

Electric potential and field between two different spheres

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Abstract

We consider a system of two spheres with different radii embedded in an infinite medium supporting an external uniform electric field. We calculate the electric potential in the whole space and the dipole moment of this system using the bispherical coordinates system. Our method is efficient enough to avoid any simplifying approximation concerning the system geometry, the external field orientation and the conductivity of the spheres. © 1998 Elsevier Science B.V. All rights reserved.

Keywords: Bispherical coordinates; Solution of Laplace's equation; Electric field between spheres; Solution of recursive equations

1. Introduction

Calculation of field or potential distributions and dipole moment associated with a regular body (sphere, ellipsoid, cube) in equilibrium with an external static field is a usual chapter of electrostatic textbooks [1–3]. Numerical calculations are necessary when the body shape is irregular. It is classical to solve the problem of two bodies in an external static field by analytical methods when the shape of the bodies is adapted to a coordinate system in which the Laplace equation can be solved (i.e. if the variables separation is possible) [4,5].

In this work we consider the classical problem of two different spheres embedded in a homogeneous and infinite medium supporting, in the absence of the spheres, a uniform static field arbitrarily oriented. The solution of the Laplace equation in the bispherical coordinates system leads us to the potential and field distributions in the whole space, especially in the area between the two spheres. Our method of resolution works in the case of spheres with different radii and with real or complex dielectric functions: it goes beyond any previous works carried out because we need no

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restrictive hypothesis [6] either on the system geometry [7–11] or on the field orientation [12] or on the perfect conductivity of the spheres [13–15].

2. Laplace’s equation in bispherical coordinates

Let us consider the bispherical coordinates defined by the three variables (β, α, φ) [4,5] defined in Fig. 1.

$$\beta = -\ln \frac{PL_2}{PL_1} \quad \text{with } -\infty < \beta < \infty, \tag{1}$$

$$\alpha = \widehat{(L_1PL_2)} \quad \text{with } 0 \leq \alpha \leq \pi. \tag{2}$$

φ , the azimuthal angle, is chosen such that $\varphi = 0$ if P belongs to the Ox axis $0 \leq \varphi < 2\pi$. They are related to the rectangular coordinates by the following

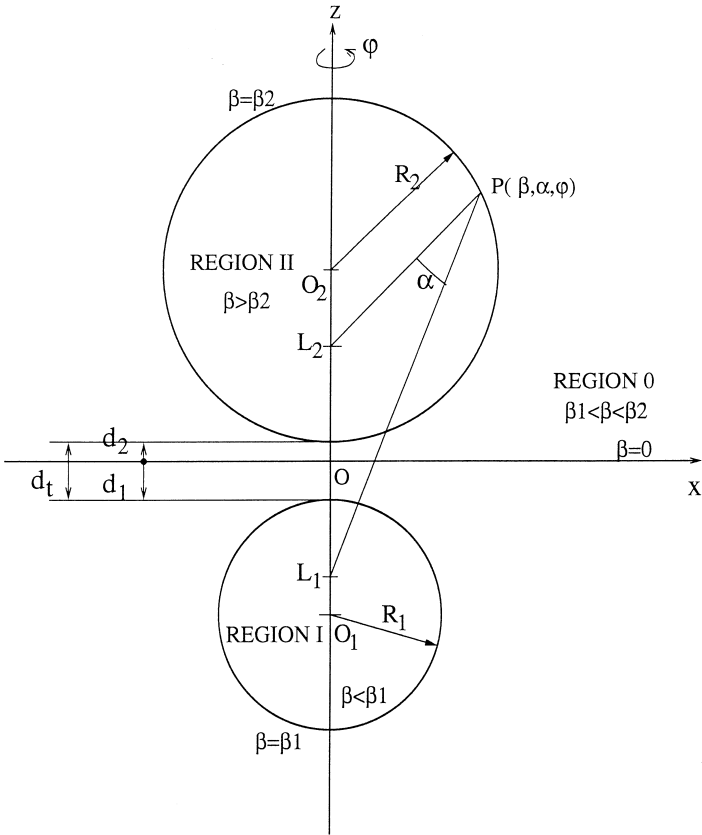


Fig. 1. The system of bispherical coordinates (β, α, φ) .

relations:

$$x = a \sin \alpha \cos \varphi / (\cosh \beta - \cos \alpha), \tag{3}$$

$$y = a \sin \alpha \sin \varphi / (\cosh \beta - \cos \alpha), \tag{4}$$

$$z = a \sinh \beta / (\cosh \beta - \cos \alpha). \tag{5}$$

The parameter $a = OL_1 = OL_2$ is adjusted to the system of two spheres with radii R_1 and R_2 , separated by the total distance d_t as previously done by Stoy [10].

In this coordinate system we solve the Laplace equation $\Delta\psi = 0$ (ψ is the electric potential) by the classical way, detailed in the textbooks by Morse and Feshbach [16] or Stratton [5]. The most general form for the solution of Laplace’s equation is given by

$$\begin{aligned} \psi(\beta, \alpha, \varphi) = aF(\alpha, \beta) & (A_{Ie} e^{-\beta(n+1/2)} + A_{II} e^{\beta(n+1/2)}) \\ & \times [A_{III} P_n^m(\cos \alpha) + A_{IV} Q_n^m(\cos \alpha)] A_V e^{im\varphi} \end{aligned} \tag{6}$$

with $F(\alpha, \beta) = \sqrt{[2(\cosh \beta - \cos \alpha)]}$ and P_n^m and Q_n^m the Legendre polynomials of first and second kinds, respectively ($n \geq 0$ and $-n \leq m \leq n$). As the Q_n^m functions have logarithmic singularities at $\alpha = \pm \pi$ we must have $A_{IV} = 0$.

