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Electrostatic potential of point charges inside dielectric oblate spheroids

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Abstract

As a sequel to a previous paper on electrostatic potential of point charges inside dielectric prolate spheroids [J. Electrostatics 66 (2008) 549-560], this note further presents the exact solution to the electrostatic problem of finding the electric potential of point charges inside a dielectric oblate spheroid that is embedded in a dissimilar dielectric medium. Numerical experiments have demonstrated the convergence of the proposed series solutions.

Keywords

Electrostatic potential; Oblate spheroid; Poisson equation; Linearized Poisson-Boltzmann equation; Spheroidal wave function

1. Introduction

As in [1], this note concerns the exact solution to the electrostatic problem of finding the electric potential of point charges inside a dielectric cavity that is embedded in a dissimilar dielectric medium. Such a problem may find its application in hybrid explicit/implicit solvent biomolecular simulations, in which biomolecules and a part of solvent molecules within a dielectric cavity are explicitly modeled while a surrounding dielectric continuum is used to model bulk effects of the solvent beyond the cavity [2]. In [1], the exact solution of the problem when the dielectric cavity is either a sphere or a prolate spheroid has been obtained by using the classical electrostatic theory. Following the same procedure as used in [1], this note will present the exact solution of the problem when the dielectric cavity is an oblate spheroid.

By the principle of linear superposition, the electrostatic problem with a single point source charge q inside a dielectric cavity only needs to be considered. It is then well-known that the total electric potential $\Psi_{\text{in}}(\mathbf{r})$ inside the cavity is given by the solution of the Poisson equation

$$\nabla \cdot (\epsilon_i \nabla \Psi_{\text{in}}(\mathbf{r})) = -4\pi q \delta(|\mathbf{r} - \mathbf{r}_s|),$$

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where ε_i is the electric permittivity of the dielectric cavity, $\mathbf{r}_s$ represents the location of the point charge, and $\delta(r)$ denotes the Dirac delta function. Outside the cavity, on the other hand, by assuming that the mobile ion concentration follows the Debye-Hückel theory, the electric field $\Psi_{\text{out}}(\mathbf{r})$ is then given by the solution of the linearized Poisson-Boltzmann equation (LPBE)

$$\nabla^2 \Psi_{\text{out}}(\mathbf{r}) - \lambda^2 \Psi_{\text{out}}(\mathbf{r}) = 0, \quad (1)$$

where λ is the inverse Debye screening length determined by the ionic concentration and the dielectric constant ε_o of the solvent medium exterior to the cavity ($\lambda = 0$ for the pure water solvent). On the interface Γ of the dielectric oblate spheroid and its surrounding dielectric medium, the following two boundary conditions are to be satisfied for the continuities of the potential and the fluxes along the normal direction

$$\Psi_{\text{out}}|_{\Gamma} = \Psi_{\text{in}}|_{\Gamma} \quad \text{and} \quad \varepsilon_o \frac{\partial \Psi_{\text{out}}}{\partial \mathbf{n}}|_{\Gamma} = \varepsilon_i \frac{\partial \Psi_{\text{in}}}{\partial \mathbf{n}}|_{\Gamma}, \quad (2)$$

where $\mathbf{n}$ is the unit outward vector normal to the surface of the cavity.

2. An oblate spheroid immersed in the pure water solvent

Let us first consider a dielectric oblate spheroid of permittivity ε_i centered at the origin and embedded in a homogeneous dielectric medium of permittivity ε_o , as shown in Fig. 1. Let further the z -axis be the non-focal axis of symmetry, and the equation for the oblate spheroid in Cartesian coordinates be

$$\frac{x^2 + y^2}{a_1^2} + \frac{z^2}{a_2^2} = 1, \quad a_1 > a_2.$$

There are several definitions of oblate spheroidal coordinates, and in this note, the oblate spheroidal coordinates (ξ, η, φ) are defined through

$$x = \frac{a}{2} \sqrt{(1+\xi^2)(1-\eta^2)} \cos \varphi, \quad y = \frac{a}{2} \sqrt{(1+\xi^2)(1-\eta^2)} \sin \varphi, \quad z = \frac{a}{2} \xi \eta,$$

where $a = 2\sqrt{a_1^2 - a_2^2}$ is the interfocal distance of the oblate spheroid, $\xi \in [0, \infty)$ is the radial variable, $\eta \in [-1, 1]$ is the angular variable, and $\varphi \in [0, 2\pi]$ is the azimuthal variable, respectively. Under this definition, the surface of constant ξ is an oblate spheroid with interfocal distance a . In particular, when $\xi = 0$, the spheroid is degenerate and flattens to the circular disk in the plane $z = 0$ with radius $a/2$. The inverse transformation from Cartesian coordinates to the oblate spheroidal coordinates is also reported here for convenience.

$$\left\{ \begin{array}{l} \text{when } z \neq 0: \\ \xi = \frac{\sqrt{(4r^2 - a^2) + \sqrt{(4r^2 - a^2)^2 + 16a^2 z^2}}}{2\sqrt{2}a}, \\ \eta = \frac{\sqrt{(4r^2 - a^2) - \sqrt{(4r^2 - a^2)^2 + 16a^2 z^2}}}{2\sqrt{2}a}, \\ \text{when } z=0: \\ \xi = \sqrt{\frac{4r^2}{a^2} - 1}, \eta = 0, \quad \text{if } r \geq \frac{a}{2}, \\ \eta = \pm \sqrt{1 - \frac{4r^2}{a^2}}, \xi = 0, \quad \text{if } r \leq \frac{a}{2}, \\ \text{where } r^2 = x^2 + y^2 + z^2, \text{ and in all cases} \\ \varphi = \arctan \frac{y}{x}. \end{array} \right.$$

