

# Maximizing bandgaps in two-dimensional photonic crystals: a variational algorithm

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September 1, 2003

## 1 Introduction

Photonic crystals are structures where the electromagnetic properties of the constituent material are periodic in space. They have been intensely studied recently [1] both for their practical applications and the theoretical challenges they pose. One area of research is the design and fabrication of structures that do *not* allow electromagnetic waves with frequencies in a certain range to propagate in them. Such structures are expected to find use as perfect mirrors and guiding structures, etc. In many applications, it is desirable that the excluded frequency range – the bandgap – be as large as possible. In this paper, we focus our attention on the design of structures with such maximal bandgaps.

The design problem that we propose to solve and ones closely related to it have been addressed before. The following brief and non-exhaustive survey is meant to give an idea of the major lines of investigation in this field. Some exact analytical studies of problems very similar to ours merit mention: a detailed examination of minimal and maximal bandgaps in the quantum-mechanical context can be found in [2], and an examination of conditions under which complete bandgaps exist in two-dimensional two-component photonic crystals can be found, for instance, in [3]. Cox and Dobson have addressed almost exactly the same problem that we do in [4], although their strategy is quite different. They impose the geometry of the lattice – for instance, a square lattice – at the outset as a constraint, whereas we allow exploration in the space of all possible lattices. Furthermore, the final optimized structure that they obtain depends on the starting structure, i.e. the solution obtained is not truly a global maximum. A number of other numerical studies (see [5] for a sample) seek to maximize bandgaps with under an even greater number of constraints imposed on the geometry of the crystal. To summarize, the starting point in each numerical approach has been to impose global constraints that the material properties must satisfy (maximum and minimum dielectric constants, for instance). We do the same. In earlier approaches, one next imposes the translational symmetry of the structure to be designed (focusing attention, for example, on square lattices only) along with – in some cases – further geometric constraints, and, finally, explores a subset of the structures that satisfy the imposed translational symmetry. Our algorithm, in contrast, involves an unrestricted exploration of *all* the structures that satisfy the initially imposed material constraints. Notably, the algorithm is polarization non-specific; it can maximize a complete bandgap (i.e. a frequency range that is excluded for all polarizations).

Two remarkable results follow quite easily from our discussion: First, that for a maximal bandgap structure where the dielectric constant is allowed to vary within a range, the dielectric constant at each point takes on either the smallest or the largest possible value. Second, that the wave-vectors corresponding to the edges of a maximal bandgap may take on values only from a very small finite subset of the Brillouin zone.

The algorithm we propose is based on incremental steps, each of which increases the size of the selected bandgap. Each step is based on a variational argument that is discussed in [7] and outlined below.

The plan of this chapter is as follows. In the next section, we present the equations relevant to the problem. Thereafter, we outline the variational argument we use and describe an algorithm to implement this in the case where the dielectric constant of the material is required to lie in a certain range. This is followed by a closer look at two exact results. Finally, some open questions relevant to this work are discussed. We have numerically implemented the algorithm; the details of the implementation will be presented elsewhere.

## 2 Maxwell equations in two-dimensional systems

Our bandgap maximization scheme, and the variational principle it is based on, work for periodic systems with any number of spatial dimensions. We choose to focus our attention on two-dimensional systems for the following reasons. The one-dimensional problem is too simple to illustrate some of the points we wish to highlight. The three-dimensional problem, however, obscures some features of the scheme with its greater algebraic complexity. Two spatial dimensions, in our view, offers a happy medium. In addition, two-dimensional photonic crystals find numerous practical application and have been actively studied analytically, numerically and in the lab. This allows our results and predictions to be tested against a large existing body of results.

The system we will analyze here is a two-dimensional photonic crystal; the bandstructure we investigate is for waves with wave-vectors lying in the same two-dimensional plane. The magnetic susceptibility of the materials constituting the crystal is assumed to be unity. The dielectric constant may, of course, vary spatially, but is assumed to be time-independent (a reasonable assumption) and frequency-independent (an assumption that is not always reasonable but is required for our scheme, in its current version, to work).

