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Author(s):   Kettunen, Henrik & Wallén, Henrik & Sihvola, Ari

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Polarizability of a dielectric hemisphere

Henrik Kettunen,[a] Henrik Wallén, and Ari Sihvola

Electromagnetics Laboratory, Helsinki University of Technology, P.O. Box 3000, FI-02015 TKK, Finland

This article presents a method for solving the polarizability of a dielectric hemispherical object as a function of its relative electric permittivity. The polarizability of a hemisphere depends on the direction of the exciting electric field. Therefore, the polarizability can be written as a dyadic consisting of two components, the axial and the transversal polarizabilities, which can be solved separately. The solution is based on an analytical approach where the electrostatic potential function is written as a series expansion. However, no closed-form solution for the coefficients of the series is found, so they must be solved from a matrix equation. This method provides very high accuracy. However, it requires construction of large matrices which consumes both time and memory. Therefore, approximative expressions for the polarizabilities with absolute error less than 10^{-5} are also presented. © *2007 American Institute of Physics*. [DOI: 10.1063/1.2769288]

I. INTRODUCTION

This article focuses on the computation of the electrostatic response of a dielectric hemispherical object when it is exposed to a uniform electric field. In a static electric field a dielectric object becomes polarized and gives rise to a secondary electric field, the main component of which is a dipolar field. Therefore, the polarized object can be considered a dipole moment. The polarizability α is a parameter which describes the magnitude of the polarization. It is defined as the ratio of the dipole moment and the magnitude of the incident field,

$$\mathbf{p} = \alpha \mathbf{E}_e, \tag{1}$$

where $\mathbf{E}_e$ is the uniform external field and $\mathbf{p}$ is the induced dipole moment.

The electric response of a single object also determines the characteristics of large mixtures of such objects. Therefore, the knowledge of polarizability is important when designing, for example, artificial composite materials by mixing dielectric inclusions into some background material.

The polarizability of a homogeneous sphere is an example which has a closed-form analytical solution.[1] If a sphere with permittivity ϵ_i is embedded in an environment with permittivity ϵ_e, the polarizability can be obtained by determining the dipole moment. It is often more convenient to write the polarizability as a dimensionless number normalized by the volume of the object V and the permittivity of the environment ϵ_e. The normalized polarizability for a sphere is

$$\alpha_n = \frac{\alpha}{V\epsilon_e} = 3\frac{\epsilon_r - 1}{\epsilon_r + 2}, \tag{2}$$

where $\epsilon_r = \epsilon_i/\epsilon_e$ is the permittivity ratio between the inclusion and the environment.

In general, when the object has no special symmetries the polarizability is dependent on the direction of the electric field. For example, the polarizability of an ellipsoid is determined by three orthogonal components. A sphere is a special case of an ellipsoid where these components become all the same. In addition to the sphere, the dielectric ellipsoid is the only example of an anisotropic object whose polarizability components have simple analytical closed-form solutions.[2]

The polarizability of an arbitrarily shaped object can be evaluated using numerical methods. There exist reported results, for example, for circular cylinders[3] and for regular polyhedra (tetrahedron, cube, octahedron, dodecahedron, and icosahedron), also known as the Platonic solids, in cases where they are ideally conducting[4] and in cases where they are dielectric with arbitrary permittivity.[5]

An interesting polarizability problem has also been the case of two spheres, separate or intersecting. Several articles considering analytical approaches to this double-sphere case can be found.[6–9]

However, polarizability of a hemisphere has not been considered before, although a hemisphere is a very simple and elementary geometry. Like a sphere, it is defined by one single parameter, its radius r. The results presented in this article are also a valuable reference in testing numerical programs which are being developed for treating more complex geometries.

For the hemisphere the relation Eq. (1) must be written in a more general form,

$$\mathbf{p} = \bar{\bar{\alpha}} \cdot \mathbf{E}_e, \tag{3}$$

where the polarizability is expressed as a dyadic. For the hemisphere, or any object with rotational symmetry which now is chosen to be with respect to the z-axis, the polarizability dyadic is of the form

$$\bar{\bar{\alpha}} = \alpha_t(\mathbf{u}_x\mathbf{u}_x + \mathbf{u}_y\mathbf{u}_y) + \alpha_z\mathbf{u}_z\mathbf{u}_z, \tag{4}$$

where α_z and α_t are the axial and the transversal polarizabilities, respectively. These polarizability components can be determined separately by solving the potential function of the hemispherical object situated in an external uniform axial and a transversal electric field. In the next section, the solution for the electrostatic potential in both of these cases is studied in a generalized case of a double hemisphere which