Oz is a symmetry axis so we separate the cases $\mathbf{E}_{\text{ext}} \parallel Oz$ and $\mathbf{E}_{\text{ext}} \perp Oz$. The first hypothesis restricts m to the single value $m = 0$, then we have a simpler form for Eq. (6):

$$\psi_{\parallel}(\beta, \alpha, \varphi) = aF(\alpha, \beta) (A'_{Ie} e^{-\beta(n+1/2)} + A'_{II} e^{\beta(n+1/2)}) P_n^0(\cos \alpha), \tag{7}$$

where A'_I and A'_{II} are real coefficients and $\psi_{\parallel}(\beta, \alpha, \varphi)$ the solution when $\mathbf{E}_{\text{ext}} \parallel Oz$.

In the second case ($\mathbf{E}_{\text{ext}} \perp Oz$) we have $m = 1$, so the Eq. (6) becomes:

$$\psi_{\perp}(\beta, \alpha, \varphi) = aF(\alpha, \beta) (B'_{Ie} e^{-\beta(n+1/2)} + B'_{II} e^{\beta(n+1/2)}) P_n^1(\cos \alpha) (\cos \varphi + i \sin \varphi), \tag{8}$$

where B'_I and B'_{II} are real coefficients and $\psi_{\perp}(\beta, \alpha, \varphi)$ the solution when the external field lies in the plane perpendicular to the symmetry axis.

The general case is obtained from the superposition of these two contributions.

3. Calculation of the potential

3.1. \mathbf{E}_{ext} parallel to the Oz axis

It is obvious that the potential is obtained from a linear combination of the solutions of the Laplace equation given by the relation (7). We distinguish three different zones.

In the first sphere ($\beta < \beta_1 < 0$):

$$\psi^{(1)} = aF(\alpha, \beta) \sum_{n=0}^{\infty} (E_n e^{(n+1/2)\beta} + F_n e^{-(n+1/2)\beta}) P_n(\cos \alpha). \tag{9}$$

In the second sphere ($\beta < \beta_2 < 0$):

$$\psi^{(2)} = aF(\alpha, \beta) \sum_{n=0}^{\infty} (A_n e^{(n+1/2)\beta} + B_n e^{-(n+1/2)\beta}) P_n(\cos \alpha). \tag{10}$$

In the embedding medium ($\beta_1 < \beta < \beta_2$) we add the contribution of the external field separately to obtain the following expansion:

$$\psi^{(0)} = -E_{\text{ext}}z + aF(\alpha, \beta) \sum_{n=0}^{\infty} (C_n e^{(n+1/2)\beta} + D_n e^{-(n+1/2)\beta}) P_n(\cos \alpha) \tag{11}$$

with $E_{\text{ext}} = \|E_{\text{ext}}\|$.

To achieve the resolution of the problem, the six coefficients A_n, B_n, C_n, D_n, E_n and F_n must be determined for each value n in the summation. Physically, the electric potential remains finite in the spheres including the points L_1 and L_2 ($\beta \rightarrow \pm \infty$) which implies $A_n = F_n = 0$ for $n \geq 0$. The potential functions are continuous across the surfaces of the spheres, hence we have $\psi^{(1)}(\beta_1) = \psi^{(0)}(\beta_1)$ and $\psi^{(2)}(\beta_2) = \psi^{(0)}(\beta_2)$.

z is developed in terms of Legendre’s polynomials [17] to obtain $\psi^{(0)}$ as a combination of Legendre’s polynomials only. Then the continuity of the potential gives the two relations:

$$E_n = E_{\text{ext}}(2n + 1) + C_n + D_n e^{-(2n+1)\beta_1}, \tag{12}$$

$$B_n = -E_{\text{ext}}(2n + 1) + D_n + C_n e^{-(2n+1)\beta_2}. \tag{13}$$

These two relations, (12) and (13), show that the potential is exactly known if C_n and D_n are determined. Two additional equations are needed to compute the coefficients C_n and D_n . The continuity of the normal component of the displacement vector across the interfaces between the spheres and the embedding medium gives us these two relations. The first one is

$$\epsilon_1 \left(\frac{\partial \psi^{(1)}}{\partial \beta} \right)_{\beta_1} = \epsilon_0 \left(\frac{\partial \psi^{(0)}}{\partial \beta} \right)_{\beta_1}. \tag{14}$$

We introduce the expansions (9) and (11) into this relation; a simple but tedious calculation [18], leads to

$$\begin{aligned} C_n U_n^{c1} + C_{n-1} V_n^{c1} + C_{n+1} W_n^{c1} + D_n U_n^{d1} + D_{n-1} V_n^{d1} + D_{n+1} W_n^{d1} \\ = E_{\text{ext}} S_n^1. \end{aligned} \tag{15}$$

In the same way, the second relation

$$\epsilon_2 \left(\frac{\partial \psi^{(2)}}{\partial \beta} \right)_{\beta_2} = \epsilon_0 \left(\frac{\partial \psi^{(0)}}{\partial \beta} \right)_{\beta_2}, \tag{16}$$

takes the new form with Eqs. (10) and (11)

$$\begin{aligned} C_n U_n^{c2} + C_{n-1} V_n^{c2} + C_{n+1} W_n^{c2} + D_n U_n^{d2} + D_{n-1} V_n^{d2} + D_{n+1} W_n^{d2} \\ = E_{\text{ext}} S_n^2. \end{aligned} \tag{17}$$

See the appendix for detailed expressions of the coefficients U, V, W, S .