Without loss of generality, let a point charge q be located at the point $\mathbf{r}_s = (\xi_0, \eta_0, \varphi_0=0)$ in the plane $y = 0$ inside the dielectric spheroid defined by the equation $\xi = \xi_1$ (so $\xi_1 \xi_0 \geq 0$), as shown in Fig. 1. Outside the spheroid ($\xi_1 \leq \xi$), the total electrostatic potential takes the form

$$\Psi_{\text{out}}(\mathbf{r}) = \frac{q}{\varepsilon_i a} \sum_{n=0}^{\infty} \sum_{m=0}^n (A_{mn} \cos m\varphi + B_{mn} \sin m\varphi) P_n^m(\eta) Q_n^m(i\xi), \quad (3)$$

and inside the spheroid ($0 \leq \xi \leq \xi_1$), it is written as

$$\Psi_{\text{in}}(\mathbf{r}) = \frac{q}{\varepsilon_i |\mathbf{r} - \mathbf{r}_s|} + \frac{q}{\varepsilon_i a} \sum_{n=0}^{\infty} \sum_{m=0}^n (C_{mn} \cos m\varphi + D_{mn} \sin m\varphi) P_n^m(\eta) P_n^m(i\xi), \quad (4)$$

where $i = \sqrt{-1}$, $P_n^m(x)$ and $Q_n^m(x)$ are the associated Legendre functions of the first kind and the second kind, respectively, and A_{mn} , B_{mn} , C_{mn} and D_{mn} are the unknown expansion coefficients.

Note that the general expansion of $1/|\mathbf{r} - \mathbf{r}_s|$ in the oblate spheroidal coordinates is given by [3–5]

$$\frac{1}{|\mathbf{r} - \mathbf{r}_s|} = \frac{1}{a} \sum_{n=0}^{\infty} \sum_{m=0}^n H_{mn} \cos m\varphi P_n^m(\eta_0) P_n^m(\eta) \begin{cases} P_n^m(i\xi_0) Q_n^m(i\xi), & \xi > \xi_0, \\ P_n^m(i\xi) Q_n^m(i\xi_0), & \xi < \xi_0, \end{cases}$$

where

$$H_{mn} = 2i(2n+1)(2 - \delta_{m0})(-1)^m \left[\frac{(n-m)!}{(n+m)!} \right]^2.$$

Here δ_{m0} is the Kronecker delta. Therefore, the total potential inside the oblate spheroid can also be written as

$$\begin{aligned}\Psi_{\text{in}}(\mathbf{r}) = & \frac{q}{\varepsilon_1 a} \sum_{l=0}^{\infty} \sum_{m=0}^n (C_{mn} \cos m\varphi + D_{mn} \sin m\varphi) P_n^m(\eta) P_n^m(i\xi) \\ & + \frac{q}{\varepsilon_1 a} \sum_{n=0}^{\infty} \sum_{m=0}^n H_{mn} \cos m\varphi P_n^m(\eta_0) P_n^m(\eta) \begin{cases} P_n^m(i\xi_0) Q_n^m(i\xi), & \xi > \xi_0, \\ P_n^m(i\xi) Q_n^m(i\xi_0), & \xi < \xi_0. \end{cases}\end{aligned}\quad (5)$$

The expansion coefficients A_{mn} , B_{mn} , C_{mn} and D_{mn} in (3) and (4) are to be determined by the boundary conditions of (2) which, under the oblate spheroidal coordinates, become

$$\Psi_{\text{out}}|_{\xi=\xi_1} = \Psi_{\text{in}}|_{\xi=\xi_1} \quad \text{and} \quad \varepsilon_0 \frac{\partial \Psi_{\text{out}}}{\partial \xi} \Big|_{\xi=\xi_1} = \varepsilon_1 \frac{\partial \Psi_{\text{in}}}{\partial \xi} \Big|_{\xi=\xi_1}.$$

Then, by using the orthogonality of $\cos m\varphi$ and $\sin m\varphi$ as well as that of $P_n^m(x)$, one can obtain $B_{mn} = D_{mn} = 0$, and

$$Q_n^m(i\xi_1) A_{mn} - P_n^m(i\xi_1) C_{mn} = H_{mn} P_n^m(\eta_0) P_n^m(i\xi_0) Q_n^m(i\xi_1), \quad (7)$$

$$\varepsilon_0 \widehat{Q}_n^m(i\xi_1) A_{mn} - \varepsilon_1 \widehat{P}_n^m(i\xi_1) C_{mn} = \varepsilon_1 H_{mn} P_n^m(\eta_0) P_n^m(i\xi_0) \widehat{Q}_n^m(i\xi_1), \quad (8)$$

where

$$\begin{aligned}\widehat{P}_n^m(i\xi_1) &= (n-m+1) P_{n+1}^m(i\xi_1) - (n+1) i\xi_1 P_n^m(i\xi_1), \\ \widehat{Q}_n^m(i\xi_1) &= (n-m+1) Q_{n+1}^m(i\xi_1) - (n+1) i\xi_1 Q_n^m(i\xi_1).\end{aligned}$$

Further solving (7) and (8) leads to

$$A_{mn} = \varepsilon_1 H_{mn} P_n^m(\eta_0) P_n^m(i\xi_0) K_{mn}^{-1} \left(P_n^m(i\xi_1) \widehat{Q}_n^m(i\xi_1) - Q_n^m(i\xi_1) \widehat{P}_n^m(i\xi_1) \right),$$

and

$$C_{mn} = (\varepsilon_1 - \varepsilon_0) H_{mn} P_n^m(\eta_0) P_n^m(i\xi_0) K_{mn}^{-1} Q_n^m(i\xi_1) \widehat{Q}_n^m(i\xi_1),$$

where

$$K_{mn} = \varepsilon_0 P_n^m(i\xi_1) \widehat{Q}_n^m(i\xi_1) - \varepsilon_1 Q_n^m(i\xi_1) \widehat{P}_n^m(i\xi_1).$$

