MAXIMIZING BAND GAPS IN TWO-DIMENSIONAL PHOTONIC CRYSTALS

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Abstract. Photonic crystals are periodic structures composed of dielectric materials, and designed to exhibit band gaps i.e., ranges of frequencies in which electromagnetic waves cannot propagate, or other interesting spectral behavior. Structures with large band gaps are of great interest for many important applications. In this paper, the problem of designing structures which exhibit maximal band gaps is considered. Admissible structures are constrained to be composed of "mixtures" of two given dielectric materials. The optimal design problem is formulated, existence of a solution is proved, a simple optimization algorithm is described, and several numerical examples are presented.

Key words. Periodic structures, band gaps, optimal design.

AMS Subject Classification. 65K10, 82D25, 49M07

1. Introduction.

We consider wave propagation in a periodic medium in $\mathbb{R}^2$, modeled by the Helmholtz equation

$$(\triangle + \omega^2 \rho) u = 0, \quad \text{in } \mathbb{R}^2, \tag{1}$$

where $\omega \in \mathbb{R}$, and ρ is real-valued and periodic. Specifically, denoting $Z = \{0, \pm 1, \pm 2, \ldots\}$, and defining the lattice $\Lambda = Z^2$, we assume

$$\rho(x + n) = \rho(x), \quad \text{for almost all } x \in \mathbb{R}^2, \text{ and all } n \in \Lambda.$$

It is further assumed that ρ belongs to the admissible set

$$ad = \{\rho \in L^\infty : 0 < a_0 \le \rho(x) \le a_1, \ \text{ a.e.}\}, \tag{2}$$

where a_0 and a_1 are fixed.

This model is motivated by the study of electromagnetic waves or acoustic waves in non-absorbing media. Figotin and Kuchment have recently proved [9, 10] that certain structures of this type admit *band gaps*, i.e. intervals (a, b) of frequencies ω in which no waves are allowed to propagate. In addition, numerous computational experiments have been carried out in the optics and physics communities in an effort to identify and characterize structures with band gaps. Interest in band gap structures is motivated largely by a wealth of important potential applications in optics, photonics, and microwaves. The reader is referred to [2, 14] for an overview of this area.

Roughly speaking, for many applications large band gaps are more desirable than small band gaps. The present paper is aimed at the general problem of finding a structure (characterized by ρ) which maximizes a band gap occurring in a specified

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portion of the spectrum. Eligible structures are constrained to lie in the admissible class *ad* defined in (2), corresponding to the physical situation in which one wishes to fabricate a structure from a "mixture" of two given dielectric materials with squared refractive indices a_0 and a_1.

The plan of this paper is as follows. After describing the underlying eigenvalue problem in Section 2, in Section 3 the optimal design problem is formulated. The existence of an optimal design is established and the generalized gradient of the objective is characterized. In Section 4, a simple minimization algorithm is proposed which takes advantage of symmetry in the structure. Numerical results are presented in Section 5. Starting from initial structures exhibiting band gaps, new structures with significantly larger gaps are obtained.

This paper concerns only the design of structures operating in the so-called E-polarization case, in which the electric field vector E is parallel to the axis of constant material parameters in $\mathbb{R}^3$. The H-polarization case is of course also of great interest; in fact it is desirable to design structures which exhibit band gaps in both E- and H-polarization modes. The full three-dimensional problem, in which the vector Maxwell equations must be retained, is of still greater importance.

Finally, let us remark that gap questions naturally arise wherever eigenvalues are studied. An idea of the breadth of these applications can be gleaned from the works of Ashbaugh, Harrell and Svirsky [1], Guiduli [11], and Olhoff and Parbery [15].

2. The family of eigenproblems. We define the periodic domain (torus)

$$\Omega = \mathbb{R}^2/Z^2.$$

Define the *first Brillouin zone* $K = [-\pi, \pi]^2$. To reduce the problem (1) over $\mathbb{R}^2$ to a family of problems over Ω, we define for $g \in L^2(\mathbb{R}^2)$ the Floquet transform $\mathcal{F}$ by

$$(\mathcal{F}g)(\alpha, x) = e^{-i\alpha\cdot x} \sum_{n\in\Lambda} g(x-n)e^{i\alpha\cdot n}, \quad \alpha \in K.$$

The sum can be considered as a Fourier series in the *quasimomentum* variable α, with values in $L^2(\Omega)$. The map $g \mapsto \mathcal{F}g$ is an isomorphism from $L^2(\mathbb{R}^2)$ to the direct product space $\int_K^{\oplus} L^2(\Omega)$, (see Kuchment [13]).

It is easy to see that formally $(\nabla + i\alpha)\mathcal{F}g = \mathcal{F}(\nabla g)$, where the gradient operation is with respect to the x variable. Under the mapping $\mathcal{F}$, equation (1) transforms to

$$[(\nabla + i\alpha)\cdot(\nabla + i\alpha) + \omega^2\rho]u_\alpha = 0 \quad \text{in } \Omega, \quad \alpha \in K, \tag{3}$$

where u_α is the transform of u. To obtain u from u_α, one computes the inverse Floquet transform.