It is important to point out that Eqs. (15) and (17) cannot be used when $d_t = 0$ and $\varepsilon_0 = \varepsilon_1$ or $\varepsilon_0 = \varepsilon_2$. If $n = 0$ the coefficients C_{-1} and D_{-1} are not defined but $V_0^{c1} = V_0^{c2} = V_0^{d1} = V_0^{d2} = 0$ so Eqs. (15) and (17) always hold for $n \geq 0$. The special case $R_1 = R_2$ and $\varepsilon_1 = \varepsilon_2$ gives $C_n = -D_n$ and we find an antisymmetric potential as in the previous papers of Love [9] and Stoy [10]. Before solving the recursive Eqs. (15) and (17) we must investigate the case $\mathbf{E}_{\text{ext}} \perp Oz$.

3.2. \mathbf{E}_{ext} perpendicular to the Oz axis

The potential in the different areas is now determined from the following expressions if $\mathbf{E}_{\text{ext}} \parallel Ox$.

In the first sphere ($\beta < \beta_1 < 0$):

$$\psi^{(1)} = aF(\alpha, \beta) \sum_{n=1}^{\infty} (E'_n e^{(n+1/2)\beta} + F'_n e^{-(n+1/2)\beta}) P_n^1(\cos \alpha) \cos \varphi. \tag{18}$$

In the second sphere ($\beta > \beta_2 > 0$):

$$\psi^{(2)} = aF(\alpha, \beta) \sum_{n=1}^{\infty} (A'_n e^{(n+1/2)\beta} + B'_n e^{-(n+1/2)\beta}) P_n^1(\cos \alpha) \cos \varphi. \tag{19}$$

In the embedding medium ($\beta_1 < \beta < \beta_2$):

$$\psi^{(0)} = -E_{\text{ext}}x + aF(\alpha, \beta) \sum_{n=1}^{\infty} (C'_n e^{(n+1/2)\beta} + D'_n e^{-(n+1/2)\beta}) P_n^1(\cos \alpha) \cos \varphi. \tag{20}$$

In this case we have $A'_n = F'_n = 0$. x is expressed in terms of Legendre's polynomials [17] and to satisfy the continuity across the surfaces of the spheres we obtain

$$B'_n = -2E_{\text{ext}} + D'_n + C'_n e^{(2n+1)\beta_2}, \tag{21}$$

$$E'_n = -2E_{\text{ext}} + C'_n + D'_n e^{-(2n+1)\beta_1}. \tag{22}$$

The two recursive equations equivalent to Eqs. (15) and (17) are obtained from the continuity of the displacement vector as in the previous case:

$$C'_n U_n^{c'1} + C'_{n-1} V_n^{c'1} + C'_{n+1} W_n^{c'1} + D'_n U_n^{d'1} + D'_{n-1} V_n^{d'1} + D'_{n+1} W_n^{d'1} = E_{\text{ext}} S_n^1 \tag{23}$$

and

$$C'_n U_n^{c'2} + C'_{n-1} V_n^{c'2} + C'_{n+1} W_n^{c'2} + D'_n U_n^{d'2} + D'_{n-1} V_n^{d'2} + D'_{n+1} W_n^{d'2} = E_{\text{ext}} S_n^2. \tag{24}$$

(The coefficients U', V', W', S' are also listed in the appendix.) The vanishing of $V_0^{c'1} = V_0^{c'2} = V_0^{d'1} = V_0^{d'2} = 0$ assesses the validity of Eqs. (23) and (24) for $n \geq 1$.

As a partial conclusion let us notice that it is sufficient to solve the recursive Eqs. (15), (17), (23) and (24) to find the potential everywhere in the space if two spheres

are embedded in a homogeneous medium with an external uniform field E_{ext} arbitrarily oriented from the Oz axis. The following section explains our method to solve these equations. This method is more general than Lin and Jin’s method [12] based on the inverse transformation and restricted to the external field parallel to the Oz axis.

4. Solution of the recursive equations

Starting from Eqs. (15) and (17) it is possible to express C_n and D_n in terms of D_n, D_{n+1}, D_{n-1} and C_n, C_{n+1}, C_{n-1} , respectively. One usual technique to reach such an expression is based on the application of Green’s function method for difference equation as suggested by Milne-Thomson [19] and used by Love [9]. Green’s functions $G_{n,N}$ and $H_{n,N}$ are the solutions of the two difference equations:

$$U_n^{c2}G_{n,N} + V_n^{c2}G_{n-1,N} + W_n^{c2}G_{n+1,N} = \delta_{n,N}, \quad N = 0, \dots, \infty, \tag{25}$$

$$U_n^{d1}H_{n,N} + V_n^{d1}H_{n-1,N} + W_n^{d1}H_{n+1,N} = \delta_{n,N}, \quad N = 0, \dots, \infty, \tag{26}$$

where δ is the Kronecker symbol. These two relations (25) and (26) are valid for $n \geq 0$ and $N \geq 0$.

