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Image systems for the reaction field inside spheroidal dielectric objects and applications

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ABSTRACT

Charges inside a dielectric object embedded in a dissimilar dielectric medium polarize the surrounding medium, which in turn makes a contribution, called the reaction field, to the electric field inside the object. In this work, we develop complete image systems for the reaction field inside a prolate or oblate spheroidal dielectric object embedded in an infinite dissimilar dielectric medium. In either case, an image system consists of a point image and a symmetric surface image over an exterior confocal spheroid that passes through the point image. As an application, the point image is applied into the generalized image charge solvation model (GICSM) and is tested in simulations of liquid water, and the results are analyzed in comparison with those obtained from the ICSM simulation as references. The results indicate that, for both the prolate and oblate cases, the single point image charge approximation for the reaction field inside the dielectric cavity of the model is good enough for the GICSM to faithfully reproduce typical static and dynamic properties of the liquid water at least when the spheroidal cavity has relatively small eccentricity.

1. Introduction

Consider a point charge q located at point $\mathbf{r}_s = (x_s, y_s, z_s)$ inside a dielectric object of electric permittivity ε_i that is embedded in a dissimilar dielectric medium of electric permittivity ε_o. The charge polarizes the surrounding dielectric medium, which in turn makes a contribution, called the reaction field, to the electric field inside the object. The electric potential at point $\mathbf{r}$ inside the object is thus given by $\Phi(\mathbf{r}) = q/(4\pi|\mathbf{r} - \mathbf{r}_s|) + \Phi_{RF}(\mathbf{r})$. Such a problem may find its application in solvation models for biomolecular simulations [1–3], for an example.

In this work, we aim to develop an image system for the reaction field $\Phi_{RF}(\mathbf{r})$, a system of fictitious sources, commonly called images, outside the object that produces the same potential as $\Phi_{RF}(\mathbf{r})$ inside the object. In the highly symmetric case that the object is spherical with radius a, it is now a textbook result that an image system may consist of one point image at the Kelvin image point $\mathbf{r}_{Kelvin} = (a/r_s)^2\mathbf{r}_s$ and a line image that extends from the Kelvin image point radially to infinity [4,5]. On the other hand, only a few studies have been dedicated to image theories for spheroidal objects [6–8], and most of them were limited to the axisymmetric case in which an exterior point charge is on the axis of symmetry. In addition, image theories have been developed for Green's function for the Laplace operator in both the prolate spheroidal geometry [9] and the general ellipsoidal geometry [10]. For example, an image system for the interior Green's function for the Laplace operator in the prolate spheroidal geometry may consist of a point image and a symmetric surface image over an exterior confocal prolate spheroid [9]. In the present work, we shall apply the same idea as used in Ref. [9] to develop an image system for the reaction field inside a prolate or oblate spheroidal dielectric object embedded in an infinite dissimilar dielectric medium.

Let the boundary S of a prolate spheroidal dielectric object be defined by

$$\frac{x^2 + y^2}{a^2} + \frac{z^2}{b^2} = 1, \tag{1}$$

where $b > a > 0$. Here the z-axis is the focal symmetry axis, and the interfocal distance is $2c$ with $c = \sqrt{b^2 - a^2}$; see Fig. 1.

The prolate spheroidal coordinates (ξ, η, ϕ) are defined through [11]

$$x = c\sqrt{(\xi^2 - 1)(1 - \eta^2)}\cos\phi, \tag{2a}$$

$$y = c\sqrt{(\xi^2 - 1)(1 - \eta^2)}\sin\phi, \tag{2b}$$

$$z = c\xi\eta, \tag{2c}$$

where $\xi \in [1, +\infty)$, $\eta \in [-1,1]$, and $\phi \in [0,2\pi]$ are the radial, angular, and azimuthal variables, respectively. The coordinate surface of