We shall find it convenient to drop the subscript on u and write (3) as

$$A_\alpha u = \lambda\rho u, \quad \text{where} \quad A_\alpha = -\Delta - 2i\alpha\cdot\nabla + |\alpha|^2. \tag{4}$$

It is not difficult to show that A_α is selfadjoint, positive semidefinite, and in possession of a compact resolvent on $L^2(\Omega)$. As a result, the spectrum of (4) is composed of a sequence of nonnegative eigenvalues each of finite multiplicity. Repeating them according to their multiplicity we denote them

$$0 \le \lambda_1(\rho,\alpha) \le \lambda_2(\rho,\alpha) \le \lambda_3(\rho,\alpha) \le \cdots \infty.$$

Let us also denote by $\mathcal{E}_k^1(\rho,\alpha)$ those eigenfunctions v, associated with $\lambda_k(\rho,\alpha)$, satisfying the normalization

$$\int_\Omega \rho|v|^2\,dx = 1.$$

In preparation for extremizing the λ_k with respect to α and ρ we record,

PROPOSITION 2.1. *For each k, (i) $\alpha \mapsto \lambda_k(\rho,\alpha)$ is continuous over K, and (ii) $\rho \mapsto \lambda_k(\rho,\alpha)$ is weak* continuous over ad.*

Proof. (i) For $\{\alpha_n\} \subset K$ and $\alpha \in K$, it is straightforward to estimate

$$\|(A_{\alpha_n} - A_\alpha)u\| \le \Big||\alpha_n|^2 - |\alpha|^2\Big| \|u\| + 4|\alpha_n - \alpha| \|A_\alpha u\|.$$

With $\alpha_n \to \alpha$, this is an equivalent condition (see Kato [12], §IV.2.6, Theorem 2.24), for the generalized convergence of A_{α_n} to A_α. That such convergence implies the convergence of the associated eigenvalues is established in Kato [12], §IV.3.5. (ii) follows the exact mode of reasoning as Prop. 4.3.i in Cox and McLaughlin [5]. Although their result was written for $\alpha = 0$ their argument requires only that A_α be elliptic. □

Formally from the Floquet transformation, one finds that all eigenfunctions ψ of the original problem

$$-\triangle\psi = \omega^2\rho\psi, \quad \text{in } \mathbb{R}^2$$

are of the form

$$\psi_\alpha(x) = \phi_\alpha(x)e^{i\alpha\cdot x}, \quad \alpha \in K,$$

where ϕ_α is an eigenfunction of the periodic problem (4). The ψ_α are Bloch functions, representing waves propagating in $\mathbb{R}^2$ with quasimomentum vector α. Frequencies at which waves can propagate (in some direction) in the medium are elements of the set

$$\mathcal{B} = \{\omega \ge 0 : \omega^2 \text{ is an eigenvalue of } A_\alpha u = \omega^2\rho u \text{ for some } \alpha \in K\}.$$

A given structure, defined by the periodic function ρ, has a *band gap* if there exists some interval $0 \le a < \omega < b < \infty$ of frequencies such that $(a,b) \cap \mathcal{B} = \emptyset$. If such a gap exists, no waves in the frequency range (a,b) can propagate.

We note that the existence of ρ giving rise to band gaps has been proved by Figotin and Kuchment [9, 10] by a constructive procedure using high-contrast materials. This insightful construction gives not only the existence of band gaps, but also their location, and estimates on gap size $|a-b|$. Furthermore, the same idea applies not only to the present case of the Helmholtz equation, but also to the more complicated Maxwell's equations in three dimensions.

3. Optimal design. We formulate the design problem, establish the existence of an optimal design, and characterize the generalized gradient of the objective in a neighborhood of the optimizer.

We begin by assuming the existence of a gap about ω_0^2 for some admissible ρ_0. More precisely, for some ρ_0 there exists an index j such that

$$\lambda_j(\rho_0, \alpha) < \omega_0^2 < \lambda_{j+1}(\rho_0, \alpha) \qquad \forall\, \alpha \in K.$$

In terms of

$$g(\rho, \alpha) \equiv \min\{\lambda_{j+1}(\rho, \alpha) - \omega_0^2, \omega_0^2 - \lambda_j(\rho, \alpha)\} \tag{5}$$

and

$$G(\rho) \equiv \inf_{\alpha \in K} g(\rho, \alpha) \tag{6}$$

our design objective is the solution of

$$\sup_{\rho \in ad} G(\rho). \tag{7}$$

This value, call it $\hat{G}$, is strictly positive so long as ρ_0 lies in *ad*. That $\hat{G}$ is indeed finite stems from the fact that $\lambda_k(\rho, \alpha)$ is dominated by $\lambda_k(a_0, \alpha)$.

