Nanostructures and Computation

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Introduction

Photonic crystals and nanophotonics employ nanoscale optical structures, on the scale of the wavelength of light, in order to produce optical phenomena far different from those in more homogeneous media. Our work has centered on three general categories of problems in nanophotonics: what new effects and devices can one achieve in such structures, how does one design devices given so many degrees of freedom, and what higher-level understanding can one develop for such complex systems. Electromagnetism also permits large-scale brute-force simulations that are essentially exact, and this has led us to a second topic of research, that of efficient numerical methods for large-scale computation. Not only have we studied advances in methods specific to electromagnetism, but we also investigate the theory and implementation of algorithms, such as FFTs, that are important for many ares of scientific computing.

1. Fast Algorithms for Spectral Methods and Signal Processing

Sponsors:
MIT Undergraduate Research Opportunities Program

Project staff:
Xuancheng Shao, Prof. S. G. Johnson

Discrete Cosine Transform (DCT) algorithms play a central role in many areas of scientific computing, from digital signal processing to spectral methods for solving partial differential equations to image and audio compression. Although considerable effort has gone into the development of efficient DCT implementations on modern computers, and we have even developed automatic techniques to optimize DCT programs (Frigo and Johnson, 2005), there has been very little progress in the underlying theory of DCT algorithms, and in particular there had been almost no progress for over 20 years in the underlying arithmetic counts of the algorithms. In 2008, we published two papers improving on the operation counts for types I–IV of the DCT (the four most common types) as well as for the modified DCT (MDCT) used in audio compression. In many cases, these seem to be the first savings of even a single addition or multiplication in DCT algorithms since the various DCT types and corresponding fast algorithms were formulated in the 1980s.

In fact, the improvement is not merely a fixed number of operations saved, but an improvement in the asymptotic constant factor from 2 $N \log N$ to $^{17}/_{9}\ N \log N$ for transforms of length N. This 6% improvement in a count long thought to be optimal, and which had resisted repeated attempts at arithmetic savings (with innumerable papers on DCT algorithms) re-opens the question of whether further improvements are possible.

2. Accurate Prediction of Casimir Forces in Nanostructured Mechanical Systems

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Prof. S. G. Johnson, Alejandro Rodriguez

Casimir forces are an interaction between uncharged objects that arise at micrometer-scale separations due to quantum vacuum-photon fluctuations. Besides their importance in basic physics research as a direct manifestation of the quantum vacuum as a measurable force, Casimir forces have important influences on cold atom trapping, superfluid films, and potentially for future nanomechanical devices. Although they were first predicted in 1948 for parallel metallic plates, Casimir forces have proven surprisingly difficult to predict for non-planar geometries; the state of the art in 2006 was the first theoretical prediction of the force between an infinite perfect-metal cylinder and an infinite perfect-metal plane. In our recent work, we have demonstrated new numerical techniques to accurately predict Casimir forces for arbitrary geometries, including arbitrary dispersive materials, which has enabled us to study a range of problems that had never previously been accurately modelled. Moreover, our approach exploits existing computational methods for classical electromagnetism that are already mature, efficient, scalable, and widely available. Although other groups have developed techniques to study specific non-planar geometries, as far as we know we have the only working code that handles any geometry without modification (given sufficient computational power), and the only working code that currently handles realistic dielectric materials. It is hard to exaggerate how exciting the opportunities are in this field—almost any geometry one can imagine has never been calculated, and very little is known about what is possible for Casimir force phenomena in complex geometries.

We have already been able to explore many new structures and have encountered phenomena very different from those in the known geometries—for example, non-monotonic variation in the force between two objects as a sidewall is brought closer (Rodriguez *et al.*, 2007), which is counter-intuitive because it contradicts the common intuition of the Casimir interaction as a monotonic attractive force. To our knowledge, this was the first accurate calculation of Casimir forces for three-body interactions, and already it exhibited surprising qualitative effects. These effects were subsequently reproduced and generalized in other geometries, in a collaboration with Profs. Kardar and Jaffe at MIT (Zaheer, 2007; Rahi, 2008).