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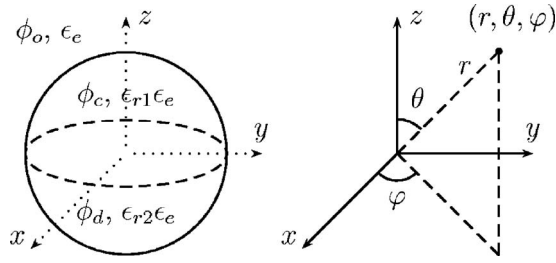[a]Electronic mail: henrik.kettunen@tkk.fi

FIG. 1. Double hemisphere located in the spherical coordinate system.

consists of two joint hemispheres with different permittivities.

The computation of the polarizability components this way however requires some effort. Therefore, also approximative expressions for the polarizabilities as functions of relative permittivity are derived by fitting interpolation curves into very accurate computed data.

II. SOLUTION OF THE ELECTROSTATIC POTENTIAL IN A HEMISPHERICAL REGION

The determination of the polarizability requires solving the electrostatic potential function in a situation where a hemispherical object is located in a uniform electric field. It is possible to examine a more general situation where the object consist of two hemispheres with different electric permittivities. Let us call such an object a double hemisphere. If the permittivity of one half of the sphere is the same as of the surrounding environment, what is left is a single hemisphere.

The solution of the electrostatic potential with material discontinuity in a spherical geometry is considered in Refs. 10–12. Let us also follow a similar procedure.

The space must now be divided into three regions: the upper and the lower regions inside the sphere with radius a and the one outside the sphere (see Fig. 1). In each region, the electrostatic potential function ϕ must satisfy the Laplace equation,

$$\nabla^2 \phi = 0. \tag{5}$$

A. Double hemisphere in an axial electric field

In the axial case the external electric field is of the form $\mathbf{E}_e = E_e \mathbf{u}_z$ (see Fig. 2) and the corresponding potential can be written as

$$\phi_e(\mathbf{r}) = -E_e z = -E_e r \cos \theta = -E_e r P_1(\cos \theta), \tag{6}$$

where $P_n(x)$ is the Legendre polynomial of order n.
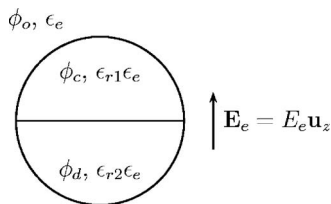

FIG. 2. Double hemisphere in an axial electric field.

The potential functions in each region can be written as series expansions as follows:

$$\phi_c(\mathbf{r}) = \sum_{k=0}^{\infty} C_k r^k P_k(\xi), \quad 0 \leq \theta \leq \frac{\pi}{2}, \quad r \leq a, \tag{7}$$

$$\phi_d(\mathbf{r}) = \sum_{k=0}^{\infty} D_k r^k P_k(\xi), \quad \frac{\pi}{2} \leq \theta \leq \pi, \quad r \leq a, \tag{8}$$

$$\phi_o(\mathbf{r}) = \sum_{n=0}^{\infty} B_n r^{-(n+1)} P_n(\xi) + \phi_e$$

$$= \sum_{n=0}^{\infty} B_n r^{-(n+1)} P_n(\xi) - E_e r P_1(\xi), \quad r > a, \tag{9}$$

where $\xi = \cos \theta$.

The unknown coefficients C_k, D_k, and B_n must be solved by applying the boundary conditions. The continuity of the potential ϕ itself is required. Also, its normal derivative multiplied by the permittivity, $\epsilon \partial \phi / \partial n$, must be a continuous function. This leads to six equations which must all be satisfied.

The Legendre polynomials have the following properties. With odd k, $P_k(0) = 0$ and with even k, $(d/d\theta)P_k(0) = 0$. Therefore, on the boundary inside the sphere, the relation between the coefficients C_k and D_k becomes

$$C_k = \eta_k D_k,$$

$$\eta_k = \begin{cases} 1, & k \text{ even} \\ \dfrac{\epsilon_{r2}}{\epsilon_{r1}}, & k \text{ odd} \end{cases}. \tag{10}$$

Solving the coefficients B_n by applying the boundary conditions on the surface of the sphere becomes more problematic because the Legendre polynomials $P_k(\xi)$ do not form an orthogonal set of functions on the intervals $0 \leq \xi \leq 1$ or $-1 \leq \xi \leq 0$. For example, on the boundary $r = a$ and $0 \leq \theta \leq \pi/2$, from which it follows that $0 \leq \xi \leq 1$, two equations can be formed based on the boundary conditions. If, with each value of k, these equations are multiplied by $P_k(\xi)$ and integrated with respect to ξ over the interval $0 \leq \xi \leq 1$, a set of k equations is obtained, each equation including an infinite sum over index n.

