ARTICLE IN PRESS

Computer Physics Communications ▮ (▮▮▮▮) ▮▮▮–▮▮▮

Contents lists available at ScienceDirect

Computer Physics Communications

journal homepage: www.elsevier.com/locate/cpc

Coulomb Green's function and image potential near a cylindrical diffuse interface

Changfeng Xue [a], Qiongwei Huang [a], Shaozhong Deng [b,*]

[a] School of Mathematics and Physics, Yancheng Institute of Technology, Yancheng, Jiangsu 224051, PR China

[b] Department of Mathematics and Statistics, University of North Carolina at Charlotte, Charlotte, NC 28223, United States

ARTICLE INFO

Article history:
Received 3 March 2015
Received in revised form
26 May 2015
Accepted 3 August 2015
Available online xxxx

Keywords:
Green's function
Image potential
Cylindrical diffuse interface

ABSTRACT

In a preceding paper [Comput. Phys. Commun. **184** (1): 51–59, 2013], we revisited the problem of calculating Coulomb Green's function and image potential near a planar diffuse interface within which the dielectric permittivity of the inhomogeneous medium changes continuously along one Cartesian direction in a transition layer between two dissimilar dielectric materials. In the present paper, we consider a cylindrical diffuse interface within which the dielectric permittivity changes continuously along the radial direction instead. First we propose a specific cylindrical diffuse interface model, termed the quasi-harmonic diffuse interface model, that can admit analytical solution for the Green's function in terms of the modified Bessel functions. Then and more importantly we develop a robust numerical method for building Green's functions for any cylindrical diffuse interface models. The main idea of the numerical method is, after dividing a diffuse interface into multiple sublayers, to approximate the dielectric permittivity profile in each one of the sublayers by one of the quasi-harmonic functional form rather than simply by a constant value as one would normally do. Next we describe how to efficiently compute well-behaved ratios, products, and logarithmic derivatives of the modified Bessel functions so as to avoid direct evaluations of individual modified Bessel functions in our formulations. Finally we conduct numerical experiments to show the effectiveness of the quasi-harmonic diffuse interface model in overcoming the divergence of the image potential, to validate the numerical method in terms of its accuracy and convergence, and to demonstrate its capability for computing Green's functions for any cylindrical diffuse interface models.

1. Introduction

Problems of calculating electrostatic potential at an arbitrary location due to a charge distribution in a dielectric medium sharing a common boundary, also called an interface, with another dissimilar dielectric medium occur frequently in many physical, chemical, and biological applications. In general, the electrostatic potential Φ at location $\mathbf{r}$ due to the presence of a point charge Q_s located at $\mathbf{r}_s$ in a medium with a spatially varying dielectric permittivity profile $\varepsilon(\mathbf{r})$ is the solution of the Poisson equation

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

where $\delta(\cdot)$ is the Dirac delta function. When the charge is a unit one ($Q_s = 1$), the potential $\Phi(\mathbf{r}, \mathbf{r}_s)$ defines the electrostatic Coulomb Green's function, denoted as $G(\mathbf{r}, \mathbf{r}_s)$, for such a system with a position dependent dielectric constant.

In [1], we revisited the problem of calculating Coulomb Green's function and image potential near a planar diffuse interface between two dielectrics in which the dielectric permittivity profile $\varepsilon(\mathbf{r})$ varies and changes continuously along only one Cartesian direction. In particular, we extended previous work in planar diffuse interfaces in two ways. Firstly, a new diffuse interface model, termed the quasi-harmonic interface model, was constructed, for which analytical calculation of Green's function and image potential is easy to achieve. Secondly and also more importantly, a robust numerical method for building Green's functions for general diffuse interface models was developed, thus opening the way to treat in principle any well-behaving and physically plausible dielectric permittivity profile for diffuse interfaces. In the present work, we shall extend our work in [1] to the case of cylindrical diffuse interfaces within which $\varepsilon(\mathbf{r})$ varies along only the radial direction. Typical areas of application of such an electrostatic problem include the study of solvation effects on

* Corresponding author. Tel.: +1 704 687 0634; fax: +1 704 687 1392.
E-mail address: shaodeng@uncc.edu (S. Deng).

http://dx.doi.org/10.1016/j.cpc.2015.08.027
0010-4655/

Please cite this article in press as: C. Xue, et al., Coulomb Green's function and image potential near a cylindrical diffuse interface, Computer Physics Communications (2015), http://dx.doi.org/10.1016/j.cpc.2015.08.027

molecules at a cylindrical interface separating two fluid phases [2] and the simulation of ion channels [3,4].