The solution of Eq. (15) is obtained from Eq. (25) as

$$C_n = \sum_{N=0}^{\infty} G_{n,N}(E_{\text{ext}}S_N^2 - D_NU_N^{d2} - D_{N-1}V_N^{d2} - D_{N-1}W_N^{d2}) = \sum_{N=0}^{\infty} G_{n,N}\bar{D}_N \tag{27}$$

and the solution of Eq. (17) from Eq. (26):

$$D_n = \sum_{N=0}^{\infty} H_{n,N}(E_{\text{ext}}S_N^1 - C_NU_N^{c1} - C_{N-1}V_N^{c1} - C_{N-1}W_N^{c1}) = \sum_{N=0}^{\infty} H_{n,N}\bar{C}_N. \tag{28}$$

Using the complementary difference equation technique previously detailed by Love and the Poincaré–Perron theorem [20] we can build Green’s functions $G_{n,N}$.

$$G_{n+1,N} = p_{n+1}G_{n,N}, \quad n \geq N, \tag{29}$$

$$G_{n-1,N} = q_{n-1}G_{n,N}, \quad n \leq N, \tag{30}$$

$$G_{N,N} = 1/(U_N^{c2} + V_N^{c2}q_{N-1} + W_N^{c2}p_{N+1}), \tag{31}$$

with

$$p_{n+1} = \frac{V_{n+1}^{c2}}{-U_{n+1}^{c2} - W_{n+1}^{c2} \times \frac{V_{n+2}^{c2}}{-U_{n+2}^{c2} - W_{n+2}^{c2} \times \dots}}, \tag{32}$$

$$q_{n-1} = \frac{W_{n-1}^{c2}}{-U_{n-1}^{c2} - V_{n-1}^{c2} \times \frac{W_{n-2}^{c2}}{-U_{n-2}^{c2} - V_{n-2}^{c2} \times \dots}}. \tag{33}$$

The coefficients p_n and q_n are continued fractions (p_n is an infinite one and q_n a finite one) and their limits if $n \rightarrow +\infty$ are $p_n \rightarrow e^{-2\beta_2}$ and $q_n \rightarrow 1$. We obtain, finally, the expression for the C_n coefficients:

$$C_n = \sum_{N=0}^{\infty} \frac{\overline{\overline{D_N}}}{q_{N-1}V_N^{c2} + U_N^{c2} + p_{N-1}W_N^{c2}} \times \left(\underbrace{\delta_{n,N} + \Theta(N-n) \prod_{l=n}^{N-1} q_l}_{G_{n,N} \text{ if } n < N} + \underbrace{\Theta(n-N) \prod_{l=N+1}^n p_l}_{G_{n,N} \text{ if } n > N} \right) \tag{34}$$

where $\Theta(N - n)$ is the Heaviside step function.

From Eqs. (26) and (28), the same derivation gives the D_n coefficients:

$$D_n = \sum_{N=0}^{\infty} \frac{\overline{\overline{C_N}}}{r_{N-1}V_N^{d1} + U_N^{d1} + s_{N-1}W_N^{d1}} \times \left(\underbrace{\delta_{n,N} + \Theta(N-n) \prod_{l=n}^{N-1} r_l}_{H_{n,N} \text{ if } n < N} + \underbrace{\Theta(n-N) \prod_{l=N+1}^n s_l}_{H_{n,N} \text{ if } n > N} \right) \tag{35}$$

(r_l and s_l have the same form as q_l and p_l , respectively, with subscript $d1$.)

Eqs. (34) and (35) are exact for $n = 0, \dots, \infty$. For the value $n = 0$, we obtain C_0 as a function of all the coefficients D_n and D_0 as a function of all the coefficients C_n :

$$C_0 = \sum_{N=0}^{\infty} \frac{\overline{\overline{D_N}}}{q_{N-1}V_N^{c2} + U_N^{c2} + p_{N-1}W_N^{c2}} \left(\delta_{0,N} + \prod_{l=0}^{N-1} q_l \right), \tag{36}$$

$$D_0 = \sum_{N=0}^{\infty} \frac{\overline{\overline{C_N}}}{r_{N-1}V_N^{d1} + U_N^{d1} + s_{N-1}W_N^{d1}} \left(\delta_{0,N} + \prod_{l=0}^{N-1} r_l \right). \tag{37}$$

Until now, we have not used the fact that the two recursive Eqs. (15) and (17) link the same coefficients C_n and D_n . So with Eqs. (15) and (17), C_{n+1} and D_{n+1} can be expressed as functions of $C_n, D_n, C_{n-1}, D_{n-1}$:

$$C_{n+1} = (\overline{\overline{Z_n^{(2)}}}W_n^{d1} - \overline{\overline{Z_n^{(1)}}}W_n^{d2})/\det_n, \tag{38}$$

$$D_{n+1} = (\overline{\overline{Z_n^{(1)}}}W_n^{c2} - \overline{\overline{Z_n^{(2)}}}W_n^{c1})/\det_n, \tag{39}$$

with

$$\det_n = W_n^{c2} W_n^{d1} - W_n^{d2} W_n^{c1} ,$$

$$\overline{Z_n^{(1)}} = E_{\text{ext}} S_n^1 - C_n U_n^{c1} - C_{n-1} V_n^{c1} - D_n U_n^{d1} - D_{n-1} V_n^{d1} ,$$

$$\overline{Z_n^{(2)}} = E_{\text{ext}} S_n^2 - C_n U_n^{c2} - C_{n-1} V_n^{c2} - D_n U_n^{d2} - D_{n-1} V_n^{d2} .$$

From the relations (38) and (39) we deduce all the coefficients C_n and D_n as a function of C_0 and D_0 . Eqs. (36) and (37) are transcendental ones, it is not possible to solve them analytically to express C_0 and D_0 , so we need to compute these two coefficients and obtain afterwards, the C_n and D_n values by increasing the parameter n . Now, we are able to express E_n and B_n from relations (12) and (13) and the potential $\psi(\beta, \alpha, \varphi)$ take an explicit form in the whole space (relations (9)–(11)) when the electric field is parallel to the Oz axis. The same process also works to obtain the contribution given by an external field perpendicular to the Oz axis and the superposition of these two contributions give the total electric potential everywhere. The electric field in bispherical coordinates is obtained by

$$E_{\text{res}}(\beta, \alpha, \varphi) = - \nabla \psi(\beta, \alpha, \varphi) = - \frac{(\cosh \beta - \cos \alpha)}{a} \left(\frac{\partial \psi}{\partial \beta}, \frac{\partial \psi}{\partial \alpha}, \frac{\partial \psi}{\partial \varphi} \times \frac{1}{\sin \alpha} \right). \tag{40}$$

As an extension of the calculation we can perform a multipole expansion of the perturbative part of the potential due to the two spheres.