The same procedure is followed on the surface of the lower hemisphere, i.e., $r = a$ and $-1 \leq \xi \leq 0$. Two more equations can be formed and, with every value of k, they are also multiplied by $P_k(\xi)$ and now integrated with respect to ξ over the interval $-1 \leq \xi \leq 0$.

Now the sets of equations obtained from the upper and the lower hemisphere must be combined. Since $P_n(\xi)$ is an even/odd polynomial when n is even/odd, the following applies for the integrals of the Legendre polynomials:

$$\int_{-1}^{0} P_n(\xi) P_k(\xi) d\xi = (-1)^{n+k} \int_{0}^{1} P_n(\xi) P_k(\xi) d\xi. \tag{11}$$

Also, the relation Eq. (10) must be taken into consideration. For every k, the coefficients B_n satisfy
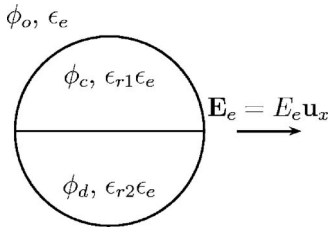
FIG. 3. Double hemisphere in a transversal electric field.

$$\sum_{n=0}^{\infty} B_n a^{-(n+2)} [\eta_k(n+1) + \eta_k k \epsilon_{r1} + (-1)^{n+k}(n+1)$$

$$+ (-1)^{n+k} k \epsilon_{r2}] U_{n,k}$$

$$= E_e [\eta_k k \epsilon_{r1} - \eta_k + (-1)^{1+k} k \epsilon_{r2} - (-1)^{1+k}] U_{1,k}, \quad (12)$$

where

$$U_{n,k} = \int_0^1 P_n(\xi) P_k(\xi) d\xi. \quad (13)$$

These integrals can be computed analytically. For their expressions, see Eq. (A18) in the Appendix.

The coefficients of the potential inside the double hemisphere are obtained from the equation system

$$\sum_{k=0}^{\infty} D_k a^k \left[\eta_k + \eta_k \frac{k \epsilon_{r1}}{n+1} + (-1)^{n+k} + (-1)^{n+k} \frac{k \epsilon_{r2}}{n+1} \right] U_{k,n}$$

$$= -E_e a \left[\frac{1}{n+1} + 1 + \frac{(-1)^{1+k}}{n+1} + (-1)^{1+k} \right] U_{1,n}, \quad (14)$$

and the coefficients C_k are obtained from the relation Eq. (10).

In computation of the polarizability, only the coefficients of the potential outside the sphere, B_n, are needed. They can be solved from the system Eq. (12) by writing it as an $N \times N$ matrix equation by taking N equations each consisting of a sum over N terms as

$$\mathbf{MB} = \mathbf{A},$$

where

$$M_{kn} = a^{-(n+2)} [\eta_k(n+1) + \eta_k k \epsilon_{r1} + (-1)^{n+k}(n+1)$$

$$+ (-1)^{n+k} k \epsilon_{r2}] U_{n,k}, \quad (15)$$

and

$$A_k = E_e [\eta_k k \epsilon_{r1} - \eta_k + (-1)^{1+k} k \epsilon_{r2} - (-1)^{1+k}] U_{1,k}. \quad (16)$$

B. Double hemisphere in a transversal electric field

In the transversal case the external electric field is no longer azimuthally symmetric. Let the direction of the field be $\mathbf{E}_e = E_e \mathbf{u}_x$ (see Fig. 3). The corresponding potential function becomes

$$\phi_e(\mathbf{r}) = -E_e x = -E_e r \sin \theta \cos \varphi = -E_e r P_1^1(\xi) \cos \varphi. \quad (17)$$

Now, a $\cos \varphi$ dependency is included and, instead of the Legendre polynomials, the associated Legendre functions $P_n^m(\xi)$ are required.

