentric spheres with the formula [9]: \(\varepsilon_{\text{eff}} = \varepsilon_0 + \frac{a V}{4 \pi \varepsilon_0 V}\), where \(V\) is the volume of the external sphere.

3. Validation and Results

In this Section, we present some numerical results obtained with a Matlab code. To demonstrate the validity of the model, we provide comparisons between such results and simulations implemented on Comsol Multiphysics. We consider the case of an external sphere with a ratio between the radius and the wavelength equal to \(10^{-8}\). The total electric field outside the sphere is the negative gradient of the electric potential \(\phi_0\). In Fig. 2, the electric field along a line of coordinates \((x, y) = ((-R_s, 0), -1.5R_s)\) is shown, in the case of an internal sphere with radius \(R_c = R_s / 2\), posed at a distance from the origin \(d = R_c / 2\). The external sphere has a relative dielectric permittivity \(\varepsilon_s = 2.25\) and the internal sphere is of a PEC (Fig. 2.a); in the second case the internal sphere is dielectric with \(\varepsilon_e = 5\) (Fig. 2.b). These comparisons show an excellent agreement between the results of our code and the simulations.
In Fig. 3, the axial component of the electric field in a point \( P = (0,0,-1.5R_e) \) is shown as a function of the distance between the centers of the two spheres. In this case, we can see that the field is strongly affected by the position of the inclusion. As we expected, the field is stronger when the inclusion is nearer to the boundary of the external sphere.

Fig. 2. Electric field components computed along a line of coordinates \( (x,y) = ((-R_e,0), (-1.5R_e)) \); in the case of a dielectric host sphere (\( \varepsilon_r = 2.25 \)) with inside: a) an eccentric PEC sphere; b) an eccentric dielectric sphere (\( \varepsilon_r = 5 \)).

Another parameter of interest is the effective permittivity. Like the polarizability, also the effective permittivity is an integral parameter, then we expect that it is not strongly affected by the position of the inclusion; however, it is strongly affected by the inclusion radius. To show this dependence, let us consider the case of two internally tangential spheres, with the radius of the internal sphere varying from zero to the radius of the external sphere, see Fig. 4.a. The permittivity of this object must vary all the way from \( \varepsilon_r \) to \( \varepsilon_r \). To emphasize this effect, we consider the case of a PEC inclusion. In Fig. 4.b, the effective permittivity as a function of the radius of the inclusion is shown. We can see that the effective permittivity grows extremely slowly with the inclusion's radius until \( R_e = 0.7R_e \). Beyond that, the increase becomes more nonlinear and tends to infinity.

Fig. 3. Electric field component as a function of the distance between the centers of the two spheres. The parameters are the same of Fig. 2.

Fig. 4. a) Geometry and b) effective permittivity of two internally tangential spheres as a function of the internal radius. The parameters of the two spheres are the same of Fig. 3.

Until now, we have analyzed dielectric and conducting spheres. Let us next focus on plasmonic composite structures. In particular we want to study the effect of the eccentricity on the position and magnitude of these resonances. We study
the case of a dielectric sphere with an eccentric plasmonic inclusion, as a generalization of a dielectric sphere with a plasmonic core. In Fig. 6, we can see the normalized polarizability, for an external sphere with relative permittivity equal to $\varepsilon_\varepsilon = 4$ and a spherical inclusion with radius $R_e = R_e/2$, as a function of the relative permittivity $\varepsilon_e$ of the inclusion. We see that, increasing the eccentricity $d$ of the inclusion, the plasmon resonance decreases in magnitude, and it vanishes for the maximum value of $d$. Therefore, we find that a dielectric sphere with a plasmonic eccentric inclusion does not present plasmon resonances for high values of the eccentricity.

4. Conclusion

In this paper, we studied the behavior of an eccentric composite core-shell structure in the presence of an external electric field. The spheres are considered with different values of the radii, relative permittivities and reciprocal positions. A quasi-static analysis has been developed in order to obtain the scattering behavior and, in particular, the polarizability and the effective permittivity of the spheres. A comparison has been presented to validate the results. We found that the polarizability of the two eccentric spheres is affected mostly by the radius of the internal sphere and weakly by the internal sphere's position. On the other hand, we demonstrated that this dependence is only on the integral behavior, while the local behavior of the electric field strongly depends on the position of the internal sphere. Finally, we considered the case of plasmonic spheres and we found that for two eccentric spheres with a plasmonic inclusion, the plasmon resonance disappears for high values of the eccentricity.

Fig. 5. Normalized polarizability of two eccentric spheres, with a dielectric external sphere with relative permittivity $\varepsilon_\varepsilon = 4$, and an internal sphere with radius $R_e = R_e/2$, as a function of the relative permittivity $\varepsilon_e$ of the internal sphere.

5. References

8. P. M. Morse and H. Feshbach, Methods of Theoretical Physics, Part II, McGraw-Hill, 1953.