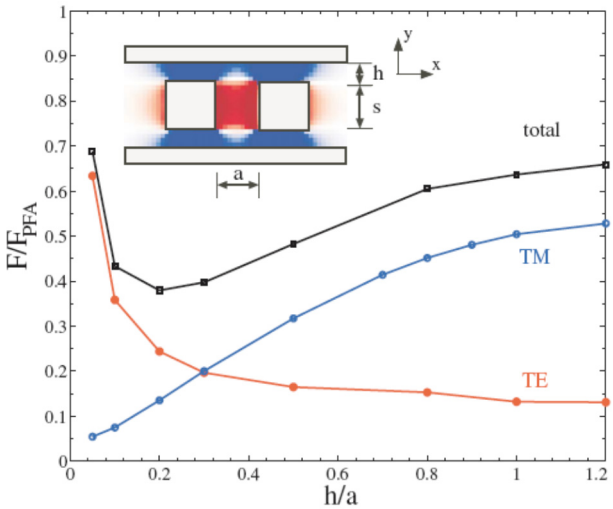

figure 1. Non-monotonic Casimir force due to multi-body interactions in a "piston"-like geometry of two blocks between metal sidewalls. Plot is force between the blocks as a function of the separation *h* between the blocks and sidewalls. Inset: schematic and plot of Casimir stress tensor (blue/white/red = negative/zero/positive) around the blocks.

3. Modeling Photonic Quasicrystals

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A. Rodriguez, A. McCauley, Dr. Y. Avniel, and Prof. S. G. Johnson

Photonic quasicrystals are aperiodic structures with long-range order, fractal (Cantor-set) spectra, and potentially high rotational symmetry and large photonic band gaps. The study of quasicrystals in two and (especially) three dimensions has been hampered, however, by the difficulty of numerically solving an aperiodic structure—unlike a periodic structure, where only the unit cell need be considered, quasicrystals seem to require large "supercells" to accurately capture their long-range order. Because quasicrystals are typically defined by irrational "slices" of higher-dimensional periodic structures, however, we have recently shown that it is possible to solve for their spectra by extending Maxwell's equations into higher dimensions—so that the entire infinite aperiodic structure can be captured by a single higher-dimensional unit cell (Rodriguez *et al.*, 2008). We believe that the formulation of this idea as a numerical approach opens the possibility of studying new classes of structures that were previously out of reach. For example, we are not aware of any numerical solutions of three-dimensional photonic quasicrystals, by any method.

As an initial proof-of-concept validation of the method, we successfully applied the method to calculate the spectrum of a one-dimensional "Fibonacci" quasicrystal, so-called because it consists of a sequence of layers A,B,AB,BAB,ABBAB,… formed of two materials A and B put together by a Fibonacci-like string-concatenation rule. Even in this simple system, we were able to use the higher-dimensional approach to demonstrate the origin of the quasicrystal band gap, exponentially localized modes, and other features that previously required large computational cells with thousands of layers to reproduce accurately but which now require only a single 2d unit cell.

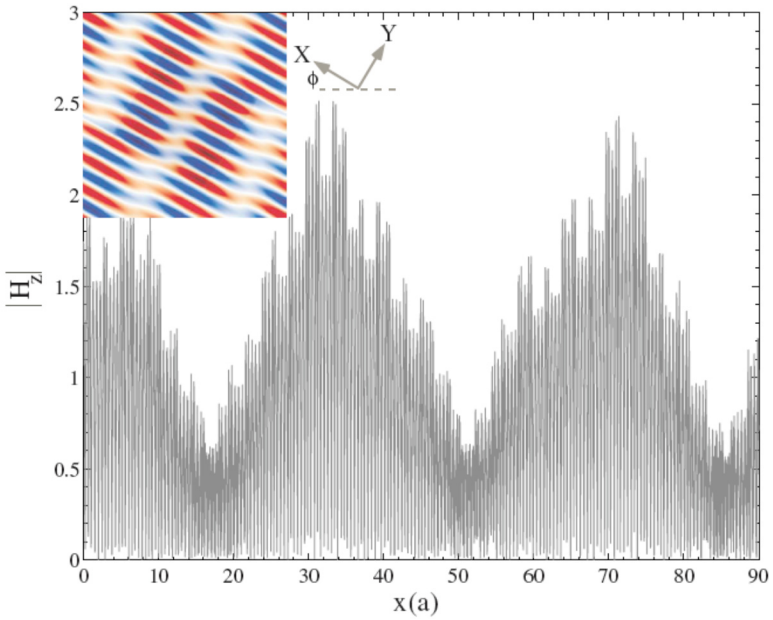

figure 2. Magnetic-field amplitude $|H_z|$ in a one-dimensional Fibonacci quasicrystal, which directly corresponds to the two-dimensional inset field pattern in a two-dimensional "superspace" where the quasicrystal is periodic.

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