The expansions of the electrostatic potential are

$$\phi_c(\mathbf{r}) = \sum_{k=1}^{\infty} C_k r^k P_k^1(\xi) \cos \varphi, \quad (18)$$

$$\phi_d(\mathbf{r}) = \sum_{k=1}^{\infty} D_k r^k P_k^1(\xi) \cos \varphi, \quad (19)$$

$$\phi_o(\mathbf{r}) = \sum_{n=1}^{\infty} B_n r^{-(n+1)} P_n^1(\xi) \cos \varphi - E_e r P_1^1(\xi) \cos \varphi. \quad (20)$$

Again, the coefficients C_k, D_k, and B_n are obtained by applying the boundary conditions and following the same procedure as in the axial case.

The associated Legendre functions $P_k^1(\xi)$ have the following properties. With even values of k, $P_k^1(0) = 0$ and with odd values of k, $(d/d\theta) P_k^1(0) = 0$. Therefore,

$$C_k = \eta_k D_k,$$

$$\eta_k = \begin{cases} 1, & k \text{ odd,} \\ \dfrac{\epsilon_{r2}}{\epsilon_{r1}}, & k \text{ even.} \end{cases} \quad (21)$$

The following equations system can be derived for B_n:

$$\sum_{n=1}^{\infty} B_n a^{-(n+2)} [\eta_k(n+1) + \eta_k k \epsilon_{r1} + (-1)^{n+k}(n+1)$$

$$+ (-1)^{n+k} k \epsilon_{r2}] U_{n,k}^1$$

$$= E_e [\eta_k k \epsilon_{r1} - \eta_k + (-1)^{1+k} k \epsilon_{r2} - (-1)^{1+k}] U_{1,k}^1, \quad (22)$$

and for D_k

$$\sum_{k=0}^{\infty} D_k a^k \left[\eta_k + \eta_k \frac{k \epsilon_{r1}}{n+1} + (-1)^{n+k} + (-1)^{n+k} \frac{k \epsilon_{r2}}{n+1} \right] U_{k,n}^1$$

$$= -E_e a \left[\frac{1}{n+1} + 1 + \frac{(-1)^{1+k}}{n+1} + (-1)^{1+k} \right] U_{1,n}^1. \quad (23)$$

The coefficients C_k are obtained from the relation Eq. (21).

The integrals

$$U_{n,k}^1 = \int_0^1 P_n^1(\xi) P_k^1(\xi) d\xi, \quad (24)$$

can also be evaluated analytically. For their expressions, see Eq. (A20) in the Appendix.

In the derivation of Eq. (22), the relation

$$\int_{-1}^0 P_n^1(\xi) P_k^1(\xi) d\xi = (-1)^{n+k} \int_0^1 P_n^1(\xi) P_k^1(\xi) d\xi, \quad (25)$$

is used. The relation Eq. (25) follows from the even/odd properties of the associated Legendre functions.

Again, the required coefficients are solved from an $N \times N$ matrix equation.

III. POLARIZABILITY OF A HEMISPHERE

If $\epsilon_{r2} = 1$, only one hemisphere is left. As stated before, the main component of the secondary electric field caused by the polarization of the object is the dipolar one. The polarized object can therefore be approximated using an electric dipole. The induced dipole moment **p** can be determined by comparing the dipolar term of the series expansion of the potential function with the potential function of an electric dipole, which is of the form[1]

$$\phi_d(\mathbf{r}) = \frac{\mathbf{p} \cdot \mathbf{u}_r}{4\pi\epsilon_e r^2}. \tag{26}$$

In the axial case the dipole is z-directed. The potential Eq. (26) becomes

$$\phi_d(\mathbf{r}) = \frac{\mathbf{p} \cdot \mathbf{u}_r}{4\pi\epsilon_e r^2} = \frac{p \cos\theta}{4\pi\epsilon_e r^2}, \tag{27}$$

and the dipolar term in the series expansion Eq. (9) is

$$\phi_d(\mathbf{r}) = \frac{B_1}{r^2} P_1(\xi) = \frac{B_1}{r^2} \cos\theta. \tag{28}$$

Therefore, the magnitude of the dipole moment is

$$p = 4\pi\epsilon_e B_1, \tag{29}$$

and the normalized axial polarizability becomes

$$\alpha_{zn} = \frac{p}{E_e \epsilon_e V} = 6\frac{B_1}{E_e a^3}. \tag{30}$$

To determine the polarizability, only the coefficient B_1 is needed. However, it cannot be solved separately. Instead, an $N \times N$ matrix equation must be constructed and all coefficients up to B_N must be solved.