In summary, the total potential inside the oblate spheroid is given by

$$\Psi_{\text{in}}(\mathbf{r}) = \frac{q}{\varepsilon_i |\mathbf{r} - \mathbf{r}_s|} + \frac{q}{\varepsilon_i a} \sum_{n=0}^{\infty} \sum_{m=0}^n (\varepsilon_i - \varepsilon_o) H_{mn} P_n^m(\eta_0) P_n^m(i\xi_0) K_{mn}^{-1} \times Q_n^m(i\xi_1) \widehat{Q}_n^m(i\xi_1) \cos m\varphi P_n^m(\eta) P_n^m(i\xi), \quad (9)$$

while the potential outside the oblate spheroid is

$$\Psi_{\text{out}}(\mathbf{r}) = \frac{q}{\varepsilon_i a} \sum_{n=0}^{\infty} \sum_{m=0}^n \varepsilon_i H_{mn} P_n^m(\eta_0) P_n^m(i\xi_0) K_{mn}^{-1} \times (P_n^m(i\xi_1) \widehat{Q}_n^m(i\xi_1) - Q_n^m(i\xi_1) \widehat{P}_n^m(i\xi_1)) \cos m\varphi P_n^m(\eta) Q_n^m(i\xi). \quad (10)$$

Similarly, when the point charge q is located at the point $\mathbf{r}_s = (\xi_0, \eta_0, \varphi_0=0)$ outside the dielectric spheroid defined by the equation $\xi = \xi_1$ (so $\xi_0 > \xi_1 > 0$), the electrostatic potential outside the spheroid takes the form

$$\Psi_{\text{out}}(\mathbf{r}) = \frac{q}{\varepsilon_o |\mathbf{r} - \mathbf{r}_s|} + \frac{q}{\varepsilon_o a} \sum_{n=0}^{\infty} \sum_{m=0}^n A_{mn} \cos m\varphi P_n^m(\eta) Q_n^m(i\xi), \quad (11)$$

or

$$\Psi_{\text{out}}(\mathbf{r}) = \frac{q}{\varepsilon_o a} \sum_{n=0}^{\infty} \sum_{m=0}^n A_{mn} \cos m\varphi P_n^m(\eta) Q_n^m(i\xi) + \frac{q}{\varepsilon_o a} \sum_{n=0}^{\infty} \sum_{m=0}^n H_{mn} \cos m\varphi P_n^m(\eta_0) P_n^m(\eta) \begin{cases} P_n^m(i\xi_0) Q_n^m(i\xi), & \xi > \xi_0, \\ P_n^m(i\xi) Q_n^m(i\xi_0), & \xi < \xi_0. \end{cases} \quad (12)$$

And on the other hand, the potential inside the spheroid can be written as

$$\Psi_{\text{in}}(\mathbf{r}) = \frac{q}{\varepsilon_o a} \sum_{n=0}^{\infty} \sum_{m=0}^n C_{mn} \cos m\varphi P_n^m(\eta) P_n^m(i\xi). \quad (13)$$

Then using the boundary conditions of (6), one can obtain

$$Q_n^m(i\xi_1) A_{mn} - P_n^m(i\xi_1) C_{mn} = -H_{mn} P_n^m(\eta_0) P_n^m(i\xi_1) Q_n^m(i\xi_0), \quad (14)$$

$$\varepsilon_o \widehat{Q}_n^m(i\xi_1) A_{mn} - \varepsilon_i \widehat{P}_n^m(i\xi_1) C_{mn} = -\varepsilon_o H_{mn} P_n^m(\eta_0) \widehat{P}_n^m(i\xi_1) Q_n^m(i\xi_0). \quad (15)$$

Solving (14) and (15) leads to

$$A_{mn} = (\varepsilon_i - \varepsilon_o) H_{mn} P_n^m(\eta_0) Q_n^m(i\xi_0) K_{mn}^{-1} P_n^m(i\xi_1) \widehat{P}_n^m(i\xi_1),$$

and

$$C_{mn} = \varepsilon_0 H_{mn} P_n^m(\eta_0) Q_n^m(i\xi_0) K_{mn}^{-1} \left(P_n^m(i\xi_1) \widehat{Q}_n^m(i\xi_1) - Q_n^m(i\xi_1) \widehat{P}_n^m(i\xi_1) \right).$$

In summary, the total potential outside the oblate spheroid is given by

$$\begin{aligned} \Psi_{\text{out}}(\mathbf{r}) = & \frac{q}{\varepsilon_0 |\mathbf{r} - \mathbf{r}_s|} + \frac{q}{\varepsilon_0 a} \sum_{n=0}^{\infty} \sum_{m=0}^n (\varepsilon_i - \varepsilon_0) H_{mn} P_n^m(\eta_0) Q_n^m(i\xi_0) K_{mn}^{-1} \\ & \times P_n^m(i\xi_1) \widehat{P}_n^m(i\xi_1) \cos m\varphi P_n^m(\eta) Q_n^m(i\xi), \end{aligned} \quad (16)$$

while the potential inside the oblate spheroid is

$$\begin{aligned} \Psi_{\text{in}}(\mathbf{r}) = & \frac{q}{\varepsilon_0 a} \sum_{n=0}^{\infty} \sum_{m=0}^n \varepsilon_0 H_{mn} P_n^m(\eta_0) Q_n^m(i\xi_0) K_{mn}^{-1} \\ & \times \left(P_n^m(i\xi_1) \widehat{Q}_n^m(i\xi_1) - Q_n^m(i\xi_1) \widehat{P}_n^m(i\xi_1) \right) \cos m\varphi P_n^m(\eta) P_n^m(i\xi). \end{aligned} \quad (17)$$

