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Band Structure Calculations of Dispersive Photonic Crystals in 3D using Holomorphic Operator Functions

Wenqiang Xiao[1], Bo Gong[2,*], Junshan Lin[3] and Jiguang Sun[4]

[1] *Beijing Computational Science Research Center, Beijing, 100193, China.*
[2] *Faculty of Science, Beijing University of Technology, Beijing, 100124, China.*
[3] *Department of Mathematics and Statistics, Auburn University, Auburn, AL 36849, United States.*
[4] *Department of Mathematical Sciences, Michigan Technological University, Houghton, MI 49931, United States.*

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Abstract. We propose a finite element method to compute the band structures of dispersive photonic crystals in 3D. The nonlinear Maxwell's eigenvalue problem is formulated as the eigenvalue problem of a holomorphic operator function. The Nédélec edge elements are employed to discretize the operators, where the divergence free condition for the electric field is realized by a mixed form using a Lagrange multiplier. The convergence of the eigenvalues is proved using the abstract approximation theory for holomorphic operator functions with the regular approximation of the edge elements. The spectral indicator method is then applied to compute the discrete eigenvalues. Numerical examples are presented demonstrating the effectiveness of the proposed method.

AMS subject classifications: 35P30, 65N25, 65N30, 78M10

Key words: Band structure, dispersive photonic crystal, Maxwell's equations, nonlinear eigenvalue problem, edge element, holomorphic operator function.

1 Introduction

Photonic crystals (PCs) are periodic structures with dielectric or metallic materials. They possess band gaps so that the propagation of light through the crystal is prohibited at specific frequencies. This property allows for designs of many optical devices with a wide range of applications, such as filters, optical communications, lasers and microwaves [18].

*Corresponding author. *Email addresses:* wqxiao@csrc.ac.cn (W. Xiao), gongbo@bjut.edu.cn (B. Gong), jzl0097@auburn.edu (J. Lin), jiguangs@mtu.edu (J. Sun)

By the Floquet-Bloch theory [22], the spectral problem related to band structures can be formulated as an eigenvalue problem of the Maxwell's equation with periodic boundary conditions in the fundamental cell.

For non-dispersive media where the permittivity and permeability are independent of the frequency, the eigenvalue problems are linear. Many successful numerical approaches have been proposed, including the plane wave method, the finite-difference time-domain method, the finite element method, the order-N method, the transfer-matrix method, etc [1, 8, 9, 14, 26, 27, 34]. In contrast, dispersive media (with frequency dependent permittivity or permeability) lead to nonlinear eigenvalue problems in general. As such the computation of the band structure is much more challenging. Existing numerical methods for nonlinear eigenvalue problems are mostly based on the Newton's iteration [28], linearization [24] or extensions of the techniques for linear problems [29, 32]. These numerical approaches often require accurate initial guesses of the eigenvalues and eigenvectors, which are not available in general. Furthermore, the convergence analysis of the algorithms is very challenging due to the nonlinearity of the problem. We also refer the readers to [23], which formulates a new stabilized quadratic eigenvalue problem to compute a particular selection of the electromagnetic Bloch variety. The discretization for the 3D Maxwell's equation brings additional difficulty to the eigenvalue computation due to the large degree of freedom (typically in the order of million). Few numerical results exist for the band structure of the dispersive photonic crystals in 3D.

In this paper, we propose a finite element method for band structure calculations of photonic crystals in 3D. Following the idea in [33, 34], we transform the problem into the eigenvalue problem of a holomorphic operator function, whose values are solution operators of the parameterized Maxwell's equations. A mixed formulation for the Maxwell's equations is used to enforce the divergence-free condition and discretized by the Nédélec edge elements. Based on the well-posedness of a related source problem [5], we show that the operator function is of Fredholm type with index zero. Employing the abstract approximation theory for holomorphic Fredholm operator functions [19, 20] and the finite element theory for Maxwell's equations, we prove the convergence of discrete eigenvalues of the holomorphic operator function. Finally, the spectral indicator method (SIM) is applied to practically calculate the eigenvalues. The SIM extends the ideas in [15, 16] for the generalized eigenvalues of non-Hermitian matrices and is particularly effective for computing eigenvalues of a holomorphic operator function.

The current paper is a non-trivial continuation of [34] in several aspects. First, [34] only deals with the 2D case — a nonlinear eigenvalue problem of the Helmholtz equation, while the current paper deals with the 3D case — a nonlinear eigenvalue problem of the Maxwell's equations. Second, only the TE case is analyzed in [34]. In this paper, a different technique is used and the convergence is proved directly for Maxwell's equations. Third, the 3D numerical examples are way more complicated and there exist only a few examples in literature including the engineering journals. We note that, in the context of finite elements, the above approach has been applied successfully to solve several nonlinear eigenvalue problems of partial differential equations [12, 33].