In the transversal case the dipole is along the x axis. The potential of the dipole becomes

$$\phi_d(\mathbf{r}) = \frac{\mathbf{p} \cdot \mathbf{u}_r}{4\pi\epsilon_e r^2} = \frac{p \sin\theta \cos\varphi}{4\pi\epsilon_e r^2}. \tag{31}$$

The dipolar term in the series expansion Eq. (20) is of the form

$$\phi_d(\mathbf{r}) = \frac{B_1}{r^2} \sin\theta \cos\varphi. \tag{32}$$

Again, the magnitude of the dipole moment becomes

$$p = 4\pi\epsilon_e B_1, \tag{33}$$

and the normalized transversal polarizability is also determined by

$$\alpha_{tn} = 6\frac{B_1}{E_e a^3}. \tag{34}$$

IV. RESULTS

The normalized polarizabilities of a hemisphere only depend on the relative permittivity. Next, the convergence of
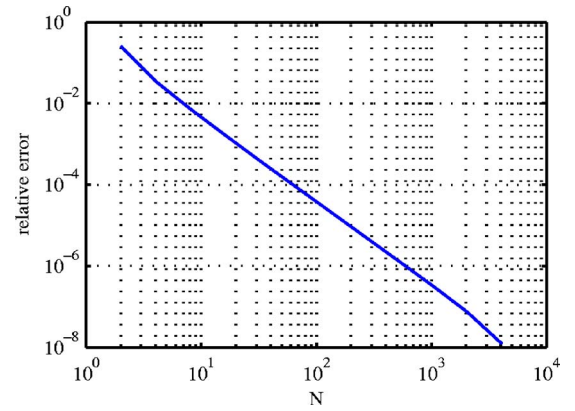

FIG. 4. (Color online) Relative error of the normalized axial polarizability as a function of matrix size N when $\epsilon_r = 10$.

the result is studied as a function of the size N of the matrix equation by choosing a hemisphere with relative electric permittivity $\epsilon_r = 10$ and computing its normalized axial polarizability α_{zn}. Let us assume that the result converges toward the real physical value, and the matrix size $N = 6500$ already gives a very accurate result α_{acc}. Now, if the polarizabilities with $N = 2^0, 2^1, 2^2, \ldots, 2^{12}$ are computed, the relative error

$$e_{rel} = \frac{|\alpha_{acc} - \alpha_{zn}|}{\alpha_{acc}},$$

can be calculated.

Figure 4 shows the relative error as a function of N. It can be seen that, already, with $N > 20$ the relative error is less than 1%. Choosing $N > 200$ should approximatively give the accuracy of 10^{-5}. The accuracies of the order of 10^{-7}, however, require $N > 1700$. The value of the permittivity ϵ_r affects the speed of convergence very little.

There are no large differences in convergence between the axial and the transversal case. In the transversal case, the result however seems to converge even slightly faster.

Figure 5 presents the normalized axial and transversal polarizabilities α_{zn} and α_{tn} of a hemisphere as functions of relative permittivity ϵ_r computed with matrix size $N = 200$. In addition, comparative results are computed using COMSOL MULTIPHYSICS, which is a commercial software based on the finite element method, FEM. The results coincide very well.
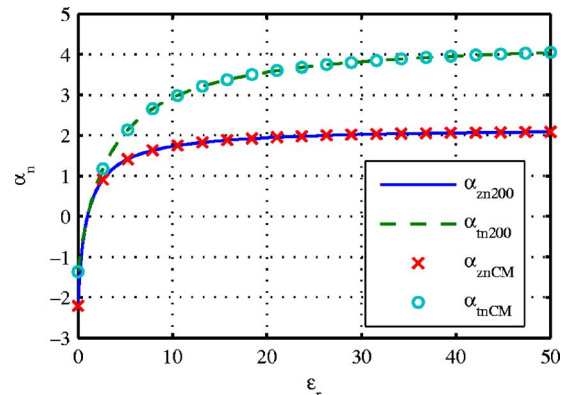

FIG. 5. (Color online) Normalized axial and transversal polarizabilities of a hemisphere as a function of relative permittivity compared with the numerical results computed using COMSOL MULTIPHYSICS.
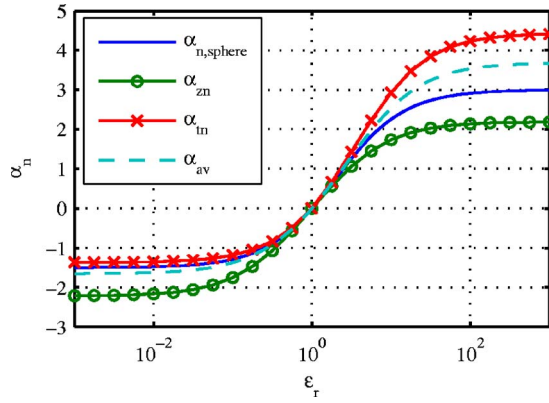
FIG. 6. (Color online) Normalized axial and transversal polarizabilities of a hemisphere and their average compared with the polarizability of a homogeneous sphere as a function of relative permittivity.