In the case E_{ext} parallel to the Oz axis the contribution of the spheres to the total potential is $\psi_p^{(0)} = \psi^{(0)} + E_{\text{ext}} z$ and we express it as decreasing powers of z with $\alpha = 0$ and $\beta \rightarrow 0$:

$$\psi_p^{(0)} = \frac{1}{z} \times \underbrace{2a^2 \sum_{n=0}^{\infty} (C_n + D_n)}_Q + \frac{1}{z^2} \times \underbrace{2a^3 \sum_{n=0}^{\infty} (2n + 1)(C_n - D_n)}_{P_z} + \dots \tag{41}$$

The first term is the net charge Q and its value is $Q = 0$ (no initial electric charge on the spheres), so $\sum_{n=0}^{\infty} (C_n + D_n) = 0$ and the second term is P_z , the dipole component along the Oz axis.

In the case E_{ext} parallel to the Ox axis, we express the potential due to the two spheres ($\psi_p^{(0)} = \psi^{(0)} + E_{\text{ext}} x$), far away from the spheres, with $\beta = \varphi = 0$ and $\alpha \rightarrow 0$ as decreasing powers of x :

$$\psi_p^{(0)} = \frac{1}{x^2} \times \underbrace{(-2a^3) \sum_{n=1}^{\infty} n(n + 1)(C'_n + D'_n)}_{P_x} + \dots \tag{42}$$

P_x is the dipole moment along the Ox axis. We can express the dipole moment of the spheres through its components: $\mathbf{P} = (P_x, 0, P_z)$

To conclude this section we would like to point out that our method can be generalized to take into account any system of recursion relations with p sets of coefficients: A_n^i, \dots, A_n^p . The previous procedure based on Green's function and difference equation is efficient if the following conditions are fulfilled:

- the recursive equations equivalent to Eqs. (15) and (17) must link three coefficients $A_n^i, A_{n-1}^i, A_{n+1}^i$ for $i = 1, \dots, p$.
- the solutions of the characteristic difference equation must be nondegenerate.
- if A_{n+1}^i are chosen as unknown quantities, they must be expressed as a function of A_n^i, A_{n-1}^i . This implies that Kramers' determinants associated with the n systems of recursive equations (generalization of relations (15) and (17)) are all different from zero. So, for $n \geq 1$, all the A_n^i can be expressed versus A_0^i ($i = 1, \dots, p$).

5. Results

5.1. E_{ext} parallel to the Oz axis

We now display selected results for fixed values of R_1, R_2, d_t and the external field $E_{\text{ext}} = (0, 0, E_0)$. In the first example we have plotted:

1. the curves corresponding to $\|\mathbf{E}_{\text{res}}\| = \text{constant}$
2. the curves corresponding to $\|\mathbf{E}_{\text{res},z}\| = \text{constant}$
3. the curves corresponding to $\|\mathbf{E}_{\text{res},x}\| = \text{constant}$

and for the other cases we restrict the results to the curves (1). The modulus of the resulting field $\|\mathbf{E}_{\text{res}}\|$ is normalized to $\|E_0\|$. Oz is a symmetry axis for the system: we need only to compute the field and its components in the plane (x, z) .

The case of Fig. 2 corresponds to the values $R_1 = 5 \text{ nm}$, $d_t = R_1$, $R_2 = 6R_1$ and $\varepsilon_1 = \varepsilon_2 = 2\varepsilon_0$. In Fig. 2a we have an enhancement of the total field E_{res} in the space between the two spheres and the maximum value corresponds to $E_{\text{res}} = 1.95E_{\text{ext}}$. However, from the dashed curve in Fig. 2a (corresponding to the ratio value 1.05), we see that the perturbation of the field near the sphere R_2 , due to the presence of the sphere, R_1 is very localized: from the centre of the large sphere when the distance exceeds $4R_2$ the field line is not quite perturbed by the presence of the small sphere. From Fig. 2b, we also see that the $E_{\text{res},z}$ component is very close to E_{res} and that is related to the weak values of the $E_{\text{res},x}$ as shown in Fig. 2c. In the same geometry, Stoy [10] has obtained the same behaviour although he has neglected the value $n = 1$ in the solution of the recursive Eqs. (23) and (24).