We will begin by establishing the notation we will use to describe our system. The primitive translation vectors  $\vec{a}_1$  and  $\vec{a}_2$  form a natural basis for describing positions in a two-dimensional periodic structure. Let the two vectors be of length  $l_1$  and  $l_2$  with an angle  $\theta$  between them. Our maximization scheme is designed to maximize over all allowed spatial dependences of dielectric constants, including all possible primitive bases. In particular, we will need to investigate effects of variations in  $l_1$ ,  $l_2$  and  $\theta$  (i.e., of distortions of the crystal). It is useful, then, to choose a notation that makes the dependence of the operators we encounter on these parameters explicit. To this end, we use tensor notation, rather than the vocabulary of the reciprocal basis that is more common in solid-state physics. We thereby gain in transparency what is, perhaps, lost through unfamiliarity. Suppose that we define our coordinates such that the region  $0 \leq x^1 < 1$ ,  $0 \leq x^2 < 1$  describes a unit cell. We begin by noting that the distance  $ds$  between two points in the relevant two-dimensional plane separated by  $dx^1\vec{a}_1 + dx^2\vec{a}_2$  (the superscripts are ‘contravariant’ indices, not exponents) is given by  $(ds)^2 = (l_1dx^1)^2 + (l_2dx^2)^2 + 2l_1l_2dx^1dx^2\cos\theta = g_{\alpha\beta}dx^\alpha dx^\beta$ . (We will use the Einstein summation convention.) This information is summarized in the matrix form of the metric tensor

$$g = \begin{pmatrix} l_1^2 & l_1l_2\cos\theta \\ l_1l_2\cos\theta & l_2^2 \end{pmatrix}.$$

With  $\partial_\alpha \equiv \partial/\partial x_\alpha$ , the (two-dimensional) Laplacian is  $g^{\alpha\beta}\partial_\alpha\partial_\beta$ ; written in matrix form, the tensor  $g^{\alpha\beta}$  is

$$g^{-1} = \frac{1}{\sin^2\theta} \begin{pmatrix} 1/l_1^2 & -\cos\theta/l_1l_2 \\ -\cos\theta/l_1l_2 & 1/l_2^2 \end{pmatrix}.$$

We consider a two-dimensional photonic crystal with a dielectric constant  $\epsilon(\vec{\mathbf{r}})$  that is periodic in two independent directions with periodicities  $\vec{a}_1$  and  $\vec{a}_2$  (that define the  $x$ - $y$  plane) and homogeneous

in the third (the  $z$ -direction), i.e.  $\epsilon(\vec{\mathbf{r}}) = \epsilon(\vec{\mathbf{r}} + n_1 \vec{\mathbf{a}}_1 + n_2 \vec{\mathbf{a}}_2 + z \hat{\mathbf{k}})$ , where  $n_1$  and  $n_2$  are integers,  $z$  is arbitrary and  $\hat{\mathbf{k}}$  is a unit vector in the  $z$ -direction. In this system, electromagnetic waves with wave vectors in the  $x$ - $y$  plane come in two distinct species, with distinct spectra:  $E$ -polarization, where the electric field vector is parallel to the  $z$ -direction; and,  $H$ -polarization, where the magnetic field vector is parallel to the  $z$ -direction. (This well-known fact is not difficult to prove; here we will merely display that the claim is self-consistent.) In order to derive the relevant equations, we may start with Maxwell 'curl' equations in the absence of free charge and free currents:

$$\vec{\nabla} \times \vec{\mathbf{E}}(\vec{\mathbf{r}}, t) = -\mu_0 \frac{\partial \vec{\mathbf{H}}(\vec{\mathbf{r}}, t)}{\partial t} \quad (1)$$

$$\vec{\nabla} \times \vec{\mathbf{H}}(\vec{\mathbf{r}}, t) = \epsilon \epsilon_0 \frac{\partial \vec{\mathbf{E}}(\vec{\mathbf{r}}, t)}{\partial t}. \quad (2)$$

