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# Bandgap optimization of two-dimensional photonic crystals using semidefinite programming and subspace methods ☆

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ABSTRACT

In this paper, we consider the optimal design of photonic crystal structures for two-dimensional square lattices. The mathematical formulation of the bandgap optimization problem leads to an infinite-dimensional Hermitian eigenvalue optimization problem parametrized by the dielectric material and the wave vector. To make the problem tractable, the original eigenvalue problem is discretized using the finite element method into a series of finite-dimensional eigenvalue problems for multiple values of the wave vector parameter. The resulting optimization problem is large-scale and non-convex, with low regularity and non-differentiable objective. By restricting to appropriate eigenspaces, we reduce the large-scale non-convex optimization problem via reparametrization to a sequence of small-scale convex semidefinite programs (SDPs) for which modern SDP solvers can be efficiently applied. Numerical results are presented for both transverse magnetic (TM) and transverse electric (TE) polarizations at several frequency bands. The optimized structures exhibit patterns which go far beyond typical physical intuition on periodic media design.


## 1. Introduction

The propagation of waves in periodic media has attracted considerable interest in recent years. This interest stems from the possibility of creating periodic structures that exhibit bandgaps in their spectrum, i.e., frequency regions in which the wave propagation is prohibited. Bandgaps occur in many wave propagation phenomena including electromagnetic, acoustic and elastic waves. Periodic structures exhibiting electromagnetic wave bandgaps, or photonic crystals, have proven very important as device components for integrated optics including frequency filters [11], waveguides [10], switches [21], and optical buffers [28].

The optimal conditions for the appearance of gaps were first studied for one-dimensional crystals by Lord Rayleigh in 1887 [18]. In a one-dimensional periodic structure, one can widen the bandgap by increasing the contrast in the refractive index and difference in width between the materials. Furthermore, it is possible to create bandgaps for any particular frequency by changing the periodicity length of the crystal. Unfortunately, however, in two or three dimensions one can only suggest rules of thumb for the existence of a bandgap in a periodic structure, since no rigorous criteria have yet been determined. This made the design of two- or three-dimensional crystals a trial and error process, being far from optimal. Indeed,

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the possibility of two- and three-dimensionally periodic crystals with corresponding two- and three-dimensional bandgaps was not suggested until 100 years after Rayleigh's discovery of photonic bandgap in one dimension, by Yablonovitch [26] and John [14] in 1987.

From a mathematical viewpoint, the calculation of the bandgap reduces to the solution of an infinite-dimensional Hermitian eigenvalue problem which is parametrized by the dielectric function and the wave vector. In the design setting, however, one wishes to know the answer to the question: which periodic structures, composed of arbitrary arrangements of two or more different materials, produce the largest bandgaps around a certain frequency? This question can be rigorously addressed by formulating an optimization problem for the parameters that represent the material properties and geometry of the periodic structure. The resulting problem is infinite-dimensional with an infinite number of constraints. After appropriate discretization in space and consideration of a finite set of wave vectors, one obtains a large-scale finite-dimensional eigenvalue problem which is non-convex and is known to be non-differentiable when eigenvalue multiplicities exist. The current state-of-the-art work done on this problem falls into two broad categories. The first kind tries to find the "optimal" band structure by parameter studies – based on prescribed inclusion shapes (e.g., circular or hexagonal inclusions) [9], fixed topology [27], or geometric considerations from the interpretation of an extensive numerical optimization study [19]. The second kind attempts to use formal topology optimization techniques [4,7,20], and level set methods [15]. Both approaches typically use gradient-based optimization methods. While these methods are attractive and have been quite successful in practice, the optimization processes employed explicitly compute the sensitivities of eigenvalues with respect to the dielectric function, which are local subgradients for such non-differentiable problem. As a result, gradient-based solution methods often suffer from the lack of regularity of the underlying problem when eigenvalue multiplicities are present, as they typically are at or near the solution.

In this paper we propose a new approach based on semidefinite programming (SDP) and subspace methods for the optimal design of photonic band structure. In the last two decades, SDP has emerged as the most important class of models in convex optimization; see [1,2,16,23,25]. SDP encompasses a huge array of convex problems as special cases, and is computationally tractable (usually comparable to least-square problems of comparable dimensions). There are three distinct properties that make SDP very suitable for the bandgap optimization problem. First, the underlying differential operator is Hermitian and positive semidefinite. Second, the objective and associated constraints involve bounds on eigenvalues of matrices. And third, as explained below, we can approximate the original non-convex optimization problem by a semidefinite program for which SDP can be well applied, thanks to its efficiency and robustness of handling this type of spectral objective and constraints.

In our approach, we first reformulate the original problem of maximizing the bandgap between two consecutive eigenvalues as an optimization problem in which we optimize the gap in eigenvalues between two orthogonal subspaces. The first eigenspace consists of eigenfunctions corresponding to eigenvalues below the bandgap, whereas the second eigenspace consists of eigenfunctions whose eigenvalues are above the bandgap. In this way, the eigenvalues are no longer present in our formulation; however, like the original problem, the exactly reformulated optimization problem is large-scale. To reduce the problem size, we truncate the high-dimensional subspaces to only a few eigenfunctions below and above the bandgap [5,17], thereby obtaining a new small-scale yet non-convex optimization problem. Finally, we keep the subspaces fixed at a given decision parameter vector and use a reparametrization of the decision variables to obtain a convex semidefinite optimization problem for which SDP solution methods can be effectively applied. We apply this approach to optimize bandgaps in two-dimensional photonic crystals for either the transverse magnetic (TM) or the transverse electric (TE) polarizations.

A detailed assessment of the computational efficiency of the proposed approach compared to alternative methods is outside the scope of this paper. We note that the performance of methods that require sensitivity information of the eigenvalues with respect to the dielectric function will deteriorate when eigenvalue multiplicities occur. The approach developed herein is designed to deal with such situations and therefore, we expect it will perform with increased robustness in complex realistic applications.

The rest of the paper is organized as follows. In Section 2 we introduce the governing differential equations and the mathematical formulation of the bandgap optimization problem. We then discuss the discretization process and present the subspace restriction approach. In Section 3 we introduce the semidefinite programming formulation of the band structure optimization, and lay out the optimization steps involved in solving the problem. Numerical results are presented in Section 4 for both the TE and TM polarizations in square lattices. Finally, in Section 5 we conclude with several remarks on anticipated future research directions.

## 2. The bandgap optimization problem

### 2.1. Governing equations

Our primary concern is the propagation of electromagnetic linear waves in periodic media, and the design of such periodic structures, or photonic crystals, to create optimal bandgaps in their spectrum. The propagation of electromagnetic waves in photonic crystals is governed by Maxwell's equations. The solutions to these equations are in general very complex functions of space and time. Due to linearity however, it is possible to separate the time dependence from the spatial dependence by expanding the solution in terms of harmonic modes – any time-varying solution can always be reconstructed by a