3. An oblate spheroid immersed in an ionic solvent

Using the oblate spheroidal coordinates, the LPBE of (1) can be written as

$$\frac{\partial}{\partial \xi} \left[(\xi^2 + 1) \frac{\partial \Psi}{\partial \xi} \right] + \frac{\partial}{\partial \eta} \left[(1 - \eta^2) \frac{\partial \Psi}{\partial \eta} \right] + \frac{\xi^2 + \eta^2}{(\xi^2 + 1)(1 - \eta^2)} \frac{\partial^2 \Psi}{\partial \varphi^2} - c^2 (\xi^2 + \eta^2) \Psi = 0,$$

where $c = (a/2) \lambda$ is the spheroidal parameter. By means of the separation of variables with

$$\Psi(\xi, \eta, \varphi) = S_{mn}(c, \eta) R_{mn}(c, i\xi) \begin{pmatrix} \cos m\varphi \\ \sin m\varphi \end{pmatrix},$$

where m and n are zero or positive integers with $n \geq m$, one can obtain the ordinary differential equations

$$\frac{d}{d\eta} \left[(1 - \eta^2) \frac{dS_{mn}(c, \eta)}{d\eta} \right] + \left[\lambda_{mn}(c) - c^2 \eta^2 - \frac{m^2}{1 - \eta^2} \right] S_{mn}(c, \eta) = 0, \quad (18)$$

$$\frac{d}{d\xi} \left[(\xi^2 + 1) \frac{dR_{mn}(c, i\xi)}{d\xi} \right] - \left[\lambda_{mn}(c) + c^2 \xi^2 - \frac{m^2}{\xi^2 + 1} \right] R_{mn}(c, i\xi) = 0, \quad (19)$$

where those values $\lambda_{mn}(c)$ for which (18) admits solutions that are finite at $\eta = \pm 1$ are eigenvalues of the differential equation (18), and $S_{mn}(c, \eta)$ and $R_{mn}(c, i\xi)$ are the eigenfunctions associated with the eigenvalue $\lambda_{mn}(c)$.

3.1 The angular function $S_{mn}(c, \eta)$

Note that Eq. (18) is exactly the same as that solved by prolate spheroidal angular wave functions for the Helmholtz equation in the standard theory, whose solutions are usually called the prolate angular functions of the first kind and the second kind. However, only the angular functions of the first kind $S_{mn}^{(1)}(c, \eta)$ are used in this paper since they are regular at $\eta = \pm 1$. Moreover, we use the following expansion in terms of the associated Legendre functions of the first kind

$$S_{mn}^{(1)}(c, \eta) = \sum_{r=0,1}^{\infty} {}'d_r^{mn}(c) P_{m+r}^m(\eta). \quad (20)$$

Here and in the sequel, the prime over the summation sign indicates that the summation is over only even values of r when $n - m$ is even, and over only odd values of r when $n - m$ is odd.

The eigenvalues $\lambda_{mn}(c)$ and the angular expansion coefficients $d_r^{mn}(c)$ in (20) satisfy the following recursion formula for $r \geq 0$ [6]

$$\alpha_r^m(c) d_{r+2}^{mn}(c) + (\beta_r^m(c) - \lambda_{mn}(c)) d_r^{mn}(c) + \gamma_r^m(c) d_{r-2}^{mn}(c) = 0, \quad (21)$$

in which

$$\alpha_r^m(c) = \frac{(2m+r+2)(2m+r+1)c^2}{(2m+2r+3)(2m+2r+5)}, \quad (22)$$

$$\beta_r^m(c) = (m+r)(m+r+1) + \frac{2(m+r)(m+r+1) - 2m^2 - 1}{(2m+2r-1)(2m+2r+3)} c^2, \quad (23)$$

$$\gamma_r^m(c) = \frac{r(r-1)c^2}{(2m+2r-3)(2m+2r-1)}. \quad (24)$$

The eigenvalues are determined by the condition that $d_r^{mn}(c) \rightarrow 0$ as $r \rightarrow \infty$, and various methods have been proposed to calculate the eigenvalues and the expansion coefficients; see [6–14] and references therein.

3.2 The radial function $R_{mn}(c, i\xi)$

In the standard theory, the prolate spheroidal radial wave function $R_{mn}(c, \xi)$ for the Helmholtz equation satisfies the differential equation

$$\frac{d}{d\xi} \left[(\xi^2 - 1) \frac{dR_{mn}(c, \xi)}{d\xi} \right] - \left[\lambda_{mn}(c) - c^2 \xi^2 + \frac{m^2}{\xi^2 - 1} \right] R_{mn}(c, \xi) = 0. \quad (25)$$

Note that Eq. (19) can be obtained from Eq. (25) by replacing ξ with $i\xi$. The standard prolate radial functions are usually expanded in a basis of spherical Bessel functions. Accordingly, the radial solution $R_{mn}(c, i\xi)$ to (19) can be expanded in the modified spherical Bessel functions [15]

$$R_{mn}^{(1)}(c, i\xi) = \frac{1}{\rho_{mn}(c)} \left(\frac{\xi^2 + 1}{\xi^2} \right)^{\frac{m}{2}} \sum_{r=0,1}^{\infty} {}_r d_r^{mn}(c) \frac{(2m+r)!}{r!} i_{m+r}(c\xi),$$

and

$$R_{mn}^{(3)}(c, i\xi) = \frac{1}{\rho_{mn}(c)} \left(\frac{\xi^2 + 1}{\xi^2} \right)^{\frac{m}{2}} \sum_{r=0,1}^{\infty} {}_r d_r^{mn}(c) \frac{(2m+r)!}{r!} k_{m+r}(c\xi), \quad (26)$$

where $i_n(r)$ and $k_n(r)$ are the modified spherical Bessel functions of the first kind and the third kind, respectively, defined as

$$i_n(r) = \sqrt{\frac{\pi}{2r}} I_{n+1/2}(r), \quad k_n(r) = \sqrt{\frac{\pi}{2r}} K_{n+1/2}(r).$$