We look for fields that satisfy these equations, and have a time dependence of  $e^{-i\omega t}$ , so that

$$\vec{\nabla} \times \vec{\mathbf{E}}(\vec{\mathbf{r}}) = i\mu_0 \omega \vec{\mathbf{H}}(\vec{\mathbf{r}}) \quad (3)$$

$$\vec{\nabla} \times \vec{\mathbf{H}}(\vec{\mathbf{r}}) = -i\epsilon \epsilon_0 \omega \vec{\mathbf{E}}(\vec{\mathbf{r}}), \quad (4)$$

from which we obtain

$$\frac{1}{\epsilon} \vec{\nabla} \times \vec{\nabla} \times \vec{\mathbf{E}}(\vec{\mathbf{r}}) = \frac{\omega^2}{c^2} \vec{\mathbf{E}}(\vec{\mathbf{r}}) \quad (5)$$

$$\vec{\nabla} \times \frac{1}{\epsilon} \vec{\nabla} \times \vec{\mathbf{H}}(\vec{\mathbf{r}}) = \frac{\omega^2}{c^2} \vec{\mathbf{H}}(\vec{\mathbf{r}}). \quad (6)$$

These equations are quite general. To proceed further, we invoke the claim regarding polarization, and use (5) for  $E$ -polarization, and (6) for  $H$ -polarization. In the former case,

$$\epsilon^{-1} g^{\alpha\beta} \partial_\alpha \partial_\beta E + \frac{\omega^2}{c^2} E = 0, \quad (7)$$

and in the latter,

$$g^{\alpha\beta} \partial_\alpha \epsilon^{-1} \partial_\beta H + \frac{\omega^2}{c^2} H = 0. \quad (8)$$

$E$  and  $H$  are the  $z$ -components of the electric field and magnetization vectors, respectively. (See [6] for details of derivation.) Each of these equations may be cast in the form  $Du = \lambda u$ , where  $D$  is a Hermitian operator. (This is useful in proving some of the results later on, where we will invoke orthogonality of the eigenmodes, as also in numerical work.) In the case of  $E$ -polarization,

$$D \equiv \epsilon^{-1/2} g^{\alpha\beta} \partial_\alpha \partial_\beta \epsilon^{-1/2} \quad (9)$$

and  $u \equiv \epsilon^{1/2} E$ . For  $H$ -polarization,

$$D \equiv g^{\alpha\beta} \partial_\alpha \epsilon^{-1} \partial_\beta \quad (10)$$

and  $u \equiv H$ . In both cases,  $\lambda \equiv -\omega^2/c^2$ . For ease of exposition, we will set  $c = 1$ .

It is well-known that the spectra of eigenvalues of the equations above display 'bands'. Given two bands, the difference between the smallest eigenvalue of the upper band and the largest eigenvalue of the lower band characterizes the bandgap. (We will focus our attention on the spectrum of  $\omega$ , rather than  $\lambda$ .) After having selected two adjacent bands, we will seek a function  $\epsilon(\vec{\mathbf{r}})$  and lattice parameters (implicit in  $g^{\alpha\beta}$  through  $l_1$ ,  $l_2$  and  $\theta$ ) that maximizes the bandgap between them. In general,  $\epsilon(\vec{\mathbf{r}})$  may be subject to imposed constraints. While the method outlined below may be used to handle a variety of constraints, we will confine ourselves to a specific one:  $\epsilon_{min} \leq \epsilon(\vec{\mathbf{r}}) \leq \epsilon_{max}$ .