The relative error for both polarizabilities is in the worst case only of the order of 10^{-5}.

Figure 6 presents the normalized axial and transversal polarizabilities of a hemisphere as a function of relative permittivity on a logarithmic scale computed with matrix size $N = 200$. They are compared with the normalized polarizability of a homogeneous sphere $\alpha_{n,\text{sphere}}$. It can be noted that α_{zn} has values smaller and α_{tn} greater than the homogeneous sphere. However, the sphere and the hemisphere are not comparable as objects in this way because the three-dimensional characteristics of the hemisphere must be taken into consideration. Therefore, the average normalized polarizability of the hemisphere, $\alpha_{\text{av}} = (\alpha_{zn} + 2\alpha_{tn})/3$, is computed and plotted. It can be seen that its absolute value is always greater than the one of the homogeneous sphere computed at certain permittivity value.

These observations seem reasonable. The dimension of the hemisphere in the transversal direction is twice as large as in the axial direction. Therefore, it is expected that its response to the electric field in the transversal direction becomes larger than in the axial direction. Also, the behavior of the average polarizability of the hemisphere makes sense, since it is known that the sphere is the geometry with the minimum absolute value of the polarizability. Any deviation from spherical symmetry therefore increases the magnitude of the average polarizability of the object.[13,14]

V. APPROXIMATIVE FORMULAS

Let us next form approximative formulas for the normalized polarizabilities by finding a fit with the computed results. It is convenient to write the formulas as Padé approximations which are of the form

$$\alpha_n(\epsilon_r) \approx \frac{P(\epsilon_r)}{Q(\epsilon_r)}, \tag{35}$$

where $P(\epsilon_r)$ and $Q(\epsilon_r)$ are polynomials of the mth order. The higher the order m is, the better the accuracy of the approximation becomes. However, with large m, the formulas become very complicated with many parameters to be fitted. In this case, the order $m = 4$ is a good compromise.

By determining the values of the polarizability beforehand at certain permittivities, the number of fitted parameters can be reduced. Let us denote $\alpha_0 = \alpha(0)$ and $\alpha_\infty = \alpha(\epsilon_r)$, when $\epsilon_r \rightarrow \infty$. The polarizability α_∞ can be solved by deriving new equation systems by substituting $\epsilon_{r1} \rightarrow \infty$ into Eqs. (12) and (22). The division by zero in computation of the polarizability with $\epsilon_r = 0$ can be avoided by turning the hemisphere around and choosing $\epsilon_{r1} = 1$ and $\epsilon_{r2} = 0$. Also, naturally $\alpha(1) = 0$.

In the axial case these values become $\alpha_0 \approx -2.215\,15$ and $\alpha_\infty \approx 2.189\,38$ and in the transversal case $\alpha_0 \approx -1.368\,53$ and $\alpha_\infty \approx 4.430\,30$.

The approximative equations become

$$\alpha_{zn}(\epsilon_r) \approx 2.18938(\epsilon_r - 1)\frac{\epsilon_r^3 + 4.91591\epsilon_r^2 + 6.45198\epsilon_r + 2.21515}{\epsilon_r^4 + 6.35053\epsilon_r^3 + 12.8989\epsilon_r^2 + 9.48877\epsilon_r + 2.18938}, \tag{36}$$

and

$$\alpha_{tn}(\epsilon_r) \approx 4.43030(\epsilon_r - 1)\frac{\epsilon_r^3 + 4.05220\epsilon_r^2 + 4.51906\epsilon_r + 1.36853}{\epsilon_r^4 + 7.71930\epsilon_r^3 + 18.7410\epsilon_r^2 + 16.5759\epsilon_r + 4.43030}. \tag{37}$$

The average normalized polarizability can be computed as $\alpha_{\text{av}} = (\alpha_{zn} + 2\alpha_{tn})/3$ or using the approximative formula,

$$\alpha_{\text{av}}(\epsilon_r) \approx 3.68332(\epsilon_r - 1)\frac{\epsilon_r^3 + 4.31762\epsilon_r^2 + 5.08292\epsilon_r + 1.65074}{\epsilon_r^4 + 7.54217\epsilon_r^3 + 17.5848\epsilon_r^2 + 14.5778\epsilon_r + 3.68332}. \tag{38}$$

With permittivity values $\epsilon_r \geq 0$, the absolute errors of these formulas are always less than 10^{-5}.