Our method is not restricted by geometrical limits, so we can take any value for the radii and the distance d_t . In Fig. 3 we have plotted the electric field for the very small value $d_t = 0.3 \text{ nm}$, and $R_1 = 10d_t$, $R_2 = 100d_t$, with $\varepsilon_1 = \varepsilon_2 = 2\varepsilon_0$. The enhancement of E_{res} between the two spheres is also evident but with a larger gradient and a maximum value $E_{\text{res}} = 2.4E_{\text{ext}}$. The low value of d_t induces a stronger interaction of

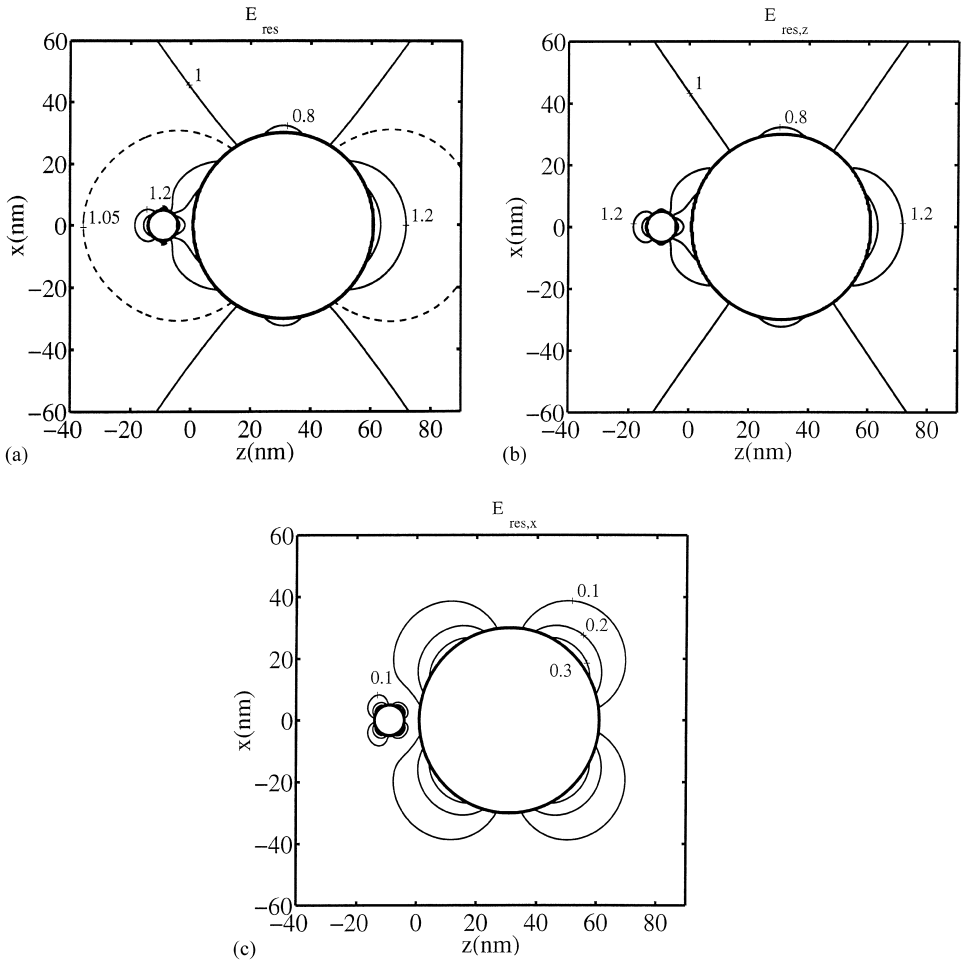


Fig. 2. The contour lines of the electric field around two spheres: $R_1 = 5 \text{ nm}$, $R_2 = 6R_1$ and $d_i = R_i$, $\epsilon_1 = \epsilon_2 = 2\epsilon_0$, $\mathbf{E}_{ext} = z \text{ V/m}$. (a) Iso-modulus curves $E_{res} = \text{constant}$, curves are separated from each other by 0.2 V/m . (b) Curves corresponding to $E_{res,z} = \text{constant}$ (separated by 0.2 V/m). (c) Curves corresponding to $E_{res,x} = \text{constant}$ (separated by 0.1 V/m).

the two spheres as pointed out by the curvature of the lines $E_{res} = \text{constant}$ in the sphere R_2 .

5.2. E_{ext} parallel to the Ox axis

For this orientation of \mathbf{E}_{res} no enhancement of the total electric field occurs between the spheres. This is related to the fact that the value of the normal component of the

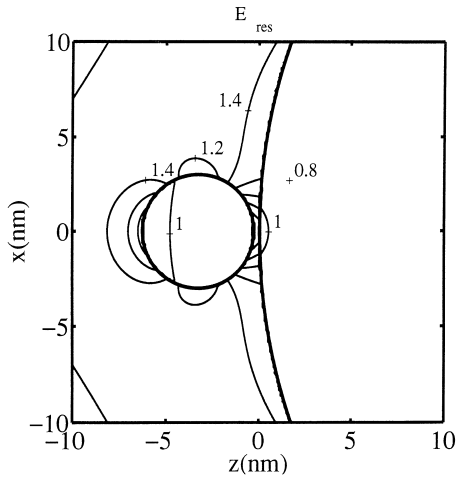


Fig. 3. As for Fig. 2a with $R_1 = 3$ nm, $R_2 = 30$ nm and $d_t = 0.3$ nm, $\epsilon_1 = \epsilon_2 = 2\epsilon_0$ (iso-modulus curves are separated by 0.2 V/m).