### 3 The variational algorithm

#### 3.1 Background

We will first review a standard but useful result. Starting with the standard eigenvalue problem  $Du = \lambda u$ , where  $D$  is a Hermitian operator, we will first investigate changes in  $\lambda$  due to changes in  $D$ . Prefixing  $\delta$  to denote ‘change in’

$$(u + \delta u)^\dagger (D + \delta D)(u + \delta u) = \lambda + \delta \lambda.$$

Retaining terms to first order in the changes, and noting that for normalized eigenfunctions,  $u^\dagger \delta u = 0$ ,

$$u^\dagger \delta D u = \delta \lambda. \quad (11)$$

Change in  $D$  is due to change  $\delta \epsilon$  in  $\epsilon$ , as well as due to changes in  $l_1, l_2$  and  $\theta$ . We may set a length scale for the problem by fixing, say,  $l_1$  (i.e.  $\delta l_1 = 0$ ). (Note that  $\omega$  is inversely proportional to the length-scale of the crystal. Therefore, bandgap maximization without a preset length-scale leads to a trivial, and singular, result.) This leaves two independent variables in the description of the periodic structure. We will choose these to be  $l \equiv l_2/l_1$  and  $p \equiv \cos \theta$ . (Since  $\cos \theta$  is monotonic in  $\theta$  within the permissible range of values of  $\theta$ , this poses no problem.) In the cases of interest,  $l$  and  $p$  occur in  $D$  through  $g^{-1}$ . Rewriting  $g^{-1}$  in terms of  $l$  and  $p$  we obtain

$$g^{-1} = \frac{1}{l_1^2(1-p^2)} \begin{pmatrix} 1 & -p/l \\ -p/l & 1/l^2 \end{pmatrix} \quad (12)$$

so that

$$\frac{\partial g^{-1}}{\partial l} = \frac{1}{l_1^2(1-p^2)} \begin{pmatrix} 0 & p/l^2 \\ p/l^2 & -2/l^3 \end{pmatrix} \quad (13)$$

and

$$\frac{\partial g^{-1}}{\partial p} = \frac{2p}{1-p^2} g^{-1} - \frac{1}{l_1^2(1-p^2)} \begin{pmatrix} 0 & 1/l \\ 1/l & 0 \end{pmatrix}. \quad (14)$$

Thus, replacing  $g^{\alpha\beta}$  by the appropriate partial derivative of  $g^{\alpha\beta}$  in  $D$  yields the corresponding variation of  $D$ , i.e.

$$\frac{\delta D}{\delta l} = \begin{cases} \epsilon^{-1/2} (\partial g^{\alpha\beta} / \partial l) \partial_\alpha \partial_\beta \epsilon^{-1/2} & : E - \text{polarization} \\ (\partial g^{\alpha\beta} / \partial l) \partial_\alpha \epsilon^{-1} \partial_\beta & : H - \text{polarization,} \end{cases} \quad (15)$$

$$\frac{\delta D}{\delta p} = \begin{cases} \epsilon^{-1/2} (\partial g^{\alpha\beta} / \partial p) \partial_\alpha \partial_\beta \epsilon^{-1/2} & : E - \text{polarization} \\ (\partial g^{\alpha\beta} / \partial p) \partial_\alpha \epsilon^{-1} \partial_\beta & : H - \text{polarization,} \end{cases} \quad (16)$$

In the case of  $E$ -polarization,

$$\begin{aligned} \delta D &= \delta \left[ \epsilon^{-1/2} g^{\alpha\beta} \partial_\alpha \partial_\beta \epsilon^{-1/2} \right] \\ &= -\frac{\delta \epsilon}{2\epsilon} D - D \frac{\delta \epsilon}{2\epsilon} + \frac{\delta D}{\delta l} \delta l + \frac{\delta D}{\delta p} \delta p \end{aligned} \quad (17)$$

so that

$$u^\dagger \delta D u = -\lambda \int_C u^* \frac{\delta \epsilon}{\epsilon} u \, d\tau + \int_C u^* \left( \frac{\delta D}{\delta l} \delta l + \frac{\delta D}{\delta p} \delta p \right) u \, d\tau, \quad (18)$$

where we use  $d\tau$  to denote the volume element of the unit cell  $C$  with boundary  $S$ .

