A Pseudo-spectral Analysis of Photonic Crystals

A. R. Baghai-Wadji
Vienna University of Technology, Vienna, Austria
Accelerated Computational Technology Group

We present a pseudo-spectral analysis of electromagnetic wave propagation in photonic crystals utilizing a suitably designed diagonalization of Maxwell's equations.

Statement of the Problem: Consider a three manifold M with the boundary surface S. Let Au=0 represent the system of linear homogeneous Maxwell's equations in M with given boundary conditions on S, and a fairly general anisotropic, or bi-anisotropic material constitution. At an arbitrary point p in M consider the local coordinate system (x,y,z) permitting separability of the fields with respect to at least one coordinate, say, z. Diagonalize Au=0 with respect to z.

On the Notion of Diagonalization: Diagonalization with respect to the coordinate z refers to as a transformation of Au=0 into an equivalent form Bv=dv. Thereby, d at the RHS denotes the derivative of v with respect to z. Diagonalized forms possess a number of distinguished properties, which will thoroughly be reviewed in this presentation. Furthermore, the existence problem of diagonalized forms, corresponding to physically realizable systems, will be investigated.

Outline of the Diagonalization Procedure: To accomplish the transformation Au=0 into Bv=dv we utilize a convenient symbolic form for representing the curl operator in terms of three constituent matrices N1, N2, N3. We find that these matrices satisfy the defining commutation relations of the Lie algebra so(3).

Next we establish a relationship between N1, N2, N3 and the proper rotation matrices R1, R2, R3. It is known that every proper rotation in three dimensional Euclidean space can be expressed in terms of a succession of three proper rotations about the x-, y-, and z axis. The corresponding one-parameter subgroups can be generated by three matrices R1, R2, and R3. Each of these matrices satisfy the following properties:

(a) They are orthonormal,
(b) they are proper (special),
(c) the group multiplication is an analytic function of their parameter,
(d) the inverse operation is an analytic function of parameter.
(e) These matrices form a one-parameter Lie group and since they are *special* and *orthonormal*, they are called the special orthogonal group in three dimensions and denoted by SO(3).

Using the properties of N1, N2, and N3 the original system of PDEs (Au=0) can be transformed into the equivalent form Bv=dv virtually *simply by inspection*.

In this presentation we will focus on the following:

(1) We apply our formulation to the analysis of strictly periodic 2D- and 3D photonic crystal models, and briefly comment on the analysis of photonic crystals with defects. To this end we discretize the transformed diagonalized form in the plane normal to the diagonalization direction, and hybridize the resulting discrete system with a suitably chosen finite difference implementation in the diagonalization direction.
(2) We discuss details of the implementation and show the superiority of our method to other techniques available in terms of the accuracy, speed, and most importantly the consistency of the numerical data: We will show that our results are always devoid of spurious modes.
(3) As a further point in our discussion we address the “defect problem” in photonic crystals. To this end we investigate the construction and properties of Wannier functions, and use an accurate numerical Fourier transform in d-dimensions without aliasing; however, with a comparable time complexity as the fast Fourier transform.
(4) We conclude by discussing alternative strategies to model defects efficiently, including the construction of problem-adapted bases by utilizing eigenfunctions of suitably constructed dual (perturbed) problems.