Here, $I(r)$ and $K(r)$ are the modified Bessel functions of the first kind and the third kind, respectively. The normalization factor $\rho_{mn}(c)$ is given by

$$\rho_{mn}(c) = \sum_{r=0,1}^{\infty} {}_r d_r^{mn}(c) \frac{(2m+r)!}{r!}.$$

When expressing the electric potential outside the oblate spheroid where $\xi \geq \xi_1 > 0$, only $R_{mn}^{(3)}(c, i\xi)$ needs to be used since it is finite outside the oblate spheroid and vanishes at $\xi = \infty$. For convenience, ${}_r d_r^{mn}(c)$ is simply denoted by d_r^{mn} , $S_{mn}^{(1)}(c, \eta)$ by $S_{mn}(\eta)$, and $R_{mn}^{(3)}(c, i\xi)$ by $R_{mn}(\xi)$, respectively, for the rest of this note. In particular, i is dropped since $R_{mn}^{(3)}(c, i\xi)$ is actually real-valued.

Finally, as pointed out in [16], $k_n(c\xi)$ approaches infinity and the expansion (26) diverges and thus becomes inadequate when the argument $c\xi$ is fairly small. This could be the case when the inverse Debye screening length λ , which is proportional to the square root of the ionic concentration of the solvent medium, is small, or when the aspect ratio of the oblate spheroid a_2/a_1 is high (so the interfocal distance a is small). This may also happen even when the aspect ratio of the oblate spheroid is low because ξ_1 , which defines the oblate spheroidal, may be small in this case. Therefore, it is desirable to deduce appropriate expressions for $R_{mn}^{(3)}(c, i\xi)$ which will be more conveniently used when the argument $c\xi$ is small [15–18]. We use an expansion modified from that given in [16], which, as far as we are aware, seems to be new. The constant multipliers are so chosen that the modified expansion is consistent with (26) when they both converge.

$$R_{m(m+2r)}^{(3)}(c, i\xi) = \frac{2m+1}{2(m)!d_0^{m(m+2r)}c^m} \cdot (\xi^2+1)^{\frac{m}{2}} \cdot \sum_{q=0}^{\infty} \omega_{2q} k_{m+q} \left(\frac{c}{2} (\sqrt{\xi^2+1} + \xi) \right) i_{m+q} \left(\frac{c}{2} (\sqrt{\xi^2+1} - \xi) \right), \quad (27)$$

$$R_{m(m+2r+1)}^{(3)}(c, i\xi) = \frac{2m+3}{(m)!d_1^{m(m+2r+1)}c^{m+1}} \cdot \xi(\xi^2+1)^{\frac{m}{2}} \cdot \sum_{q=0}^{\infty} \omega_{2q+1} k_{m+q+1} \left(\frac{c}{2} (\sqrt{\xi^2+1} + \xi) \right) i_{m+q+1} \left(\frac{c}{2} (\sqrt{\xi^2+1} - \xi) \right), \quad (28)$$

where the coefficients ω_{2q} 's and ω_{2q+1} 's are

$$\begin{aligned} \omega_{2q} &= (2m+2q+1) \sum_{s=0}^q \sum_{t=s}^q (-1)^{t+q} 2^{m+2s+1} \\ &\cdot \frac{(2m+q+t)!(2m+2s)!(2t)!(t+m+s)!}{t!(m+t)!(q-t)!(2s)!(t-s)!(2t+2m+2s+1)!} d_{2s}^{m(m+2r)}, \\ \omega_{2q+1} &= (2m+2q+3) \sum_{s=0}^q \sum_{t=s}^q (-1)^{t+q} 2^{m+2s+2} \\ &\cdot \frac{(2m+q+t+2)!(2m+2s+1)!(2t+1)!(t+m+s+1)!}{t!(m+t+1)!(q-t)!(2s+1)!(t-s)!(2t+2m+2s+3)!} d_{2s+1}^{m(m+2r+1)}. \end{aligned}$$

3.3 Series solution of the electric potential

Let us consider again a point charge q located at the point $\mathbf{r}_s = (\xi_0, \eta_0, \varphi_0 = 0)$ in the plane $y = 0$ inside the dielectric oblate spheroid defined by the equation $\xi = \xi_1$ (so $\xi_1 > \xi_0 \geq 0$); see Fig. 1. Inside the spheroid, the total potential still takes the forms (4) and (5). On the other hand, since the potential outside the oblate spheroid ($\xi_1 \leq \xi$) must be finite and vanishes at $\xi = \infty$, it should take on the form

$$\Psi_{\text{out}}(\mathbf{r}) = \frac{q}{\varepsilon_i a} \sum_{n=0}^{\infty} \sum_{m=0}^n (A_{mn} \cos m\varphi + B_{mn} \sin m\varphi) S_{mn}(\eta) R_{mn}(\xi), \quad (29)$$

where A_{mn} and B_{mn} are the unknown expansion coefficients.