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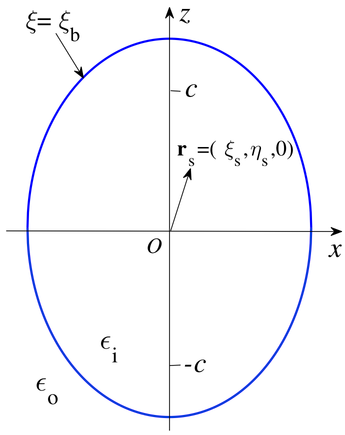

Fig. 1. A prolate spheroid is centered at the origin, its focal symmetry axis is aligned with the z-axis, and the interfocal distance is $2c$. In terms of the prolate spheroidal coordinates (ξ, η, ϕ) defined in the main text, the prolate spheroid is represented by $\xi = \xi_b$. A point source q is located at $\mathbf{r}_s = (\xi_s, \eta_s, 0)$ inside the prolate spheroid. The spheroidal object has dielectric permittivity ε_i, while the infinite surrounding exterior to the object has dielectric permittivity ε_o, respectively.

constant $\xi \geq 1$ is a prolate spheroid, denoted by S_ξ, confocal to the reference prolate spheroid S of this coordinate system. In particular, S_{ξ_b}: $\xi = \xi_b$ with $\xi_b = b/c$ is the prolate spheroid S, and S_1: $\xi = 1$ corresponds to the focal line of the prolate spheroid S, respectively. Note that, in general, a confocal prolate spheroid S_ξ specified by some constant $\xi > 1$ can be written as

$$\frac{x^2 + y^2}{c^2(\xi^2 - 1)} + \frac{z^2}{c^2\xi^2} = 1.$$

We assume, without loss of any generality, that the point charge q is located at point $\mathbf{r}_s$ in the plane $y = 0$ inside the spheroid so $\mathbf{r}_s = (x_s, 0, z_s)$ or $\mathbf{r}_s = (\xi_s, \eta_s, 0)$ with $1 \leq \xi_s < \xi_b$. Then the reaction field at point $\mathbf{r}$ inside the spheroidal object ($1 \leq \xi < \xi_b$) is given by the series expansion [12]:

$$\Phi_{RF}(\mathbf{r}) = \frac{q}{4\pi\varepsilon_i c} \sum_{n=0}^{\infty} \sum_{m=0}^{n} A_{mn} H_{mn} P_n^m(\xi_s) P_n^m(\eta_s) P_n^m(\xi) P_n^m(\eta) \cos(m\phi), \tag{3}$$

where

$$A_{mn} = \frac{(\varepsilon_i - \varepsilon_o) Q_n^m(\xi_b) Q_n^{m\prime}(\xi_b)}{\varepsilon_o P_n^m(\xi_b) Q_n^{m\prime}(\xi_b) - \varepsilon_i P_n^{m\prime}(\xi_b) Q_n^m(\xi_b)}.$$

Here, $P_n^m(x)$ and $Q_n^m(x)$, $n = 0,1, \cdots$ and $m = 0,1, \cdots, n$, are the associated Legendre functions of the first and second kinds, respectively, and

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

where δ_{m0} is the Kronecker delta. Note that $P_n^m(x)$ and $Q_n^m(x)$ with real argument $x > 1$ and non-negative integer degree n and order m with $n \geq m$ are often called the prolate spheroidal harmonics of the first and second kinds [13], respectively.

In Ref. [3], the reaction field is computed by the point image charge approximation:

$$\Phi_{RF}(\mathbf{r}) \approx \frac{q_{\text{Prolate}}}{4\pi\varepsilon_i |\mathbf{r} - \mathbf{r}_{\text{Prolate}}|}, \tag{4}$$

where

$$q_{\text{Prolate}} = \frac{\varepsilon_i - \varepsilon_o}{\varepsilon_i + \varepsilon_o} \frac{Q_0(\xi_s)}{Q_0(\xi_b)} q, \tag{5}$$

and

$$\mathbf{r}_{\text{Prolate}} = \frac{Q_0(\xi_b)}{Q_0(\xi_s)} \left(\frac{Q_1^1(\xi_s) P_1^1(\xi_b)}{Q_1^1(\xi_b) P_1^1(\xi_s)} x_s, \frac{Q_1^1(\xi_s) P_1^1(\xi_b)}{Q_1^1(\xi_b) P_1^1(\xi_s)} y_s, \frac{Q_1(\xi_s) P_1(\xi_b)}{Q_1(\xi_b) P_1(\xi_s)} z_s \right).$$