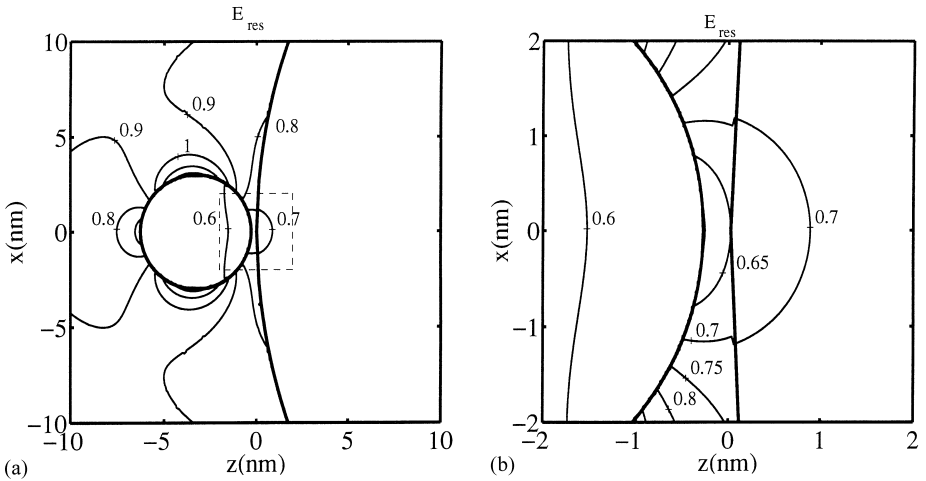


Fig. 4. The contour lines of the electric field around two spheres as in Fig. 3 except the value $E_{ext} = x$ V/m. (a) Iso-modulus curves $E_{res} = \text{constant}$ (separated by 0.1 V/m). (b) Enlargement of the dashed area of (a) (iso-modulus curves are separated by 0.05 V/m).

electric field at the spheres surfaces is very small. For an arrangement like in Fig. 3, the iso-modulus lines $\|E_{res}\| = \text{constant}$ are plotted in Fig. 4a, and Fig. 4b is an enlargement of the area between the spheres.

6. Numerical processing

The first stage of our work is the computation of coefficients C_0 and D_0 from Eqs. (36) and (37). These equations can be written as

$$f(C_0, D_0) = C_0 - \sum_{N=0}^{\infty} \frac{\overline{D}_N}{q_{N-1} V_N^{c2} + U_N^{c2} + p_{N-1} W_N^{c2}} \left(\delta_{0,N} + \prod_{l=0}^{N-1} q_l \right) = 0, \quad (43)$$

$$g(C_0, D_0) = D_0 - \sum_{N=0}^{\infty} \frac{\overline{C}_N}{r_{N-1} V_N^{d1} + U_N^{d1} + s_{N-1} W_N^{d1}} \left(\delta_{0,N} + \prod_{l=0}^{N-1} r_l \right) = 0. \quad (44)$$

We solve this system of two non-linear functions of two variables (or four non-linear functions of four variables if we work with complex numbers) using a routine of NAG library (C05NBF) which is based upon the MINPACK routine HYBRID [21]. From initial values of C_0 and D_0 the NAG routine chooses the correction at each step as a convex combination of the Newton method and scaled gradient direction.

The starting point is to choose $C_0 = 0$ and $D_0 = 0$. From Eqs. (38) and (39) with $n = 1$ it is easy to compute the coefficients C_1 and D_1 . Increasing n and using the coefficients given in appendix (U, V, W, S) we compute \overline{C}_n and \overline{D}_n for any n . Now, we still have to compute $f(C_0, D_0)$ and $g(C_0, D_0)$. \overline{D}_n and \overline{C}_n are obtained from C_n and D_n and the relations (27) and (28). The continued fractions are obtained from the coefficients U, V, W . Once we have all these parameters, we obtain an assessment of $f(C_0, D_0)$ and $g(C_0, D_0)$. The routine NAG computes the new variables C_0 and D_0 and the cycle then starts again until the functions $f(C_0, D_0)$ and $g(C_0, D_0)$ converge to zero.

The computing of all the infinite sums used here, is stopped when the difference between the $(n + 1)$ th and n th orders of the sums normalized by the $(n + 1)$ th order is lower than a predetermined value: the convergence criterion. We provide in Table 1 some results about different values of the convergence criterion and time computing [22] for C_0 and D_0 . We have taken as examples $R_1 = 300$ nm, $R_2 = 30$ nm for $d_t = 5$,

Table 1

d_t (nm)	$\varepsilon_1 = \varepsilon_2$	Criterion	n_{NAG}	Time (s) to compute $C_0, D_0 (C_1, D_1)$	$\ E_{\text{res}}\ $	$n_{\text{iteration}}$
5	2	10^{-6}	8	4.0 (5.5)	2.14835627	215
5	2	10^{-8}	8	5.0 (6.5)	2.14835531	259
3	2	10^{-6}	8	7.0 (10.0)	2.29307728	287
3	2	10^{-8}	8	8.5 (12.0)	2.29307619	344
1	2	10^{-6}	9	37.5 (45.0)	2.50104052	528
1	2	10^{-8}	8	38.0 (52.5)	2.50104170	628
5	(-6.29 + i2.04216)	10^{-6}	8	5.5 (5.5)	55.93995802	200
5	(-6.29 + i2.04216)	10^{-8}	8	6.5 (6.5)	55.93998348	244
3	(-6.29 + i2.04216)	10^{-6}	8	10.0 (10.0)	127.22515855	254
3	(-6.29 + i2.04216)	10^{-8}	8	12.5 (12.0)	127.22521565	311
1	(-6.29 + i2.04216)	10^{-6}	8	44.5 (45.5)	406.35362358	455
1	(-6.29 + i2.04216)	10^{-8}	8	53.5 (52.5)	406.35381793	556

3, 1 nm and two different dielectric functions: $\varepsilon_1 = \varepsilon_2 = 2\varepsilon_0$ and $\varepsilon_1 = \varepsilon_2 = (-6.29 + i2.04216)\varepsilon_0$ (which is the ε gold value at 2.3 eV).