One may proceed similarly in the case of  $H$ -polarization:

$$\begin{aligned}
u^\dagger \delta D u &= \int_C u^* g^{\alpha\beta} \partial_\alpha \delta(\epsilon^{-1}) \partial_\beta u \, d\tau + \int_C u^* \left( \frac{\delta D}{\delta l} \delta l + \frac{\delta D}{\delta p} \delta p \right) u \, d\tau \\
&= \int_S u^* \delta(\epsilon^{-1}) g^{\alpha\beta} (\partial_\alpha u) \hat{n}_\beta \, dA - \int_C \delta(\epsilon^{-1}) g^{\alpha\beta} (\partial_\alpha u^*) (\partial_\beta u) \, d\tau \\
&\quad + \int_C u^* \left( \frac{\delta D}{\delta l} \delta l + \frac{\delta D}{\delta p} \delta p \right) u \, d\tau \\
&= - \int_C \delta(\epsilon^{-1}) g^{\alpha\beta} (\partial_\alpha u^*) (\partial_\beta u) \, d\tau + \int_C u^* \left( \frac{\delta D}{\delta l} \delta l + \frac{\delta D}{\delta p} \delta p \right) u \, d\tau. \tag{19}
\end{aligned}$$

Recall that  $\lambda = -\omega^2$  and  $u^\dagger \delta D u = \delta\lambda = -2\omega\delta\omega$ . Substituting these in (18) and (19), we have the following:

$$\frac{\delta\omega}{\delta\epsilon} = \begin{cases} -\omega|u|^2/2\epsilon & : E\text{-polarization} \\ -g^{\alpha\beta} (\partial_\alpha u^*) (\partial_\beta u) / 2\omega\epsilon & : H\text{-polarization,} \end{cases} \tag{20}$$

and, for both polarizations,

$$\frac{\partial\omega}{\partial l} = -\frac{1}{2\omega} \int_C u^* \frac{\delta D}{\delta l} u \, d\tau \tag{21}$$

$$\frac{\partial\omega}{\partial p} = -\frac{1}{2\omega} \int_C u^* \frac{\delta D}{\delta p} u \, d\tau \tag{22}$$

It is not  $\omega$  but, rather, a difference  $\omega_2 - \omega_1$ , that we seek to maximize with respect to variations in  $\epsilon$ ,  $l$  and  $p$  in our iterative design scheme. Consider, first, changes in  $l$ . In an iterative scheme, it is straightforward to determine if  $\partial\omega_2/\partial l - \partial\omega_1/\partial l$  is positive or negative, and make a small positive or negative change in  $l$ , respectively. Changes in  $p$  may be implemented similarly.

Let us now consider variations in  $\epsilon$ . We would like to tailor variations in  $\epsilon$  so that  $\delta(\omega_2 - \omega_1) > 0$ . This is achieved if  $\delta\epsilon > 0$  wherever  $\delta\omega_2/\delta\epsilon > \delta\omega_1/\delta\epsilon$ , and vice versa. (Note that this is a 'pixel by pixel' process, so that the change in  $\epsilon$  in each 'pixel' (i.e. a small discretized neighborhood within the unit cell) may be different from the change in another 'pixel'.) If  $\epsilon = \epsilon_{max}$  ( $\epsilon = \epsilon_{min}$ ), it is impossible to achieve  $\delta\epsilon > 0$  ( $\delta\epsilon < 0$ ). Therefore, maximal  $\omega_2 - \omega_1$  is expected when  $\epsilon = \epsilon_{max}$  wherever  $\delta\omega_2/\delta\epsilon > \delta\omega_1/\delta\epsilon$ , and  $\epsilon = \epsilon_{min}$  wherever  $\delta\omega_2/\delta\epsilon < \delta\omega_1/\delta\epsilon$ . Note that no explicit reference to polarization has been made;  $\omega_1$  and  $\omega_2$  may even be eigenvalues corresponding to different polarizations. This makes it possible for our algorithm to maximize the size of complete bandgaps.