Once again, by using the orthogonality of $\cos m\varphi$ and $\sin m\varphi$ together with the boundary conditions of (6), one can obtain $B_{mn} = D_{mn} = 0$, and

$$\sum_{n=m}^{\infty} [S_{mn}(\eta) R_{mn}(\xi_1) A_{mn} - P_n^m(\eta) P_n^m(i\xi_1) C_{mn}] = \sum_{n=m}^{\infty} H_{mn} P_n^m(\eta) P_n^m(\eta_0) P_n^m(i\xi_0) Q_n^m(i\xi_1), \quad (30)$$

$$\sum_{n=m}^{\infty} [\varepsilon_0 S_{mn}(\eta) R'_{mn}(\xi_1) A_{mn} - i\varepsilon_i P_n^m(\eta) P_n^{m'}(i\xi_1) C_{mn}] = i \sum_{n=m}^{\infty} \varepsilon_i H_{mn} P_n^m(\eta) P_n^m(\eta_0) P_n^m(i\xi_0) Q_n^{m'}(i\xi_1). \quad (31)$$

Using (20) to rewrite $S_{mn}(\eta)$ in series of the associated Legendre polynomials, and then applying the orthogonality of the associated Legendre polynomials, one can arrive at the following equations for the expansion coefficients

$$\sum_{r=0,1}^{\infty} {}_r d_{n-m}^{m(m+r)} R_{m(m+r)}(\xi_1) A_{m(m+r)} - P_n^m(i\xi_1) C_{mn} = H_{mn} P_n^m(\eta_0) P_n^m(i\xi_0) Q_n^m(i\xi_1), \quad (32)$$

$$\varepsilon_0 \sum_{r=0,1}^{\infty} {}_r d_{n-m}^{m(m+r)} R'_{m(m+r)}(\xi_1) A_{m(m+r)} - i\varepsilon_1 P_n^{m'}(i\xi_1) C_{mn} = i\varepsilon_1 H_{mn} P_n^m(\eta_0) P_n^m(i\xi_0) Q_n^{m'}(i\xi_1). \quad (33)$$

For a fixed value of m , (32) and (33) for all $n = m, m+1, \dots$, constitute a system of an infinite set of equations, but the system can be completely decoupled into two independent systems, one for $A_{mm}, A_{m(m+2)}, \dots, C_{mm}, C_{m(m+2)}, \dots$, and the other for $A_{m(m+1)}, A_{m(m+3)}, \dots, C_{m(m+1)}, C_{m(m+3)}, \dots$.

In practice, the series expansion of the angular function $S_{mn}(\eta)$, Eq. (20), is presumed to be a convergent representation. Hence, one can perform the computation based on a finite set of equations. More specifically, let us assume that the series expansions of the potentials are truncated as

$$\Psi_{\text{out}}(\mathbf{r}) \approx \frac{q}{\varepsilon_i a} \sum_{n=0}^N \sum_{m=0}^n A_{mn} \cos m\varphi S_{mn}(\eta) R_{mn}(\xi), \quad (34)$$

and

$$\Psi_{\text{in}}(\mathbf{r}) \approx \frac{q}{\varepsilon_i |\mathbf{r} - \mathbf{r}_s|} + \frac{q}{\varepsilon_i a} \sum_{n=0}^N \sum_{m=0}^n C_{mn} \cos m\varphi P_n^m(\eta) P_n^m(i\xi), \quad (35)$$

where N , the truncation number of the summation over n , must be large enough to make the truncation error negligible for a certain physical application. Accordingly, for each fixed m ($0 \leq m \leq N$), the regular oblate spheroidal wave functions $S_{mn}(\eta)$, $n = m, m+1, \dots, N$, are truncated as

$$S_{mn}(\eta) \approx \sum_{r=0,1}^{r_{mn}} {}_r d_r^{mn} P_{m+r}^m(\eta), \quad (36)$$

where $r_{mn} = (N - m) - \sigma$. Here $\sigma = 0$ if $N - m$ is even, and $\sigma = 1$ if $N - m$ is odd.

Then for each fixed m , the expansion coefficients $A_{m,m}, A_{m,m+1}, \dots, A_{m,N}$ are obtained by solving the following two independent systems

$$\widetilde{\mathcal{K}}_{\sigma} \widetilde{\mathbf{A}}_{\sigma} = \widetilde{\mathbf{F}}_{\sigma}, \quad \sigma=0, 1, \quad (37)$$

where

$$\widetilde{\mathcal{K}}_{\sigma} = \begin{bmatrix} k_{\sigma,\sigma} & k_{\sigma,\sigma+2} & \cdots & k_{\sigma,\sigma+2N_m^{(\sigma)}} \\ k_{\sigma+2,\sigma} & k_{\sigma+2,\sigma+2} & \cdots & k_{\sigma+2,\sigma+2N_m^{(\sigma)}} \\ \vdots & \vdots & \ddots & \vdots \\ k_{\sigma+2N_m^{(\sigma)},\sigma} & k_{\sigma+2N_m^{(\sigma)},\sigma+2} & \cdots & k_{\sigma+2N_m^{(\sigma)},\sigma+2N_m^{(\sigma)}} \end{bmatrix},$$

and

$$\widetilde{\mathbf{A}}_{\sigma} = \begin{pmatrix} A_{m,m+\sigma} \\ A_{m,m+\sigma+2} \\ \vdots \\ A_{m,m+\sigma+2N_m^{(\sigma)}} \end{pmatrix}, \quad \widetilde{\mathbf{F}}_{\sigma} = \begin{pmatrix} f_{\sigma} \\ f_{\sigma+2} \\ \vdots \\ f_{\sigma+2N_m^{(\sigma)}} \end{pmatrix}.$$

Here

$$\begin{aligned} k_{st} &= \varepsilon_i \widehat{a}_{st} \widehat{b}_s - \varepsilon_0 \widehat{a}_{st} b_s, \\ f_s &= \varepsilon_i (g_s \widehat{b}_s - \widehat{g}_s b_s), \\ a_{sr} &= d_s^{m(m+r)} R_{m(m+r)}(\xi_1), \\ \widehat{a}_{sr} &= d_s^{m(m+r)} R'_{m(m+r)}(\xi_1), \\ b_s &= P_{m+s}^m(i\xi_1), \\ \widehat{b}_s &= i P_{m+s}^{m'}(i\xi_1), \\ g_s &= H_{m(m+s)} P_{m+s}^m(\eta_0) P_{m+s}^m(i\xi_0) Q_{m+s}^m(i\xi_1), \\ \widehat{g}_s &= i H_{m(m+s)} P_{m+s}^m(\eta_0) P_{m+s}^{m'}(i\xi_0) Q_{m+s}^{m'}(i\xi_1). \end{aligned}$$

And $N_m^{(\sigma)}$ is defined as

$$N_m^{(0)} = N_m^{(1)} = \frac{N-m-1}{2}$$

if $N-m$ is odd, and as

$$N_m^{(0)} = \frac{N-m}{2}, \quad N_m^{(1)} = \frac{N-m-2}{2}$$

if $N-m$ is even.