When $\varepsilon(\mathbf{r})$ varies along only the radial direction, one can employ the cylindrical coordinates $\mathbf{r} = (\rho, \phi, z)$. Without loss of generality, we assume the point charge Q_s is located at $\mathbf{r}_s = (\rho_s, \phi_s = 0, z_s = 0)$. Then the Coulomb Green's function $G(\mathbf{r}, \mathbf{r}_s) = G(\rho, \phi, z; \rho_s)$ can be expanded in a Fourier–Bessel form [5] as

$$G(\mathbf{r}, \mathbf{r}_s) = \int_0^\infty dk \cos(kz) \sum_{n=0}^{\infty} \left(\frac{2-\delta_{n0}}{2\pi^2}\right) \cos(n\phi) \hat{G}_n(k, \rho, \rho_s), \tag{1.2}$$

where δ_{n0} is the Kronecker delta. By substituting this Fourier–Bessel form into (1.1), one can find that the radial Green's function $\hat{G}_n(k, \rho, \rho_s)$ satisfies the following mono-dimensional differential equation

$$\frac{1}{\rho}\frac{d}{d\rho}\left[\rho\varepsilon(\rho)\frac{d}{d\rho}\hat{G}_n(k, \rho, \rho_s)\right] - \left(k^2 + \frac{n^2}{\rho^2}\right)\varepsilon(\rho)\hat{G}_n(k, \rho, \rho_s) = -\frac{4\pi}{\rho}\delta(\rho - \rho_s) \tag{1.3}$$

with the boundary condition that $\hat{G}_n(k, \rho, \rho_s)$ is finite as $\rho \to 0$ and, on the other hand, $\hat{G}_n(k, \rho, \rho_s) \to 0$ as $\rho \to \infty$.

If the dielectric permittivity were also independent of ρ, say $\varepsilon(\rho) \equiv \varepsilon_s$ with $\varepsilon_s = \varepsilon(\rho_s)$, then (1.3) would reduce to the following inhomogeneous modified Bessel equation:

$$\frac{1}{\rho}\frac{d}{d\rho}\left[\rho\frac{d}{d\rho}\hat{G}_n(k, \rho, \rho_s)\right] - \left(k^2 + \frac{n^2}{\rho^2}\right)\hat{G}_n(k, \rho, \rho_s) = -\frac{4\pi}{\rho\varepsilon_s}\delta(\rho - \rho_s), \tag{1.4}$$

whose solution, denoted by $\hat{G}_n^S(k, \rho, \rho_s)$, can be found in [5] and is

$$\hat{G}_n^S(k, \rho, \rho_s) = \begin{cases} \dfrac{4\pi}{\varepsilon_s} I_n(k\rho_s)K_n(k\rho), & \text{if } \rho \ge \rho_s, \\ \dfrac{4\pi}{\varepsilon_s} K_n(k\rho_s)I_n(k\rho), & \text{if } \rho \le \rho_s. \end{cases} \tag{1.5}$$

Here, $I_n(\rho)$ and $K_n(\rho)$ are the modified Bessel functions of the first and the second kind which are monotonically increasing and decreasing with respect to $\rho > 0$, respectively. Fig. 1 shows some typical radial Green's functions $\hat{G}_n^S(k, \rho, 0.5)$ of a homogeneous medium, namely, vacuum ($\varepsilon_s = 1$). As can be seen, when ρ is fixed, $\hat{G}_n^S(k, \rho, \rho_s)$ converges to zero as $n \to \infty$ and also as $k \to \infty$. However, it converges to zero much slower as $n \to \infty$ than as $k \to \infty$. It should be pointed out that, the unit of ρ is nm, but in the actual numerical implementation, it is converted to Bohr radius. In other words, the actual ρ value plugged into $I_n(k\rho)$ and $K_n(k\rho)$ is $10\rho/0.52917706$.

The corresponding Coulomb Green's function would be the Green's function in the homogeneous medium of dielectric constant ε_s, namely, $G(\mathbf{r}, \mathbf{r}_s) = 1/(\varepsilon_s|\mathbf{r} - \mathbf{r}_s|)$. So

$$\frac{1}{\varepsilon_s|\mathbf{r} - \mathbf{r}_s|} = \begin{cases} \dfrac{1}{\varepsilon_s}\displaystyle\int_0^\infty dk \cos(kz) \sum_{n=0}^{\infty} \mathcal{K}_n \cos(n\phi) I_n(k\rho_s)K_n(k\rho), \\ \quad \text{if } \rho \ge \rho_s, \\ \dfrac{1}{\varepsilon_s}\displaystyle\int_0^\infty dk \cos(kz) \sum_{n=0}^{\infty} \mathcal{K}_n \cos(n\phi) K_n(k\rho_s)I_n(k\rho), \\ \quad \text{if } \rho \le \rho_s, \end{cases} \tag{1.6}$$