### 3.2 The algorithm

The preceding discussion suggests the following iterative algorithm to a maximal bandgap:

0. Choose  $l$  and  $p$  (i.e. periodicity of  $\epsilon(\vec{\mathbf{r}})$ ), and the adjacent bands that straddle the bandgap to be maximized. Initialize with an arbitrary (but appropriately periodic)  $\epsilon(\vec{\mathbf{r}})$ .
1. Determine, using  $\epsilon(\vec{\mathbf{r}})$ , the spectrum of eigenvalues  $\omega$  and the wavefunctions  $u$ .
2. Determine the wavefunctions that correspond to the smallest eigenvalue of the upper band ( $u_2$  and  $\omega_2$ ) and the largest eigenvalue of the lower band ( $u_1$  and  $\omega_1$ ).
3. Make one or more of the following *small* changes:
  - a.  $\delta\epsilon$  in  $\epsilon(\vec{\mathbf{r}})$ :  $\delta\epsilon \geq 0$  wherever  $\delta\omega_2/\delta\epsilon > \delta\omega_1/\delta\epsilon$  (determined using the expressions in (20)), and vice versa. (Maintain consistency with the constraint  $\epsilon_{min} \leq \epsilon(\vec{\mathbf{r}}) \leq \epsilon_{max}$ .)
  - b.  $\delta l$  in  $l$ ;  $\delta l$  has the same sign as  $\partial\omega_2/\partial l - \partial\omega_1/\partial l$ .

c.  $\delta p$  in  $p$ ;  $\delta p$  has the same sign as  $\partial\omega_2/\partial p - \partial\omega_1/\partial p$ .

4. Go to **1** unless termination/convergence criteria are met.

A discussion of some of the finer points of each step follows.

The initialization step requires the lattice parameters as input, both to establish a length scale and to fix the translational symmetry of the system. It is in this sense – and this sense only – that the maximum attained is not global. (Observe that, due to the scaling properties of the eigenvalue equations, maximization without an imposed length scale is trivial.)

Considerable work [8, 9] has been done towards numerical solution of the eigenvalue equations for arbitrary  $\epsilon(\vec{r})$ . The usual practice is to first discretize the space in some manner, then select a reasonably dense subset of wave-vectors from the Brillouin zone and, finally, obtain the eigenvalues corresponding to each wave-vector.

Remarkably, it turns out that it may not necessary to perform a complete bandstructure computation at each iteration to implement our scheme. We will show (in section 3.3) that, *in the optimized structure*, the edges of the relevant bands (i.e. the ones for which the bandgap was maximized) may only be located at wave-vector  $\vec{k}$  values with components 0,  $(0, \pi)$ ,  $(\pi, 0)$  and  $(\pi, \pi)$ ! In addition, numerical results obtained so far indicate that even in the intermediate iterative steps (where the crystal structure is not yet optimized), it is sufficient to confine our search to these  $\vec{k}$  values.

### 3.3 Consequences: Two important results

We will show, first, that in the optimized structure, the edges of the relevant bands may occur only at certain values of the wave-vector. To see this, note first that, since  $\epsilon(\vec{r})$  is real, Bloch wave-vectors  $\pm\vec{k}$  have degenerate spectra, say with frequency  $\omega$ . Therefore, any arbitrary linear combination  $u = \alpha u_{\vec{k}} + \beta u_{-\vec{k}}$  is an eigenfunction, too, with frequency  $\omega$ . Note, too, from our earlier discussion (equation (20) and following paragraph), that either of the wavefunctions  $u = u_2$  or  $u = u_1$  that straddle the bandgap *in the optimized structure* must be such that  $|u|^2$  ( or  $g^{\alpha\beta}(\partial_\alpha u^*)(\partial_\beta u)$ ) has the same translational symmetry as the underlying lattice. Bloch's theorem allows us to write  $u_{\vec{k}} = v_{\vec{k}} e^{ik_\mu x^\mu}$ , where  $v_{\vec{k}}$  is periodic in each of the coordinates with period 1. Now,