PROPOSITION 3.1. *The mapping $\rho \mapsto G(\rho)$ attains its maximum on ad.*

Proof. As *ad* is weak* compact there exists a weak* convergent sequence $\rho_n \to \hat{\rho}$ for which $G(\rho_n) \to \hat{G}$. It follows immediately from Proposition 2.1.i that we may choose $\hat{\alpha} \in K$ such that $G(\hat{\rho}) = g(\hat{\rho}, \hat{\alpha})$. From Proposition 2.1.ii we deduce that $g(\rho_n, \hat{\alpha}) \to g(\hat{\rho}, \hat{\alpha}) = G(\hat{\rho})$. Finally, as $G(\rho_n) \leq g(\rho_n, \hat{\alpha})$ it follows that

$$\lim_n G(\rho_n) \leq \lim_n g(\rho_n, \hat{\alpha}),$$

i.e., $\hat{G} \leq G(\hat{\rho})$. $\square$

In order to characterize and/or approximate this optimal structure, $\hat{\rho}$, one requires knowledge of the gradient of G. With respect to (5) and (6) we recognize three obstacles to the classical differentiability of G. First, the minimum of a family of smooth functions is itself smooth only when the minimum is attained at precisely one point. Note that G is defined in terms of two minimums, neither of which are known to be attained at singletons. The third obstacle stems from the (related) fact that $\rho \mapsto \lambda_j(\rho, \alpha)$ and $\rho \mapsto \lambda_{j+1}(\rho, \alpha)$ are not smooth where they are multiple and such multiplicities may not be ruled out, *a priori*. As these latter functions are however Lipschitz the same may be said of g and G and hence it makes sense to speak of the generalized gradient, in the sense of Clarke, of G.

More precisely, (see Clarke [3], Theorem 2.8.2), the generalized gradient of G lies in the weak* closed convex hull of the collection of points obtained by evaluating the generalized gradient of $\rho \mapsto g(\rho, \alpha)$ at those α at which the infimum is attained in (6). That is

$$\partial G(\rho) \subset \overline{\text{co}}^*\{\partial_\rho g(\rho,\alpha) : \alpha \in \text{Argmin}\, g(\rho,\cdot)\}.$$

As it follows directly from (5) and [3], Prop. 2.3.12, that

$$\partial_\rho g(\rho,\alpha) \subset \text{co}\,\{\partial_\rho \lambda_{j+1}(\rho,\alpha), -\partial_\rho \lambda_j(\rho,\alpha)\},$$

and, almost as directly, from Cox [4], Theorem 1, that

$$\partial_\rho \lambda_k(\rho,\alpha) = \text{co}\,\{-\lambda_k(\rho,\alpha)|v|^2 : v \in \mathcal{E}_k^1(\rho,\alpha)\}, \quad k = j, j+1, \tag{8}$$

we find

$$\begin{aligned} \partial G(\rho) \;\subset\; \overline{\text{co}}^*\{&\text{co}\,\{\text{co}\,\{-\lambda_{j+1}(\rho,\alpha)|v|^2 : v \in \mathcal{E}_{j+1}^1(\rho,\alpha)\}, \\ &\text{co}\,\{\lambda_j(\rho,\alpha)|v|^2 : v \in \mathcal{E}_j^1(\rho,\alpha)\}\} : \alpha \in \text{Argmin}\, g(\rho,\cdot)\}. \end{aligned} \tag{9}$$

With respect to our earlier remarks we note that the triple layering of convex hulls precisely mirrors the three obstacles to classical differentiability. In order to justify this calculation it remains only to give a careful derivation of (8). To this end we define

$$F(\rho,\alpha,u) \equiv \langle \rho^{1/2} T_\alpha(\rho) \rho^{1/2} u, u\rangle \quad \text{and} \quad T_\alpha(\rho) \equiv (A_\alpha - \omega_0^2 \rho)^{-1}$$

and establish

Proposition 3.2. *(i) The maximum in*

$$\frac{1}{\lambda_{j+1}(\rho,\alpha) - \omega_0^2} = \max_{\|u\|_2=1} F(\rho,\alpha,u), \tag{10}$$

is attained at $\mathcal{E}_{j+1}^1(\rho,\alpha)$. (ii) The mapping $F(\cdot,\alpha,u)$ is uniformly Lipschitz in a neighborhood of $\hat\rho$.

Proof. (i) As $\rho^{1/2}T_\alpha(\rho)\rho^{1/2}$ is compact and selfadjoint on $L^2(\Omega)$, the maximum in (10) is attained at an eigenfunction of $\rho^{1/2}T_\alpha(\rho)\rho^{1/2}$ associated with its largest positive eigenvalue. More precisely, with $1/z$ denoting the value of (10), there exists a unit vector u for which

$$\rho^{1/2}(A_\alpha - \omega_0^2\rho)^{-1}\rho^{1/2}u = u/z,$$

or, in other words,

$$z\rho^{1/2}u = (A_\alpha - \omega_0^2\rho)\rho^{-1/2}u.$$

Setting $v = \rho^{-1/2}u$ and rearranging, we find

$$A_\alpha v = (\omega_0^2 + z)\rho v.$$

This reveals that $\omega_0^2 + z = \lambda_k(\rho,\alpha)$ for some k. As z is the smallest such number it follows that $k = j+1$.

