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High-Order Spectral Simulation of Graphene Ribbons

David P. Nicholls

Department of Mathematics, Statistics, and Computer Science, University of Illinois at Chicago, Chicago, IL 60607, USA.

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Abstract. The plasmonics of graphene and other two-dimensional materials has attracted enormous amounts of attention in the scientific literature over the past decade. Both the possibility of exciting plasmons in the terahertz to midinfrared regime, and the active tunability of graphene via electrical gating or chemical doping has generated a great deal of excitement among engineers seeking sensing devices which operate in this regime. Consequently there is significant demand for robust and highly accurate computational capabilities which can incorporate such materials. Standard volumetric approaches can answer this demand, but require vast computational resources in exchange. Here we describe an algorithm which addresses this issue in two ways, first, we model the graphene layer with a surface current which is applicable to a wide class of two-dimensional materials. In addition, we reformulate the governing volumetric equations in terms of surface quantities using Dirichlet-Neumann Operators. These surface equations can be numerically simulated in an efficient, stable, and accurate fashion using a novel High-Order Perturbation of Envelopes methodology. We utilize an implementation of this algorithm to study absorbance spectra of TM polarized plane-waves scattered by a periodic grid of graphene ribbons.

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Key words: Layered media, two-dimensional materials, graphene, electromagnetic scattering, high-order spectral methods, high-order perturbation of envelopes methods.

1 Introduction

The discovery of graphene and other two-dimensional materials has been truly transformative to the fields of photonics and plasmonics. The mechanical, chemical, and electronic properties of these single atom thick materials are remarkable. While several materials such as black phosphorous [25] and hexagonal Boron Nitride (hBN) [23] have shown promise for use in devices, the most well-studied is graphene [10, 13, 14, 16, 37].

Graphene is a single layer of carbon atoms in a honeycomb lattice which was first isolated experimentally in 2004 [28] resulting in the 2010 Nobel Prize in Physics to Geim [14] and Novoselov [37]. Graphene plasmons have become important for devices operating in the terahertz to mid-infrared regime [24] where such phenomena are supported. For a complete discussion of graphene including modeling, device design, and particular applications, we refer the interested reader to the survey article of Bludov, Ferriera, Peres, and Vasilevskiy [4] and the text of Goncalves and Peres [18].

In light of all of this there is an understandable desire amongst scientists and engineers to simulate structures featuring two-dimensional materials numerically. A most natural approach is to solve the volumetric Maxwell equations either in the time or frequency domain where the graphene is modeled with an effective permittivity supported in a *thin* layer, or as a surface current with an effective conductivity at the interface between two layers. In either case commercial black-box Finite Element Method (FEM) software such as COMSOL Multiphysics^{TM} [7] is typically utilized, however, these simulations are quite costly due to their low-order accuracy and volumetric character.

In our recent contribution [34] we described an approach which overcomes both of these limitations by not only restating the frequency domain governing equations in terms of *interfacial* unknowns, but also describing a High-Order Spectral (HOS) algorithm which recovers solutions with remarkable accuracy (typically machine precision) with a very modest number of unknowns. A subtlety of our approach is that, in order to close the system of equations, surface integral operators must be introduced which connect interface traces of the scattered fields (Dirichlet data) to their surface normal derivatives (Neumann data). Such Dirichlet-Neumann Operators (DNOs) have been widely used and studied in the simulation of linear wave scattering, e.g., for enforcing far-field boundary conditions transparently [2,3,8,9,15,19,21,22,35] and interfacial formulations of scattering problems [27,29,32,34,36].

One way to generate plasmonic responses in photonic devices is to introduce periodicity to the structure in question. This can be done in a number of ways, and in our earlier work we focused upon two-dimensional materials deposited on periodic, corrugated grating structures. Here the height/slope of the grating *shape* was viewed as a perturbation parameter and the resulting High-Order Perturbation of Shapes (HOPS) scheme sought high order corrections to the trivially computed flat-interface, solid graphene configuration. While such devices are important, it is much easier (and more common) to create a structure with *flat* interfaces upon which periodically spaced ribbons of graphene are mounted. In this contribution we model this design by multiplying the (constant) current function by an *envelope* function which transitions between one (where the graphene is deposited) to zero (where graphene is absent). Our numerical procedure views this envelope function as a perturbation of the identity function, and we term our scheme a High-Order Perturbation of Envelopes (HOPE) algorithm.

With this approach we will not only rigorously demonstrate that the scattered fields depend analytically upon this envelope perturbation parameter, but also show that a numerical scheme can be built upon the resulting recursions. The algorithm is both robust