where

$$\mathcal{K}_n = \frac{4 - 2\delta_{n0}}{\pi}. \tag{1.7}$$

For this dielectric environment, the image potential of a point charge Q_s, also called the self-polarization potential in the literature, represents the effect of the spatially varying permittivity on the potential at the position of the point charge itself. In other words, the image potential of the charged particle Q_s is calculated from the screened Coulomb potential $\Phi(\mathbf{r}, \mathbf{r}_s)$ by taking $\mathbf{r} = \mathbf{r}_s$, excluding the direct Coulomb interaction from $\Phi(\mathbf{r}, \mathbf{r}_s)$, and then dividing by 2, namely,

$$\Phi_{\text{img}}(\mathbf{r}_s) = \frac{1}{2}\int_0^\infty dk \sum_{n=0}^{\infty}\left(\frac{2-\delta_{n0}}{2\pi^2}\right) F_n(k, \rho_s), \tag{1.8}$$

in which the image potential amplitude $F_n(k, \rho_s)$ is defined as

$$F_n(k, \rho_s) = Q_s\left[\hat{G}_n(k, \rho_s, \rho_s) - \hat{G}_n^S(k, \rho_s, \rho_s)\right]. \tag{1.9}$$

Accordingly, the image or self-polarization potential energy is

$$V_{\text{img}}(\mathbf{r}) = Q_s\Phi_{\text{img}}(\mathbf{r}) = \frac{Q_s^2}{2}\int_0^\infty dk \sum_{n=0}^{\infty}\left(\frac{2-\delta_{n0}}{2\pi^2}\right) \times \left[\hat{G}_n(k, \rho_s, \rho_s) - \hat{G}_n^S(k, \rho_s, \rho_s)\right]. \tag{1.10}$$

In the present work, we shall focus on the calculation of radial Green's function $\hat{G}_n(k, \rho, \rho_s)$. While Green's function and image potential near a planar diffuse interface have been investigated quite extensively (see e.g. [6–11] and references therein), to the best of the authors' knowledge, however, Coulomb Green's function and image potential near a cylindrical diffuse interface have not been discussed in the literature. As such, we shall extend our work in [1] from planar diffuse interfaces to cylindrical ones. We will present a specific cylindrical diffuse interface model for which analytical calculation of Green's function $\hat{G}_n(k, \rho, \rho_s)$ is easy to achieve by using the modified Bessel functions. We will also present a robust numerical method that can be applied to calculate Green's function $\hat{G}_n(k, \rho, \rho_s)$ for general cylindrical diffuse interface models where the dielectric permittivity can change continuously along the radial direction in an arbitrary way.

The paper is organized as follows. In Section 2 we include the analytical solution of Green's function and image potential for the step-like dielectric interface model. In Section 3, the quasi-harmonic diffuse interface model is constructed, for which analytical calculation of Green's function $\hat{G}_n(k, \rho, \rho_s)$ is presented. In Section 4, the robust numerical method for building Green's function $\hat{G}_n(k, \rho, \rho_s)$ for general diffuse interface models is developed. In Section 5, computation of ratios, products, and logarithmic derivatives of the modified Bessel function is briefly discussed. Results of some illustrative numerical experiments are presented in Section 6, and conclusion is given in Section 7.

To conclude this section, we introduce some shorthand notations in order to make formulations easier. For $n = 0, 1, \ldots,$ we let $u_n(\rho)$ and $v_n(\rho)$ be the ratios of the modified Bessel functions of the first and the second kind, namely,

$$u_n(\rho) = \frac{I_n(\rho)}{K_n(\rho)} \quad \text{and} \quad v_n(\rho) = \frac{K_n(\rho)}{I_n(\rho)}, \tag{1.11}$$

and $\widetilde{I}_n(\rho)$ and $\widetilde{K}_n(\rho)$ be the logarithmic derivatives of the modified Bessel functions, namely,

$$\widetilde{I}_n(\rho) = \frac{I_n'(\rho)}{I_n(\rho)} \quad \text{and} \quad \widetilde{K}_n(\rho) = \frac{K_n'(\rho)}{K_n(\rho)}. \tag{1.12}$$

Please cite this article in press as: C. Xue, et al., Coulomb Green's function and image potential near a cylindrical diffuse interface, Computer Physics Communications (2015), http://dx.doi.org/10.1016/j.cpc.2015.08.027