(ii) Owing to the existence of a gap and the strong continuity of $(\rho,\alpha)\mapsto\lambda_k(\rho,\alpha)$ for $k=j$ and $k=j+1$, there exists a $\delta>0$ and an $M<\infty$ such that

$$\|T_\alpha(\rho)\|\le M \qquad \forall\,\|\rho-\hat\rho\|_\infty<\delta,\ \alpha\in K.$$

For such ρ_1 and ρ_2 the resolvent identity permits the simple representation

$$T_\alpha(\rho_1)-T_\alpha(\rho_2)=\omega_0^2T_\alpha(\rho_1)(\rho_1-\rho_2)T_\alpha(\rho_2).$$

We exploit this in

$$\begin{aligned} F(\rho_1,\alpha,u)-F(\rho_2,\alpha,u) &= \langle\sqrt{\rho_1}T_\alpha(\rho_1)\sqrt{\rho_1}u-\sqrt{\rho_2}T_\alpha(\rho_2)\sqrt{\rho_2}u,u\rangle\\ &= \langle\omega_0^2T_\alpha(\rho_1)(\rho_1-\rho_2)T_\alpha(\rho_2)u,u\rangle\\ &\quad+\langle\sqrt{\rho_1}T_\alpha(\rho_2)(\sqrt{\rho_1}-\sqrt{\rho_2})u,u\rangle\\ &\quad+\langle(\sqrt{\rho_1}-\sqrt{\rho_2})T_\alpha(\rho_2)\sqrt{\rho_2}u,u\rangle. \end{aligned}$$

Each of these terms is easily estimable. In particular,

$$\langle\omega_0^2T_\alpha(\rho_1)(\rho_1-\rho_2)T_\alpha(\rho_2)u,u\rangle\le\omega_0^2M^2\|\rho_1-\rho_2\|_\infty$$

and

$$\langle\sqrt{\rho_1}T_\alpha(\rho_2)(\sqrt{\rho_1}-\sqrt{\rho_2})u,u\rangle+\langle(\sqrt{\rho_1}-\sqrt{\rho_2})T_\alpha(\rho_2)\sqrt{\rho_2}u,u\rangle\le\sqrt{a_1/a_0}M\|\rho_1-\rho_2\|_\infty,$$

where, for the latter we have supposed $a_0\le\rho_j(x)\le a_1$. Exchanging the roles of ρ_1 and ρ_2 we arrive at

$$|F(\rho_1,\alpha,u)-F(\rho_2,\alpha,u)|\le(\omega_0^2M^2+\sqrt{a_1/a_0}M)\|\rho_1-\rho_2\|_\infty,$$

as announced. □

From here one may argue exactly as in [4], Lemma 2 and so arrive at (8).

4. Generalized gradient ascent algorithm. Inspection of the generalized gradient (9) reveals that all one needs to calculate $\partial G(\rho)$ are the eigenfunctions associated with eigenvalues $\lambda_k(\rho,\alpha)$ and $\lambda_{k+1}(\rho,\alpha)$ for values of α at which the infimum over α is attained. Most techniques for computing eigenvalues simultaneously yield associated eigenvectors. Since the eigenvalues must be calculated to evaluate $G(\rho)$, the set of direction vectors which define $\partial G(\rho)$ can be obtained at essentially no additional computational cost, excluding storage considerations.

Since $\partial G(\rho)$ is never zero and may typically contain numerous direction vectors, standard gradient-based optimization algorithms designed for smooth functions would probably not perform well. Several general-purpose methods for nonsmooth optimization problems of this type have been developed, see for example [16, 17]. However, because of the structure of the present problem, we have elected to implement a simple special-purpose generalized gradient ascent algorithm. Our intent here is merely to describe the basic algorithm and illustrate (in the next section) its application. Convergence of the algorithm remains to be studied.

Recall that

$$ad = \{\rho \in L^\infty(\Omega) : a_0 \le \rho(x) \le a_1 \ \text{ a.e.}\}$$

is the admissible set of designs. Define the projection $P : L^1(\Omega) \to ad$ almost everywhere by

$$(Pf)(x) = \begin{cases} a_0 & \text{if } f(x) < a_0, \\ a_1 & \text{if } a_1 < f(x), \\ f(x) & \text{otherwise.} \end{cases}$$

Basic algorithm:

1. Choose initial $\rho_0 \in ad$ such that ρ_0 exhibits at least one band gap and such that the center frequency ω_0 lies within a gap.

2. For $k = 0, 1, 2, \ldots,$ convergence,

   a. Choose a direction $s_k \in \partial G(\rho_k)$ and a step size t_k to yield an increase in G,

   b. Set $\rho_{k+1} = P(\rho_k + t_k s_k)$.

   end

In step 2, "convergence" is interpreted to mean that the step length has become sufficiently small. Note that since we are projecting each step back into the admissible class ad, it cannot be assured that $0 \in \partial G(\rho_k)$ will hold when the iteration stops.

The key part of the algorithm is step 2a. Since there may be many linearly independent step directions in $\partial G(\rho_k)$, testing each of them at each step is not practical. Thus a linear subproblem is solved as follows. Let $\{q_1, \ldots, q_n\}$ be a set of direction vectors such that $\partial G(\rho_k) = \text{co}\,\{q_1, \ldots, q_n\}$, i.e. $q_j = \pm\lambda(\rho_k, \alpha)|v|^2$, where v is a normalized eigenfunction corresponding to an eigenvalue at the boundary of the gap. Each q_j is roughly the gradient of a function $g_j(\rho)$ which represents the distance from a particular eigenvalue at a particular α, to ω_0^2. We seek a step direction s in the form

$$s = \sum_{j=1}^{n} \beta_j q_j, \qquad \text{where } 0 \le \beta_j \le 1 \text{ and } \sum \beta_j = 1.$$

