

# A Robust Numerical Method for Generalized Coulomb and Self-Polarization Potentials of Dielectric Spheroids

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**Abstract.** By utilizing a novel quasi-harmonic three-layer dielectric model for the interface between a dielectric spheroid and the surrounding dissimilar dielectric medium, a robust numerical method for calculating the generalized Coulomb and self-polarization potentials of the dielectric spheroid is presented in this paper. The proposed numerical method can not only overcome the inherent mathematical divergence in the self-polarization energy which arises for the simplest step-like model of the dielectric interface, but also completely eliminate the potential numerical divergence which may occur in other treatments. Numerical experiments have demonstrated the convergence of the proposed numerical method as the number of the steps used to discretize the translation layer in a general three-layer dielectric model goes to infinity.

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**Key words:** Generalized Coulomb potential, self-polarization potential, quantum dot, hybrid solvation model, Poisson equation.

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## 1 Introduction

In this paper, we are concerned with the calculation of the generalized Coulomb potential energy  $V_c$  between two particles inside or outside a dielectric object with the coordinates  $\mathbf{r}$  and  $\mathbf{r}_s$ , and the charges  $e$  and  $e_s$ , respectively, which can be evaluated through  $V_c(\mathbf{r}, \mathbf{r}_s) = e\Phi(\mathbf{r}, \mathbf{r}_s)$ , where  $\Phi(\mathbf{r}, \mathbf{r}_s)$  is the electrostatic potential that verifies the Poisson equation

$$\nabla \cdot \varepsilon(\mathbf{r}) \nabla \Phi(\mathbf{r}, \mathbf{r}_s) = -4\pi e_s \delta(\mathbf{r} - \mathbf{r}_s). \quad (1.1)$$

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Here,  $\varepsilon(\mathbf{r})$  is the spatially dependent dielectric function, and  $\delta(\dots)$  is the Dirac delta function. Two representative applications of such a problem include the calculation of self-polarization energies of quantum dots (QDs) with finite confinement barriers [1–3], and the calculation of electrostatic interactions in the so-called hybrid explicit/implicit solvation models for treating electrostatic interactions in biomolecular simulations [4], in which the bio-macromolecule together with the solvent molecules in closest proximity of the biomolecule are modeled explicitly with assigned partial charges embedded in a dielectric cavity, and outside the cavity, the solvent is treated implicitly as a dissimilar dielectric continuum.

The three-dimensional solution of the Poisson equation (1.1), even assuming the spherical or spheroidal geometry and only the radial dependence for  $\varepsilon(\mathbf{r})$ , is quite complicated to find since Eq. (1.1) is a second-order differential equation with a variable, spatially dependent coefficient. Therefore, for simplicity, in most theoretical studies of the underlying applications, macroscopic dielectric constants  $\varepsilon_i$  and  $\varepsilon_o$  are assigned for the object (a QD or the dielectric cavity in a hybrid solvation model) and the surrounding medium (the QD matrix or the implicit solvent in the hybrid solvation model), respectively, leading to a sharp jump in the dielectric constant at the object surface. In this case, it is well-known from classical electromagnetism that the presence of a charged particle inside the dielectric object polarizes the surrounding dissimilar dielectric medium, which consequently induces charges at the object surface that have the same or opposite sign as the source charge if the dielectric constant inside the object is higher (the typical situation for QDs) or lower (the typical situation for hybrid solvation models) than that outside. In turn, a new potential energy, usually called the self-polarization energy, arises due to the mutual interaction between the source and its own induced charges.

For the above step-like dielectric model, analytical solutions of the generalized Coulomb and self-polarization potential energies exist for both the spherical and the spheroidal geometries, but unfortunately, there are a few disadvantages of this simple model as well. By construction, all the induced charges will be localized at the object surface of zero width so that both the real and the induced charges can coincide at the same location, giving rise to a self-polarization energy that diverges at the object surface. Besides, the sharp transition from  $\varepsilon_i$  to  $\varepsilon_o$  in the dielectric constant at the object surface is clearly unphysical due to interdiffusion between the object and the surrounding medium.

For the spherical geometry, several solutions have been proposed to overcome the inherent mathematical divergence of the step-like dielectric model, including the regularization method [5, 6] (which can be applied to the spheroidal geometry as well), and a more rigorous three-layer dielectric model proposed by Bolcatto and Proetto [3, 7] in which the step-like dielectric function is replaced by a continuous radial dielectric function  $\varepsilon(r)$  that changes smoothly from the object value  $\varepsilon_i$  to the medium value  $\varepsilon_o$  within a thin translation layer around the object surface. As a direct consequence of such a three-layer model, the induced charges are spread along the translation layer and the mathematical divergence in the self-polarization energy disappears. In fact, Bolcatto *et al.* actually developed a numerical method for the generalized Coulomb and self-polarization