$$\begin{aligned} |u|^2 &= |\alpha u_{\vec{k}}|^2 + |\beta u_{-\vec{k}}|^2 + 2\text{Re} \alpha^* \beta u_{\vec{k}}^* u_{-\vec{k}} \\ &= |\alpha v_{\vec{k}}|^2 + |\beta v_{-\vec{k}}|^2 + 2|\alpha\beta v_{\vec{k}} v_{-\vec{k}}| \cos(2k_\mu x^\mu + \theta), \end{aligned} \quad (23)$$

where  $\alpha^* \beta u_{\vec{k}}^* u_{-\vec{k}} = |\alpha\beta v_{\vec{k}} v_{-\vec{k}}| e^{-i\theta}$ , and  $\theta$  is periodic in each of the coordinates with period 1. The first two terms in (23) are explicitly periodic in each of the coordinates with period 1. In order that the third term satisfies this requirement, we must have

$$\cos[2k_\mu(x^\mu + n^\mu) + \theta] = \cos(2k_\mu x^\mu + \theta) \quad (24)$$

with arbitrary integers  $n^\mu$  and for all  $x^\mu$ . This is possible only if  $2k_\mu$  is a multiple of  $\pi$ . Limiting values to  $-\pi < k_\mu \leq \pi$ , the only possible values of  $k_\mu$  are 0 and  $\pi$ . Thus, the band-edges in a maximal-band-gap producing configuration of  $\epsilon(\vec{r})$  in a 2D lattice *must* be at wave-vectors 0,  $(0, \pi)$ ,  $(\pi, 0)$  and  $(\pi, \pi)$ !

Another remarkable result – referred to towards the end of section 3.1 and hinted at in step **3** of the algorithm – is the ‘maximum-contrast’ rule: if  $\epsilon(\vec{r})$  is allowed to vary arbitrarily between two limits then maximal bandgaps are obtained when  $\epsilon(\vec{r})$  attains one or the other extremal value at each point. The argument runs as follows: at each point, and at each iterative step,  $\delta(\omega_2 - \omega_1)/\delta\epsilon$  is either positive, negative or zero. To increase the bandgap  $\omega_2 - \omega_1$ , increase (decrease)  $\epsilon$  by a small amount where  $\delta(\omega_2 - \omega_1)/\delta\epsilon$  is positive (negative). Since  $\delta(\omega_2 - \omega_1)/\delta\epsilon$  can be zero in only a set of measure zero, the iterative process stops when the increase (or decrease) in  $\epsilon$  is no longer possible – i.e. when  $\epsilon$  takes on either its maximum or minimum value at every point (except in a set of measure zero where  $\delta(\omega_2 - \omega_1)\delta\epsilon$  is zero). (See [7] for a related detailed discussion.)

### 3.4 Open questions

We discuss here some open questions regarding our algorithm, and a few related possibilities for further research.

One question that we have not answered here is whether the iterative algorithm converges. In a one-dimensional system (where exact results may be obtained otherwise and where  $E$ - and  $H$ -polarization spectra are degenerate), the algorithm does indeed result in rapid convergence to expected results. In 2D, numerical results obtained so far provide very strong evidence in favor of convergence. These results will be presented elsewhere [9].

An additional question related to convergence of numerical results is whether it suffices to confine our iterative search to the four points in wave-vector space outside which the band-edges in the final optimized structure cannot lie. If it does suffice, then each iterative step in the algorithm could be speeded up enormously. Numerical computations recently carried out provide strong evidence that the answer is in the affirmative.

Yet another open question relates to what other constraints on  $\epsilon(\vec{r})$  our approach can handle in a relatively straightforward manner, or, indeed, what other sets of constraints are reasonable to impose. A number of studies – cited in the introduction – impose, in addition to the constraint we have used, constraints on the geometry of the photonic crystal. Our strategy can, of course, handle these, although not always as efficiently as strategies tailored to specific situations.

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