The expected change in g_j due to the step s is

$$\langle g, q_j \rangle = (A\beta)_j, \qquad \text{where } A = (a_{ij}) = \langle q_i, q_j \rangle,$$

and $\beta = (\beta_1, \beta_2, \ldots, \beta_n)^T$. The goal of choosing a step is to maximize over β the smallest expected change in g_j. In other words, we wish to solve the subproblem

$$\begin{aligned} & \max_{\beta} \min_{1 \le j \le n} (A\beta)_j, \\ \text{subject to} \quad & 0 \le \beta_j \le 1, \quad j = 1, \ldots, n \\ & \sum_{j=1}^{n} \beta_j = 1. \end{aligned}$$

This is easily reformulated as a standard form linear program in $n+1$ variables (see eg. [6], chapter 14) and solved by the simplex method. The resulting $s_k = \sum \beta_j q_j$ is taken as the step direction, and the iteration proceeds. The step sizes t_k are chosen by specifying some initial value t_0 at the first step, then decreasing the current t_k by $1/2$ each time a step fails to produce an increase in the objective function.

In the practical implementation of the algorithm, in order to restrict the range of $\alpha \in K$ which must be searched when calculating $G(\rho)$ and $\partial G(\rho)$, we make the assumption that the optimal ρ has some symmetry. Symmetry in ρ is reflected in symmetry in the argument α, as we now briefly point out.

Consider the Rayleigh quotient

$$R_\alpha(u) = \frac{\langle A_\alpha u, u \rangle}{\langle \rho u, u \rangle}.$$

Let Q be a real orthogonal 2×2 matrix. Q can be regarded as an operator mapping Ω into itself by defining Qx equal to the matrix Q times x, modulo Z^2. Similarly Q maps K into itself by defining $Q\alpha$ modulo $2\pi Z^2$ for $\alpha \in K$.

LEMMA 4.1. *Suppose that the coefficient ρ admits the symmetry $\rho(x) = \rho(Qx)$. Let $\tilde{u}(x) = u(Qx)$. Then $R_\alpha(u) = R_{Q\alpha}(\tilde{u})$.*

Proof. By change of variables one finds easily that

$$\langle \rho u, u \rangle = \langle \rho \tilde{u}, \tilde{u} \rangle, \quad \text{and} \quad \langle A_\alpha u, u \rangle = \langle A_{Q\alpha} \tilde{u}, \tilde{u} \rangle.$$

□

We conclude from the Lemma that if u is a stationary point of R_α then $\tilde{u}$ is a stationary point of $R_{Q\alpha}$. It follows that the eigenvalues associated with R_α and $R_{Q\alpha}$ coincide.

Assuming that ρ is invariant under the transformations:

$$(x_1, x_2) \mapsto (-x_1, -x_2), \quad (x_1, x_2) \mapsto (-x_1, x_2), \quad (x_1, x_2) \mapsto (x_2, x_1), \tag{11}$$

all possible eigenvalues associated with R_α for any $\alpha \in K$, must then occur with α restricted to the triangular region

$$T_1 = \{\alpha = (\alpha_1, \alpha_2) : \ 0 \le \alpha_1 \le \pi, \ \ 0 \le \alpha_2 \le \alpha_1\}.$$

Consequently, to search for band gaps associated with ρ with the symmetries (11), it suffices to take $\alpha \in T_1$ rather than $\alpha \in K$ (see Figure 1).

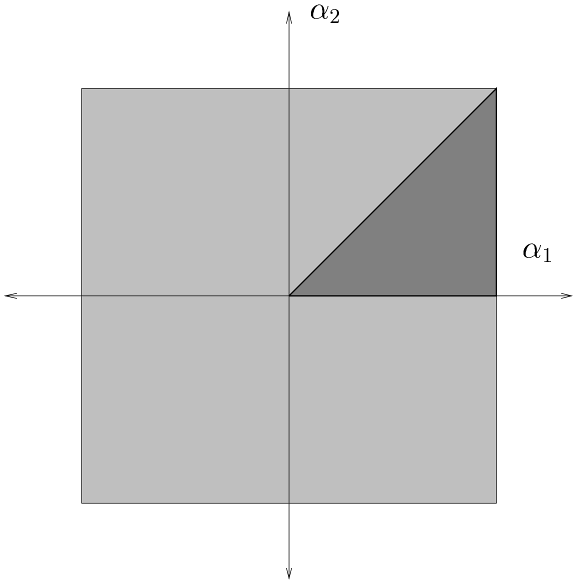

FIG. 1. *Shaded triangle region illustrates a "search region" in First Brillouin zone for ρ with symmetries (11).*

Roughly speaking, there are only certain direction vectors in $\partial G(\rho)$ which preserve the symmetries (11) in ρ. These can be computed by restricting α to the triangular region T_1, calculating the corresponding generalized gradient, then symmetrizing the result. The effect is to greatly reduce the number of α parameters which must be searched, at the cost of the tacit assumption that the optimal design has symmetries (11).