The point image charge approximation of the reaction field $\Phi_{RF}(\mathbf{r})$ by (4) is easy to use; it was, however, obtained by an intelligent but still empirical guess [3]. In addition, the location of this point image, $\mathbf{r}_{\text{Prolate}}$, does not depend on the dielectric constants of the system. In this work, we first aim to develop another point image charge approximation for the reaction field $\Phi_{RF}(\mathbf{r})$ inside a prolate spheroidal object that is mathematically more rigorous, and whose strength and location shall both depend on the dielectric constants of the system.

To conclude this section, we briefly review some related elements of the surface prolate spheroidal harmonics defined as

$$C_n^m(\eta, \phi) = P_n^m(\eta) \cos(m\phi),$$

$$S_n^m(\eta, \phi) = P_n^m(\eta) \sin(m\phi),$$

for $n = 0,1, \cdots$ and $m = 0,1, \cdots, n$. They are orthogonal over a confocal prolate spheroid S_ξ with respect to the geometrical weighting function:

$$w_\xi(\eta) = \frac{1}{c^2\sqrt{(\xi^2 - \eta^2)(\xi^2 - 1)}}.$$

Indeed, we have the following orthogonality relation:

$$\oint_{S_\xi} S_n^m(\eta, \phi) S_N^M(\eta, \phi) w_\xi(\eta) \mathrm{d}s_\xi(\eta, \phi) = \gamma_{mn} \delta_{nN} \delta_{mM}, \ (M > 0, \ m > 0)$$

$$\oint_{S_\xi} S_n^m(\eta, \phi) C_N^M(\eta, \phi) w_\xi(\eta) \mathrm{d}s_\xi(\eta, \phi) = 0,$$

$$\oint_{S_\xi} C_n^m(\eta, \phi) C_N^M(\eta, \phi) w_\xi(\eta) \mathrm{d}s_\xi(\eta, \phi) = \gamma_{mn} \delta_{nN} \delta_{mM},$$

where δ_{ij} is the Kronecker delta, the differential surface element over S_ξ is

$$\mathrm{d}s_\xi(\eta, \phi) = h_\eta h_\phi \mathrm{d}\eta \mathrm{d}\phi,$$

with the metric coefficients for the prolate spheroidal coordinates being given by

$$h_\xi(\xi, \eta) = c\sqrt{(\xi^2 - \eta^2)/(\xi^2 - 1)},$$

$$h_\eta(\xi, \eta) = c\sqrt{(\xi^2 - \eta^2)/(1 - \eta^2)},$$

$$h_\phi(\xi, \eta) = c\sqrt{(\xi^2 - 1)(1 - \eta^2)},$$

and the normalization constant γ_{mn} is

$$\gamma_{mn} = \frac{2(n + m)!}{(2n + 1)(n - m)!}(1 + \delta_{m0})\pi.$$

The surface prolate spheroidal harmonics form a complete set of eigen-functions over S_ξ. As such, any smooth function f defined over S_ξ can be expanded in terms of the surface prolate spheroidal harmonics. Furthermore, if f is even with respect to ϕ, then it can be expanded in terms of only the even surface prolate spheroidal harmonics $C_n^m(\eta, \phi)$, namely,

$$f(\eta, \phi) = \sum_{n=0}^{\infty} \sum_{m=0}^{n} c_{mn} C_n^m(\eta, \phi),$$

with the coefficients c_{mn} given by

$$c_{mn} = \frac{1}{\gamma_{mn}} \oint_{S_\xi} f(\eta, \phi) C_n^m(\eta, \phi) w_\xi(\eta) \mathrm{d}s_\xi(\eta, \phi).$$

2. Image system for the reaction field inside prolate spheroidal objects

As mentioned earlier, an image system for the reaction field $\Phi_{RF}(\mathbf{r})$ inside a dielectric object is a system of fictitious sources outside the

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