The expansion coefficients $C_{m,m}$, $C_{m,m+1}$, ..., $C_{m,N}$ can then be calculated using

$$\widetilde{\mathcal{B}}_\sigma \widetilde{\mathbf{C}}_\sigma = \widetilde{\mathcal{N}}_\sigma \widetilde{\mathbf{A}}_\sigma - \widetilde{\mathbf{G}}_\sigma, \quad \sigma=0, 1,$$

where

$$\widetilde{\mathcal{B}}_\sigma = \text{diag}(b_\sigma, b_{\sigma+2}, \dots, b_{\sigma+2N_m^{(\sigma)}}),$$

$$\widetilde{\mathcal{N}}_\sigma = \begin{bmatrix} a_{\sigma,\sigma} & a_{\sigma,\sigma+2} & \cdots & a_{\sigma,\sigma+2N_m^{(\sigma)}} \\ a_{\sigma+2,\sigma} & a_{\sigma+2,\sigma+2} & \cdots & a_{\sigma+2,\sigma+2N_m^{(\sigma)}} \\ \vdots & \vdots & \ddots & \vdots \\ a_{\sigma+2N_m^{(\sigma)},\sigma} & a_{\sigma+2N_m^{(\sigma)},\sigma+2} & \cdots & a_{\sigma+2N_m^{(\sigma)},\sigma+2N_m^{(\sigma)}} \end{bmatrix},$$

and

$$\widetilde{\mathbf{C}}_\sigma = \begin{pmatrix} C_{m,m+\sigma} \\ C_{m,m+\sigma+2} \\ \vdots \\ C_{m,m+\sigma+2N_m^{(\sigma)}} \end{pmatrix}, \quad \widetilde{\mathbf{G}}_\sigma = \begin{pmatrix} g_\sigma \\ g_{\sigma+2} \\ \vdots \\ g_{\sigma+2N_m^{(\sigma)}} \end{pmatrix}.$$

4. Numerical examples

To illustrate the simulated electric potential of point charges inside oblate spheroids using the direct series expansions (9) and (10), we let an oblate spheroid of dielectric constant $\varepsilon_i = 2$ be embedded in a dielectric medium of dielectric constant $\varepsilon_0 = 8$. The oblate spheroid is defined by $(x^2 + y^2)/4 + z^2 = 1$, which leads to $\xi_1 = 0.57735$. Figs. 2(a)–(b) show the equipotential contours in the plane $y = 0$ for the computed total potential with using $N = 20$ due to a unit point charge inside this oblate spheroid located at the point $\mathbf{x}_0 = (1, 0, 0)$ ($\xi_0 = 0$) or $\mathbf{x}_0 = (1, 0, 0.5)$ ($\xi_0 = 0.344532$), respectively. As been exhibited, the electric potential is continuous but its normal derivative is discontinuous across the spheroidal surface.

To investigate the convergence of the series expansions (9) and (10), the electric potentials due to point charges at four typical locations computed with using different N values are compared to those computed with using $N = 20$. Fig. 3 plots the relative error E of the computed electric potential $\Psi(\mathbf{x}_i)$ at 101^3 observation points $\mathbf{x}_i$ uniformly located inside the rectangular box $[-2.5, 2.5]^2 \times [-1.5, 1.5]$ for various N values, where

$$E = \left(\frac{\sum_{i=1}^{101^3} |\Psi(\mathbf{x}_i) - \bar{\Psi}(\mathbf{x}_i)|^2}{\sum_{i=1}^{101^3} |\Psi(\mathbf{x}_i)|^2} \right)^{1/2}.$$

Here $\Psi(\mathbf{x}_i)$ represents the potential at $\mathbf{x}_i$ obtained by using the series expansions with $N = 20$. First of all, for all four cases the series solutions (9) and (10) have been shown numerically convergent, and the error decreases monotonically as N increases. Second, the convergence rate clearly depends on where the point charge is located at. In particular, when the point charge is close to the spheroidal boundary, the convergence rate shall be slow, requiring a large number of terms to achieve high accuracy in the potential field. For instance, the series solutions

converge much faster for the $\mathbf{x}_0 = (0, 0, 0)$ ($\xi_0 = 0$) and $\mathbf{x}_0 = (1, 0, 0)$ ($\xi_0 = 0$) cases than for the $\mathbf{x}_0 = (0, 0, 0.5)$ ($\xi_0 = 0.288675$) and $\mathbf{x}_0 = (1, 0, 0.5)$ ($\xi_0 = 0.344532$) cases.

Similarly, to illustrate the simulated electric potential due to point charges outside oblate spheroids using the direct series expansions (16) and (17), Figs. 4(a)-(b) plot the equipotential contours in the plane $y = 0$ for the computed total potential with using $N = 20$ due to a unit point charge located at the point $\mathbf{x}_0 = (3, 0, 0)$ ($\xi_0 = 0$) or $\mathbf{x}_0 = (3, 0, 1.5)$ ($\xi_0 = 1.732051$) outside the same oblate spheroid, respectively.