We conclude this section with a final note on the practical implementation of the algorithm. Because of numerical inaccuracies one would expect that a step would rarely fall *exactly* upon a manifold of degeneracy. Nevertheless if one is near such a manifold, direction vectors from the generalized gradient at the degeneracy hold useful information. For this reason, we found it beneficial to create an error tolerance ϵ, and consider gradient directions from any point within a ball of radius ϵ as "effectively" in the generalized gradient set at the current point. This approach avoids excessively small step sizes near degeneracies.

5. Numerical experiments. To implement the gradient descent algorithm described above, we used a finite element discretization coupled with a preconditioned subspace iteration method for the computation of the eigenvalues/eigenvectors [7]. The method is quite efficient, and is particularly well suited for use in an optimization setting. Many other techniques exist for band structure calculations; see for example [8] and the references therein.

In all of the following examples we use two materials: one with dielectric constant $a_0 = 1$ and the second with dielectric constant $a_1 = 9$ (refractive index 3), representing a typical value for a high-index dielectric material in the optical frequency range. We have also run experiments with different material contrasts. Generally speaking, as one might expect, higher contrast materials allow structures with larger bandgaps.

In the first example we take as an initial guess the periodic array of high-index "rods" pictured in Figure 2a. This structure admits a gap between bands 3 and 4, with magnitude of approximately 0.045. The center frequency ω_0 was chosen roughly in the center of the gap, and a few hundred steps of the algorithm were taken, resulting in a new structure with a larger gap. We found that by moving ω_0 higher within the new gap and optimizing again, an even larger gap could be obtained. This was repeated several times until $\omega_0 = 0.575$ was reached, resulting in the structure shown in Figure 2b. The gap for this structure is 0.128, almost three times as large as the initial gap. The density of states for the optimized structure is shown in Figure 2c. The total number of gradient steps in the optimization was 1620, although the algorithm could have been stopped earlier since the last several hundred steps produced extremely small changes in ρ_k. With a more sophisticated steplength selection strategy, the number of steps could probably be reduced significantly.

Experiments indicate that the problem does appear to admit local optima. Figure 3 illustrates another example in which the gap between bands 3 and 4 is maximized, but this time using a different starting guess. A structure entirely different than that shown in Figure 2 emerges, and in fact the gap is significantly larger: 0.172 compared to 0.128.

Figure 4 shows an example which indicates that it may be possible to modify the algorithm to produce a structure with a band gap even without an initial guess which has a gap. In this example the initial guess does have a substantial gap between bands 7 and 8, however between bands 6 and 7 it has only a tiny gap (roughly 0.005 on the scale as plotted). By placing ω_0 within this gap, the algorithm was able to "peel off" band 7 and produce a structure with a large gap between bands 6 and 7, as shown in figure 4b. This leads to the idea that if one were to begin with a pseudogap structure (a structure which has an α-dependent separation between two bands, but not a true band gap) and replace the constant ω_0 with a function $\omega_0(\alpha)$ which lies within the pseudogap, a true gap could be produced by iteratively pushing the bands away from $\omega_0(\alpha)$ with steps produced by the basic algorithm described here, while homotopically deforming $\omega_0(\alpha)$ into a constant. A more complete discussion of this idea will be presented elsewhere.

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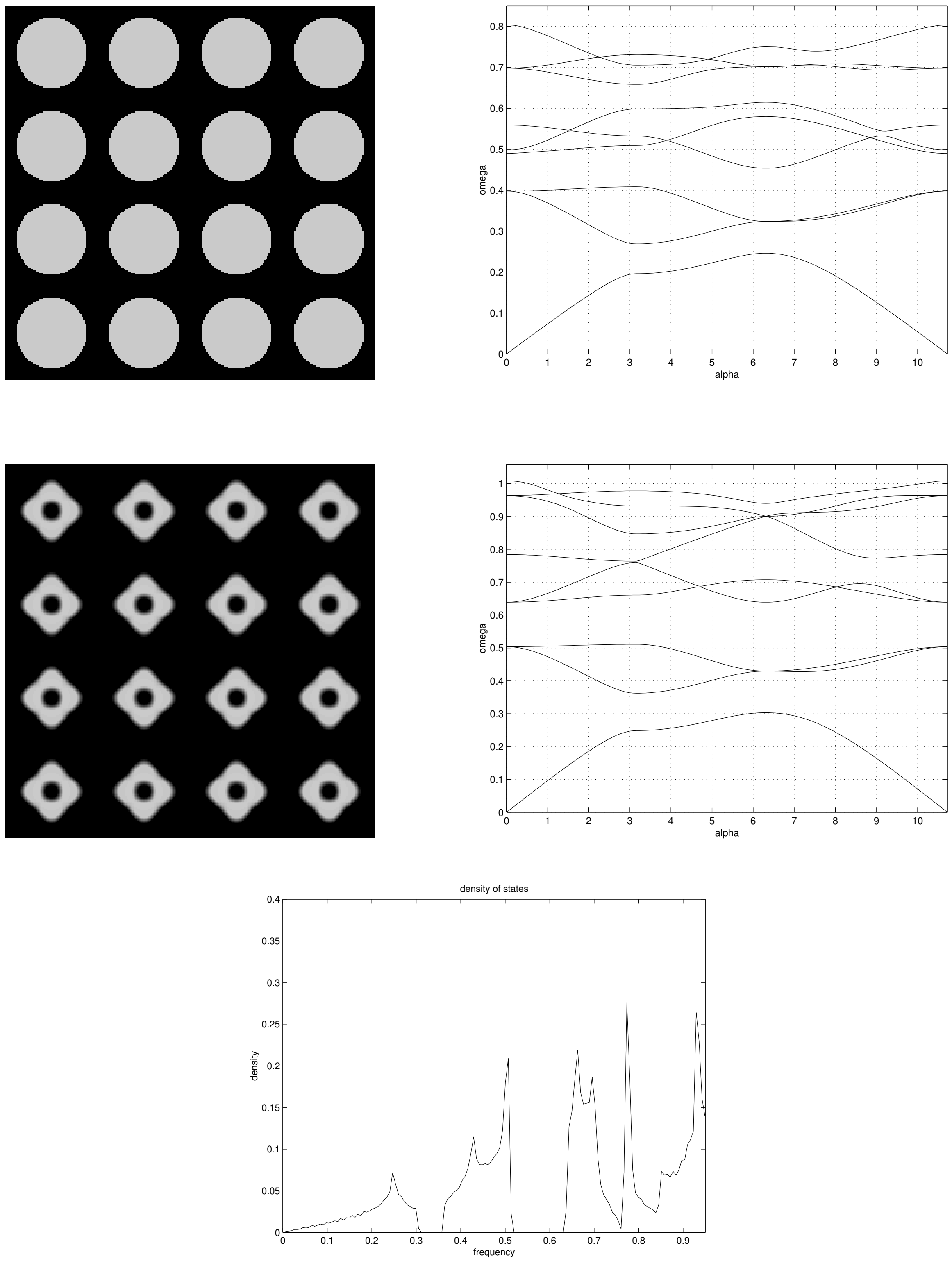