VI. CONCLUSIONS

In this article, the polarizability of a homogeneous hemispherical object was considered. The polarizability consisted of two components, the axial polarizability α_z and the transversal polarizability α_t. A method, based on an analytical approach where the potential functions were written as series expansions, was presented. However, the coefficients of the expansions could not be solved separately and an equation

system of N equations each including a sum over N terms was constructed and written as a matrix equation. All matrix elements, however, were analytically evaluable. With large matrices, this method provided very accurate results. Also, easy-to-use approximative formulas for the polarizabilities were presented. Hopefully, the reader will find these results useful. At least, they provide a reliable reference in testing numerical methods.

The polarizability of the object does not, however, give the whole picture of the electric response of the object because the polarizability is determined only by the dipolar part of the response. Only for spheres is the response purely dipolar. Deviations from elliptic geometries give rise to higher order field components. These components, however, decay very fast as a function of distance. For example, in the case of the hemisphere, the sharp edge has a significant effect on the electric response. The electric field is actually known to be singular near the edge.[15,16]

The method described in this article is based on solving all the coefficients of the series expansion outside the hemisphere. This means that also the higher order components up to the order N can be determined at the same time. Also, the expressions for the coefficients inside the hemisphere are presented. Therefore, it is possible to solve the potential functions and the electric fields in the whole space.

An obvious situation would be a dielectric hemisphere located for example in vacuum where $\epsilon_r = \epsilon_i/\epsilon_e > 1$. This method can also be used in a situation of a hemispherical hole in a dielectric environment where $0 < \epsilon_r < 1$. In computation there are actually no restrictions for even negative values of permittivity. The interest toward the negative permittivity has increased along with the research of artificial materials with tunable material parameters. Also, for metals with optical and UV frequencies, the real part of permittivity can actually be negative. The electric response of an object can be assumed to behave somewhat differently with negative values of permittivity than with positive, natural, permittivities. This can be seen also from Eq. (2). With $\epsilon_r = -2$, the polarizability of a sphere is singular. In the case of the hemisphere the situation seems much more complex, providing a new area for future research.

ACKNOWLEDGMENTS

APPENDIX: COMPUTATION OF THE INTEGRALS

Solving the equation systems Eqs. (12) and (22) requires computing the integrals

$$U_{n,k} = \int_0^1 P_n(\xi) P_k(\xi) d\xi, \tag{A1}$$

$$U_{n,k}^1 = \int_0^1 P_n^1(\xi) P_k^1(\xi) d\xi, \tag{A2}$$

where $P_n^m(\xi)$ are the associated Legendre functions, which can be constructed by using the Legendre polynomials $P_n(\xi)$,[17]

$$P_n^m(\xi) = (-1)^m (1 - \xi^2)^{m/2} \frac{d^m}{d\xi^m} P_n(\xi). \tag{A3}$$

Let us begin with the integral $U_{n,k}^1$. By applying the formula Eq. (A3), it can be written as

$$U_{n,k}^1 = \int_0^1 (1 - \xi^2) \frac{d}{d\xi} P_n(\xi) \frac{d}{d\xi} P_k(\xi) d\xi. \tag{A4}$$

Then, the partial integration gives

$$U_{n,k}^1 = \Big/_0^1 (1 - \xi^2) \frac{d}{d\xi} P_n(\xi) P_k(\xi)$$
$$- \int_0^1 \left[-2\xi \frac{d}{d\xi} P_n(\xi) + (1 - \xi^2) \frac{d}{d\xi^2} P_n(\xi) \right] P_k(\xi) d\xi. \tag{A5}$$

The latter term can be modified by applying the Legendre differential equation,[17]

$$(1 - z^2) \frac{d^2 w(z)}{dz^2} - 2z \frac{dw(z)}{dz} + \left[n(n+1) - \frac{m}{1 - z^2} \right] w(z) = 0. \tag{A6}$$

Therefore, $P_n(\xi)$ satisfies

$$(1 - \xi^2) \frac{d^2}{d\xi^2} P_n(\xi) - 2\xi \frac{d}{d\xi} P_n(\xi) = -n(n+1) P_n(\xi). \tag{A7}$$