We now consider the situation that the dissimilar dielectric medium outside a dielectric oblate spheroid is an ionic solvent, in which the electrostatic potential due to a point charge inside the oblate spheroid is approximated using the direct expansions (34) and (35). The inverse Debye screening length in the LPBE of (1) is assumed to be $\lambda = 4/a$ so the spheroidal parameter is $c = 2$. Again we let an oblate spheroid of dielectric constant $\varepsilon_i = 2$ be embedded in a dielectric medium of dielectric constant $\varepsilon_o = 8$, but we first consider an oblate spheroid with relatively low ellipticity of $1/4$ defined by $(x^2 + y^2)/4 + 4z^2/9 = 1$, which leads to $\xi_1 = 1.133893$. Therefore, the expansion (26) for $R_{mn}^{(3)}(c, i\xi)$ can be and is actually used in programming since in this case $c\xi > 2$. Figs. 5(a)-(b) again show the equipotential contours in the plane $y = 0$ for the computed total potential with using $N = 20$ due to a unit point charge inside this oblate spheroid located at the point $\mathbf{x}_0 = (1, 0, 0)$ ($\xi_0 = 0$) or $\mathbf{x}_0 = (1, 0, 0.75)$ ($\xi_0 = 0.718262$), respectively.

Next we consider the oblate spheroid with relatively high ellipticity of $1/2$ defined by $(x^2 + y^2)/4 + z^2 = 1$, which leads to $\xi_1 = 0.57735$. For this case, the expansion (26) for $R_{mn}^{(3)}(c, i\xi)$ has been found inadequate so the expansion described by (27)–(28) is instead used. Figs. 6(a)-(b) plot the equipotential contours in the plane $y = 0$ for the computed total potential with using $N = 20$ due to a unit point charge inside this oblate spheroid located at the point $\mathbf{x}_0 = (1, 0, 0)$ ($\xi_0 = 0$) or $\mathbf{x}_0 = (1, 0, 0.5)$ ($\xi_0 = 0.344532$), respectively.

Finally, the series expansions (34) and (35) can be demonstrated to be numerically convergent with the convergence rate depending on the location of the source charge. To this end, for the foregoing oblate spheroids defined by $(x^2 + y^2)/4 + 4z^2/9 = 1$ and $(x^2 + y^2)/4 + z^2 = 1$ respectively, the electric potentials due to point charges at four typical locations computed with using different N values are again compared to those computed with using $N = 20$. Figs. 7(a)-(b) plot the relative error E of the computed electric potential at 101^3 observation points uniformly located inside the rectangular box $[-1.25a_1, 1.25a_1]^2 \times [-1.5a_2, 1.5a_2]$ for various N values. As shown in Fig. 7, for both oblate spheroids, the series solutions converge for all four charge locations, but they converge much slower when the source charge is closer to the spheroidal boundary. For example, in the case of $(x^2 + y^2)/4 + 4z^2/9 = 1$, the series solutions converge much faster for the $\mathbf{x}_0 = (0, 0, 0)$ ($\xi_0 = 0$) and $\mathbf{x}_0 = (1, 0, 0)$ ($\xi_0 = 0$) cases than for the $\mathbf{x}_0 = (0, 0, 0.75)$ ($\xi_0 = 0.566947$) and $\mathbf{x}_0 = (1, 0, 0.75)$ ($\xi_0 = 0.718262$) cases. In addition, the results shown in Fig. 7 appear to have demonstrated that the convergence rate is slower for oblate spheroids of higher ellipticity, agreeing with the common understanding that oblate spheroids of higher ellipticity or oblateness are more difficult to handle.

5. Conclusions

In this paper, the series expansions of the electric potential of point charges inside a dielectric oblate spheroid are presented in terms of the associated Legendre functions or the spheroidal wave functions, depending on whether the surrounding dissimilar dielectric medium of the spheroid is ionic or non-ionic. Numerical experiments have demonstrated the convergence of the series solutions for both cases.

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Fig. 1.
A point charge and a dielectric oblate spheroid.

Fig. 2.

Equipotential contours in the plane $y = 0$ for the computed total potential due to a unit point charge located at the point $\mathbf{x}_0 = (1, 0, 0)$ or $\mathbf{x}_0 = (1, 0, 0.5)$ inside the oblate spheroid $(x^2 + y^2)/4 + z^2 = 1$, respectively.

Fig. 3.
Illustration of the convergence rate of the series solutions (9) and (10).

Fig. 4.

Equipotential contours in the plane $y = 0$ for the computed total potential due to a unit point charge located at the point $\mathbf{x}_0 = (3, 0, 0)$ or $\mathbf{x}_0 = (3, 0, 1.5)$ outside the oblate spheroid $(x^2 + y^2)/4 + z^2 = 1$, respectively.

Fig. 5. Equipotential contours in the plane $y = 0$ for the computed total potential due to a unit point charge located at the point $\mathbf{x}_0 = (1, 0, 0)$ or $\mathbf{x}_0 = (1, 0, 0.75)$ inside the oblate spheroid $(x^2 + y^2)/4 + 4z^2/9 = 1$, respectively.

Fig. 6.

Equipotential contours in the plane $y = 0$ for the computed total potential due to a unit point charge located at the point $\mathbf{x}_0 = (1, 0, 0)$ or $\mathbf{x}_0 = (1, 0, 0.5)$ inside the oblate spheroid $(x^2 + y^2)/4 + z^2 = 1$, respectively.

Fig. 7.

Illustration of the convergence rate of the series solutions (34) and (35) for oblate spheroids of different ellipticity. (a) The oblate spheroid is $(x^2 + y^2)/4 + 4z^2/9 = 1$ and the expansion (26) is used for $R_{mn}^{(3)}(c, i\xi)$; (b) The oblate spheroid is $(x^2 + y^2)/4 + z^2 = 1$ and the expansion (27)–(28) is used for $R_{mn}^{(3)}(c, i\xi)$.