FIG. 2. *Maximizing gap between bands 3-4. a.) Initial guess and corresponding bands, b.) optimized structure and corresponding bands, c.) density of states for optimized structure, gap = 0.128. For grayscale images in a.) and b.), light color indicates high-index material $\rho = 9$; dark indicates low-index material $\rho = 1$. A 4×4 array of cells is shown for clarity only. All computations were done on a single cell. The α parameter varies along the boundary of the shaded rectangle shown in Figure 1.*

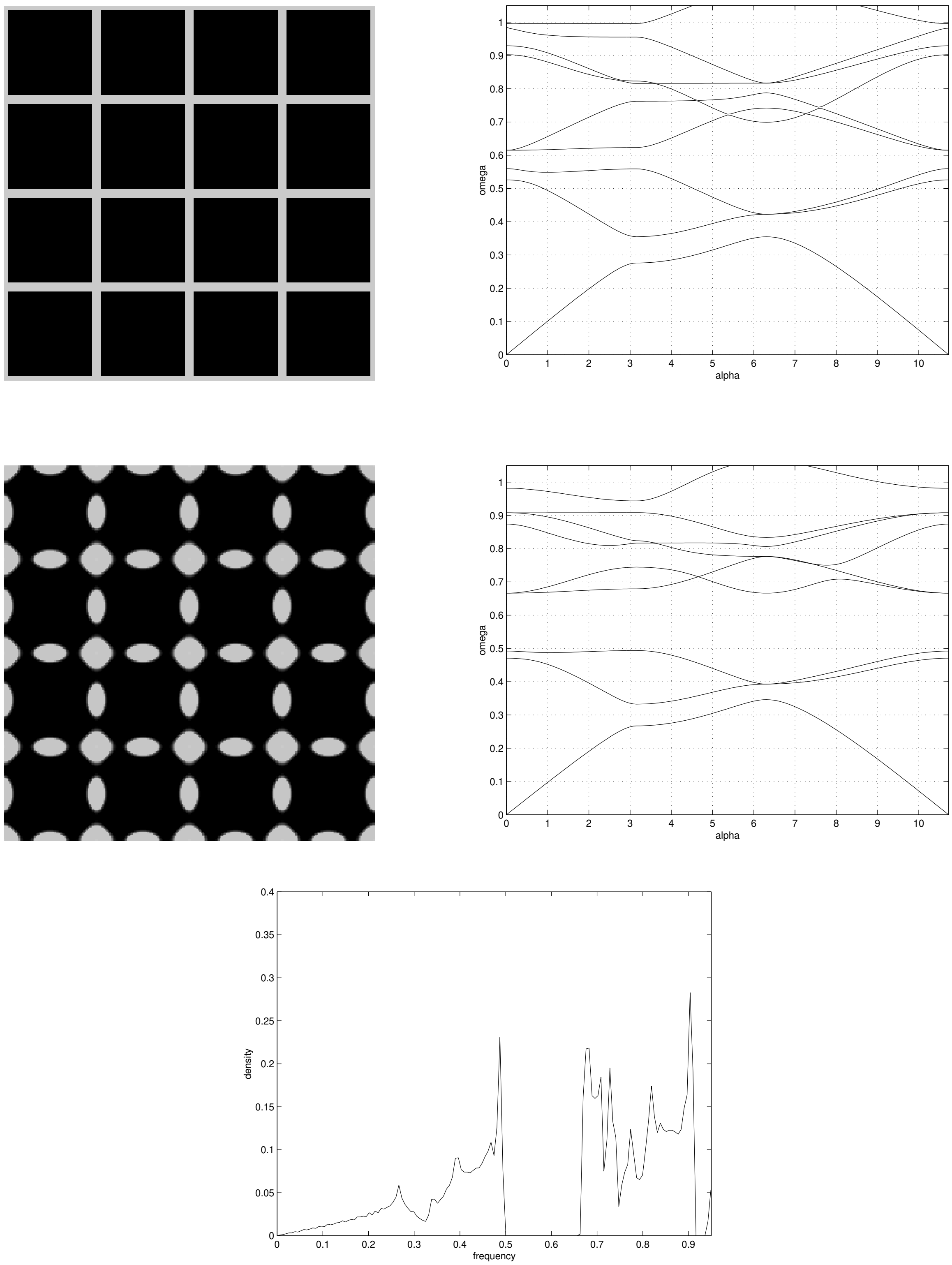