Here n_{NAG} is the number of iterations for the routine NAG to find C_0, D_0 with $f(C_0, D_0)$ and $g(C_0, D_0)$ lower than 10^{-10} , $\|E_{\text{res}}\|$ is the field computed at the origin ($x = y = z = 0$) and $n_{\text{iteration}}$ the number of iterations to obtain $\|E_{\text{res}}\|$ at this point.

If the dielectric constant increases, the convergence is slower. We have the same behaviour when d_t decreases (if $d_t = 0, \beta_1 = \beta_2 = 0$ then the programme is breaking down because the exponential in the coefficients U, V, W, S vanishes).

For the coefficients C_1 and D_1 the time of computation are quite the same.

The advantage of this processing compared to other methods which discretize the spheres (finite difference, finite elements, discrete dipole approximation) is that we need only a little of memory (lower than 3 Mo in our case).

7. Conclusions

We have solved the Laplace equation in the bispherical coordinate system for two different spheres embedded in a uniform field without any simplifying approximation. Our method allows us to study the electric interaction between these spheres. Such a solution is also suitable for the case of two non-perfectly conductive spheres illuminated by an electromagnetic wave, if the geometry satisfies the Rayleigh approximation ($R_1 + R_2 + d_t \ll \lambda/10$). In this case, the Laplace equation is a really good approximation for the Helmholtz equation [23] and we obtain the local field between two absorbing spheres. From this point of view we can use it in many cases of physical interest such as surface enhanced Raman scattering [24], plasmon resonances [23] of metallic particles whatever their relative distance and radii may be.

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Appendix A. Coefficients of the recursive equations

We first define χ_1 and χ_2 :

$$\chi_1 = (\varepsilon_0 + \varepsilon_1)/(\varepsilon_0 - \varepsilon_1),$$

$$\chi_2 = (\varepsilon_0 + \varepsilon_2)/(\varepsilon_0 - \varepsilon_2),$$

so the coefficients in the Eqs. (15) and (17) can be expressed as

$$U_n^{c1} = -e^{(n+1/2)\beta_1}(0.5 \sinh \beta_1 + (n + \frac{1}{2})\cosh \beta_1),$$

$$U_n^{d1} = e^{-(n+1/2)\beta_1}(-0.5 \sinh \beta_1 + \chi_1(n + \frac{1}{2})\cosh \beta_1),$$

$$V_n^{c1} = \frac{n}{2} e^{(n-1/2)\beta_1}, \quad V_n^{d1} = -\frac{n}{2} \chi_1 e^{-(n-1/2)\beta_1},$$

$$W_n^{c1} = \frac{(n+1)}{2} e^{(n+3/2)\beta_1}, \quad W_n^{d1} = -\frac{(n+1)}{2} \chi_1 e^{-(n+3/2)\beta_1},$$

$$S_n^1 = e^{(n+1/2)\beta_1} (n e^{-\beta_1} - (n+1) e^{\beta_1}),$$

$$U_n^{c2} = -e^{(n+1/2)\beta_2} (0.5 \sinh \beta_2 + \chi_2 (n + \frac{1}{2}) \cosh \beta_2),$$

$$U_n^{d2} = e^{-(n+1/2)\beta_2} (-0.5 \sinh \beta_2 + (n + \frac{1}{2}) \cosh \beta_2),$$

$$V_n^{c2} = \frac{n}{2} \chi_2 e^{(n-1/2)\beta_2}, \quad V_n^{d2} = -\frac{n}{2} e^{-(n-1/2)\beta_2},$$

$$W_n^{c2} = \frac{(n+1)}{2} \chi_2 e^{(n+3/2)\beta_2}, \quad W_n^{d2} = -\frac{(n+1)}{2} e^{-(n+3/2)\beta_2},$$

$$S_n^2 = -e^{-(n+1/2)\beta_2} (n e^{\beta_2} - (n+1) e^{-\beta_2}).$$

The coefficients in Eqs. (23) and (24) have a similar form:

$$U_n^{c'1} = -e^{(n+1/2)\beta_1} (\sinh \beta_1 + (2n+1) \cosh \beta_1),$$

$$U_n^{d'1} = e^{-(n+1/2)\beta_1} (-\sinh \beta_1 + \chi_1 (2n+1) \cosh \beta_1),$$

$$V_n^{c'1} = (n-1) e^{(n-1/2)\beta_1}, \quad V_n^{d'1} = -(n-1) \chi_1 e^{-(n-1/2)\beta_1},$$

$$W_n^{c'1} = (n+2) e^{(n+3/2)\beta_1}, \quad W_n^{d'1} = -(n+2) \chi_1 e^{-(n+3/2)\beta_1},$$

$$S_n^1 = 2e^{(n+1/2)\beta_1} (-e^{\beta_1} + e^{-\beta_1}),$$

$$U_n^{c'2} = -e^{(n+1/2)\beta_2} (\sinh \beta_2 + \chi_2 (2n+1) \cosh \beta_2),$$

$$U_n^{d'2} = e^{-(n+1/2)\beta_2} (-\sinh \beta_2 + (2n+1) \cosh \beta_2),$$

$$V_n^{c'2} = (n-1) \chi_2 e^{(n-1/2)\beta_2}, \quad V_n^{d'2} = -(n-1) e^{-(n-1/2)\beta_2},$$

$$W_n^{c'2} = (n+2) \chi_2 e^{(n+3/2)\beta_2}, \quad W_n^{d'2} = -(n+2) e^{-(n+3/2)\beta_2},$$

$$S_n^2 = 2e^{-(n+1/2)\beta_2} (-e^{\beta_2} + e^{-\beta_2}).$$

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