Substitution of Eq. (A7) into Eq. (A5) gives

$$U_{n,k}^1 = -\frac{d}{d\xi} P_n(0) P_k(0) + n(n+1) \int_0^1 P_n(\xi) P_k(\xi) d\xi$$
$$= -\frac{d}{d\xi} P_n(0) P_k(0) + n(n+1) U_{n,k}. \tag{A8}$$

Then, by substituting the known values[17]

$$P_n(0) = \frac{1}{\sqrt{\pi}} \cos\left(\frac{\pi}{2} n\right) \frac{\Gamma(n/2 + 1/2)}{\Gamma(n/2 + 1)}, \tag{A9}$$

$$\frac{d}{d\xi} P_n(0) = \frac{2}{\sqrt{\pi}} \sin\left(\frac{\pi}{2} n\right) \frac{\Gamma(n/2 + 1)}{\Gamma(n/2 + 1/2)}, \tag{A10}$$

Eq. (A8) gives

$$U_{n,k}^1 = -\frac{2}{\pi} \sin\left(\frac{\pi}{2} n\right) \cos\left(\frac{\pi}{2} k\right) A_{n,k} + n(n+1) U_{n,k}, \tag{A11}$$

where

$$A_{n,k} = \frac{\Gamma(n/2 + 1)}{\Gamma(n/2 + 1/2)} \frac{\Gamma(k/2 + 1/2)}{\Gamma(k/2 + 1)}. \tag{A12}$$

In the integrals Eqs. (A1) and (A2), the indices n and k can be interchanged. For example,

$$U_{n,k}^1 = \int_0^1 P_n^1(\xi) P_k^1(\xi) \, \mathrm{d}\xi = \int_0^1 P_k^1(\xi) P_n^1(\xi) \, \mathrm{d}\xi = U_{k,n}^1.$$
(A13)

Then, also in the Eq. (A11), indices must be interchangeable. It can be written

$$U_{n,k}^1 = U_{k,n}^1 = -\frac{2}{\pi} \sin\left(\frac{\pi}{2}k\right) \cos\left(\frac{\pi}{2}n\right) A_{k,n} + k(k+1) U_{k,n}.$$
(A14)

One can also note that

$$A_{k,n} = \frac{\Gamma(k/2+1)}{\Gamma(k/2+1/2)} \frac{\Gamma(n/2+1/2)}{\Gamma(n/2+1)} = \frac{1}{A_{n,k}}.$$
(A15)

From Eqs. (A11) and (A14), we obtain

$$U_{n,k} = \frac{2}{\pi} \left[\frac{\sin(\pi/2n)\cos(\pi/2k) A_{n,k}}{n(n+1)-k(k+1)} - \frac{\sin(\pi/2k)\cos(\pi/2n) A_{k,n}}{n(n+1)-k(k+1)} \right].$$
(A16)

The preceding integral can be also found in the literature.[18]

From Eqs. (A11) and (A14), it also follows that

$$U_{n,k}^1 = \frac{2}{\pi} \left[\frac{k(k+1)\sin(\pi/2n)\cos(\pi/2k) A_{n,k}}{n(n+1)-k(k+1)} - \frac{n(n+1)\sin(\pi/2k)\cos(\pi/2n) A_{k,n}}{n(n+1)-k(k+1)} \right].$$
(A17)

Finally, the integral Eq. (A1) can be expressed as

$$U_{n,k} = \begin{cases} \dfrac{1}{2n+1}, & n=k \\ 0, & n \neq k, \quad n+k \quad \text{even} \\ f_{n,k}, & \text{otherwise} \end{cases},$$
(A18)

where

$$f_{n,k} = \frac{2}{\pi} \left[\frac{\sin(\pi/2n)\cos(\pi/2k) A_{n,k}}{n(n+1)-k(k+1)} - \frac{\sin(\pi/2k)\cos(\pi/2n) A_{k,n}}{n(n+1)-k(k+1)} \right],$$
(A19)

and the integral Eq. (A2) as

$$U_{n,k}^1 = \begin{cases} \dfrac{n(n+1)}{2n+1}, & n=k \\ 0, & n \neq k, \quad n+k \quad \text{even} \\ f_{n,k}^1, & \text{otherwise} \end{cases},$$
(A20)

where

$$f_{n,k}^1 = \frac{2}{\pi} \left[\frac{k(k+1)\sin(\pi/2n)\cos(\pi/2k) A_{n,k}}{n(n+1)-k(k+1)} - \frac{n(n+1)\sin(\pi/2k)\cos(\pi/2n) A_{k,n}}{n(n+1)-k(k+1)} \right].$$
(A21)

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