Appl. Comput. Harmon. Anal. 34 (2013) 445–468

Contents lists available at SciVerse ScienceDirect

Applied and Computational Harmonic Analysis

www.elsevier.com/locate/acha

On the polarizability and capacitance of the cube

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ARTICLE INFO

Article history:
Received 10 April 2012
Accepted 17 July 2012
Available online 20 July 2012
Communicated by Gregory Beylkin

Keywords:
Electrostatic boundary value problem
Lipschitz domain
Polarizability
Capacitance
Spectral measure
Layer potential
Continuous spectrum
Sobolev space
Multilevel solver
Cube

ABSTRACT

An efficient integral equation based solver is constructed for the electrostatic problem on domains with cuboidal inclusions. It can be used to compute the polarizability of a dielectric cube in a dielectric background medium at virtually every permittivity ratio for which it exists. For example, polarizabilities accurate to between five and ten digits are obtained (as complex limits) for negative permittivity ratios in minutes on a standard workstation. In passing, the capacitance of the unit cube is determined with unprecedented accuracy. With full rigor, we develop a natural mathematical framework suited for the study of the polarizability of Lipschitz domains. Several aspects of polarizabilities and their representing measures are clarified, including limiting behavior both when approaching the support of the measure and when deforming smooth domains into a non-smooth domain. The success of the mathematical theory is achieved through symmetrization arguments for layer potentials.

1. Introduction

The determination of polarizabilities and capacitances of inclusions of various shapes has a long history in computational electromagnetics. Inclusions with smooth surfaces are, by now, rather standard to treat. When surfaces are non-smooth, however, the situation is different. Numerical solvers can run into problems related to stability and resolution. Particularly so in three dimensions and for certain permittivity combinations. Solutions may not converge or results could be hard to interpret. See [44,45,51] and references therein. The situation on the theoretical side is similar. When, and in what sense do solutions exist? Such questions are in the mainstream of contemporary research in harmonic analysis. Coincidentally, also in applied physics (plasmonics) there is a growing interest in solving electrostatic problems on domains with structural discontinuities and a concern about the sufficiency of available solvers [19,54].

This paper addresses several fundamental issues related to the problems just mentioned. We construct a stable solver for the polarizability and capacitance of a cube based on an integral equation using the adjoint of the double layer potential. We compute solutions of unprecedented accuracy and interpret the results within a rigorous mathematical framework. The reason for working with a cube is twofold. First, the cube has the advantage that its geometric difficulties are concentrated to edges and corners, since its faces are flat. Integral equation techniques, which often excel for boundary value problems in two dimensions, typically suffer from loss of accuracy in the discretization of weakly singular integral operators on curved surfaces in three dimensions. Here we need not worry about that. Secondly, cubes are actually common in plasmonic applications.

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1063-5203/$ – see front matter
http://dx.doi.org/10.1016/j.acha.2012.07.006

In the purely theoretical sections we begin by collecting a number of results and recent advances in the theory of layer potentials associated with the Laplacian in Lipschitz domains. The most obvious reason for this is that the invertibility study of layer potentials leads to the solution of the boundary value problem implicit in the definition of polarizability, and is as such the basis for both the mathematical and numerical aspects of this paper. Furthermore, the properties of the polarizability for a non-smooth domain such as a cube are quite subtle, and it is our ambition to provide a solid theoretical foundation for the problem at hand, giving a careful and detailed exposition of a mathematical framework that clarifies a number of points.

Since the double layer potential is not self-adjoint in the L^2-pairing, we develop certain symmetrization techniques for it, in particular extending the work of Khavinson, Putinar and Shapiro [31] to the case of a non-smooth domain. These techniques are used to prove the unique existence of the polarizability itself for a Lipschitz domain, as well as of a corresponding representing measure [18]. We present a thorough discussion of the smooth case, the limiting behavior in passing from the smooth to the non-smooth case, and ultimately the general case. Concerning the last point, a condition ensuring that the representing measure has no singular part is given, and it is proven that in the support of the absolutely continuous part of the measure, the polarizability can not be given a direct interpretation in terms of a potential with finite energy solving the related boundary value problem.

The paper is organized as follows: Section 2 formulates the electrostatic problem and defines the polarizability. Existence issues and representations are reviewed in Section 3. For ease of reading, rigorous statements and proofs are deferred to Sections 4 and 5. The capacitance is discussed in Section 6. Section 7 reviews the state of the art with regard to numerical schemes. Section 8 gives a necessary background to the present solver. New development takes place in Section 9. The last sections contain numerical examples performed in MATLAB. Section 10 illustrates the effects of rounding corners and Section 11 is about the cube.

The main conclusion of the paper is that, from a numerical viewpoint, it is an advantage to let cubes have sharp edges and corners as opposed to the common practice of rounding them slightly. Furthermore, the representing measure for the polarizability of the cube is determined, and a new benchmark for the capacitance of the unit cube is established.

2. The electrostatic problem and the polarizability

Let a domain V, an inclusion with surface S and permittivity ϵ_2, be embedded in an infinite space. The exterior to the closure of V is denoted E and has permittivity ϵ_1. Let ν_r be the exterior unit normal of S at position r.

We seek a potential $U(r)$, continuous in $E \cup S \cup V$, which satisfies the electrostatic equation

$$\Delta U(r) = 0, \quad r \in E \cup V, \tag{1}$$

subject to the boundary conditions on the limits of normal derivatives

$$\epsilon_1 \frac{\partial}{\partial \nu_r} U^{\text{ext}}(r) = \epsilon_2 \frac{\partial}{\partial \nu_r} U^{\text{int}}(r) \tag{2}$$

and behavior at infinity

$$\lim_{r\to\infty} \nabla U(r) = e. \tag{3}$$

Here superscripts ext and int denote limits from the exterior or interior of S, respectively, and e is an applied unit field. Eqs. (1)–(3) constitute a partial differential equation formulation of the electrostatic problem. Proposition 5.1 gives a strict interpretation of what it means for a potential $U(r)$ to solve this problem, in particular expressing (2) in a distribution sense.

For the construction of solutions to (1)–(3) we make use of fundamental solutions to the Laplace equation in two and three dimensions

$$G\bigl(r, r'\bigr) = -\frac{1}{2\pi} \log\bigl|r - r'\bigr| \quad \text{and} \quad G\bigl(r, r'\bigr) = \frac{1}{4\pi} \frac{1}{|r - r'|}, \tag{4}$$

and represent $U(r)$ in terms of a single layer density $\rho(r)$ as

$$U(r) = e \cdot r + \int_S G\bigl(r, r'\bigr)\rho\bigl(r'\bigr)\, \mathrm{d}\sigma_{r'}, \tag{5}$$

where $\mathrm{d}\sigma$ is an element of surface area.

The representation (5) satisfies (1) and (3). Its insertion in (2) gives the integral equation for $\rho(r)$

$$\rho(r) + 2\lambda \int_S \frac{\partial}{\partial \nu_r} G\bigl(r, r'\bigr)\rho\bigl(r'\bigr)\, \mathrm{d}\sigma_{r'} = -2\lambda(e \cdot \nu_r), \quad r \in S, \tag{6}$$