FIG. 3. *Maximizing gap between bands 3-4. a.) Initial guess and corresponding bands, b.) optimized structure and corresponding bands, c.) density of states for optimized structure, gap = 0.172.*

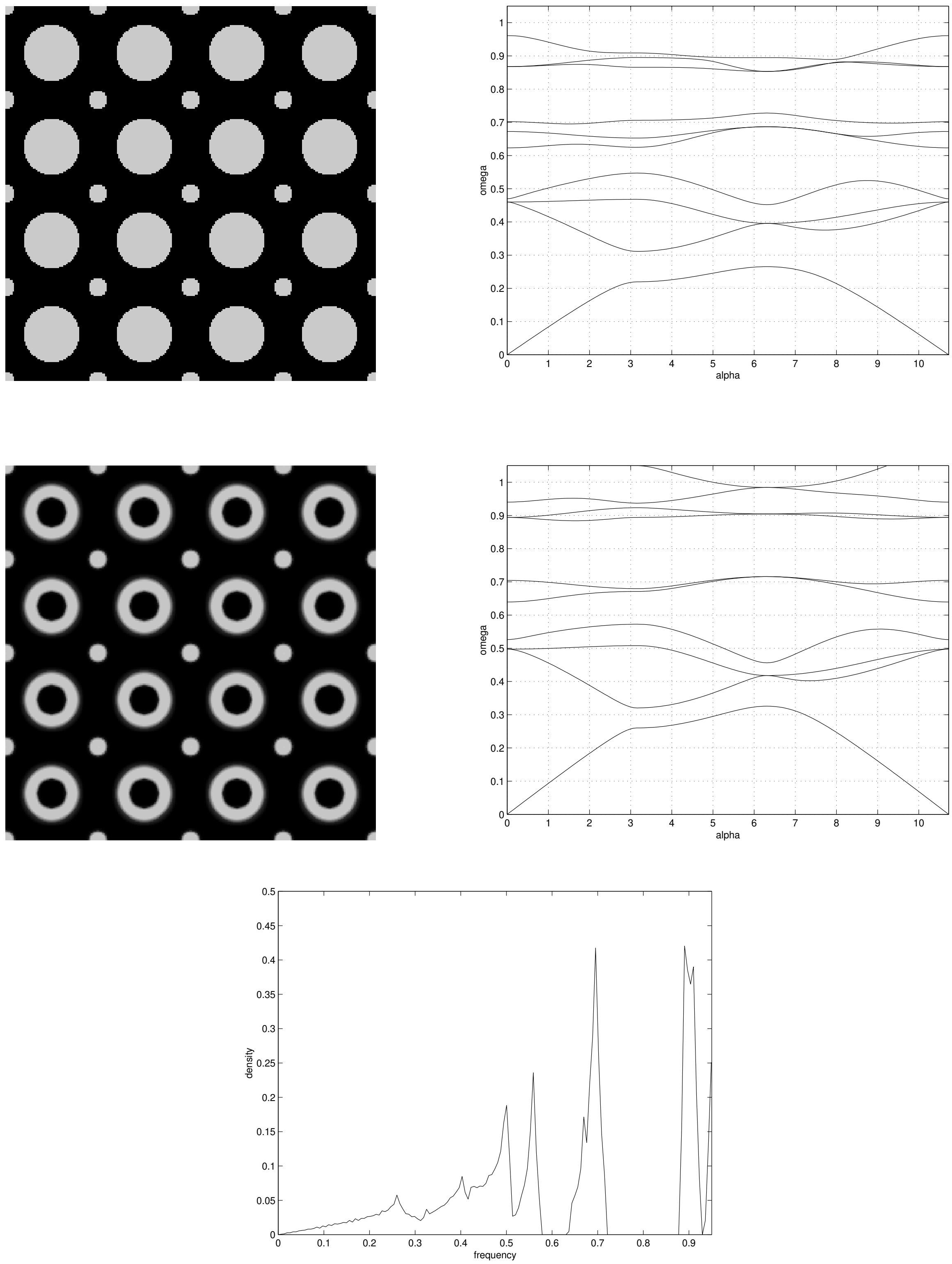

FIG. 4. *Maximizing gap between bands 6-7. a.) Initial guess and corresponding bands (note large gap is between bands 7-8, not 6-7; see discussion), b.) optimized structure and corresponding bands, c.) density of states for optimized structure, gap = 0.168.*

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