Optimal Design of Photonic Bandgap Crystals

Fadil Santosa
School of Mathematics
University of Minnesota

joint work with David Dobson (Utah)

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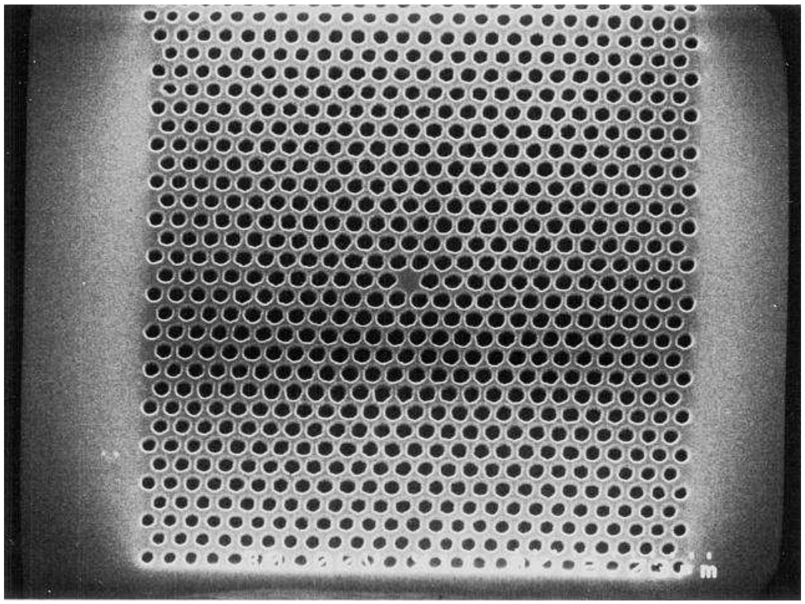
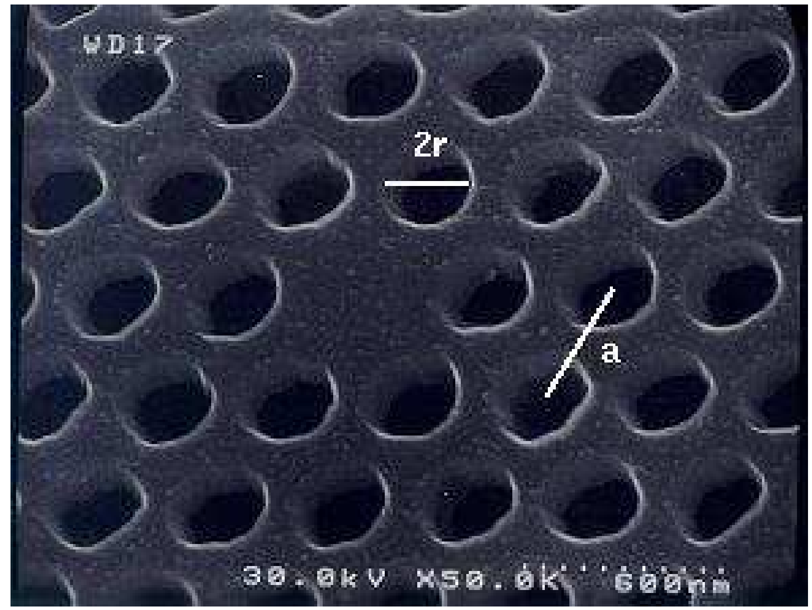
Outline

- Introduction to photonic band gap structures
- Designing eigenfunctions
- Well-posed formulations
- A numerical approach
- Examples
- Discussion

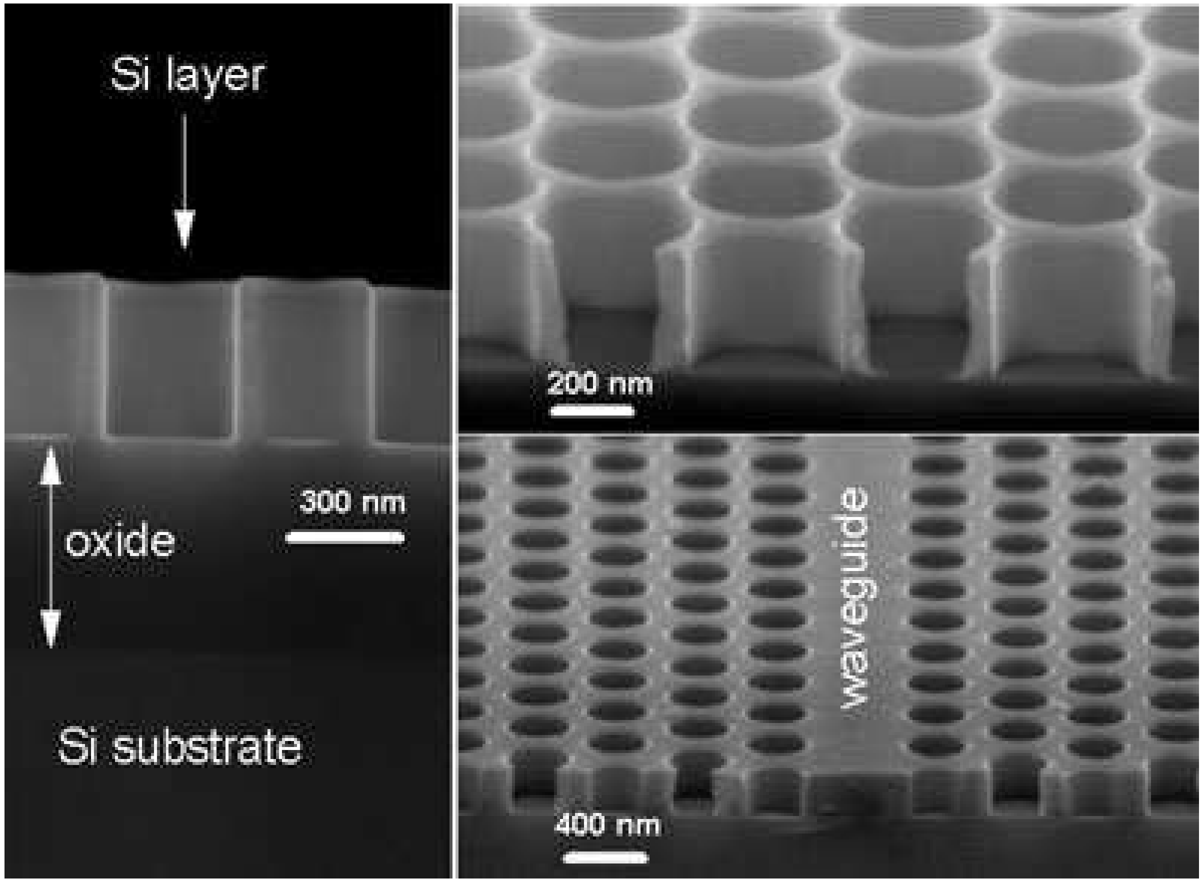
What they are making and why





Photonic Band Gap (PBG) structures are nanostructures with periodic index of refraction through which light can propagate.

Photonic band gap phenomenon refers to the existence of a certain frequency band in which waves having frequency in that band cannot propagate in the structure.



To make an optical device out of a photonic band gap (PBG) structure, defects are patterned into the periodic structure. These defects can be designed to localize and guide waves within the structure.

Possible applications

Photonic band gap structures are optical equivalent of electronic circuits.

The dream:

- Fully optical networks
- Computer interconnects

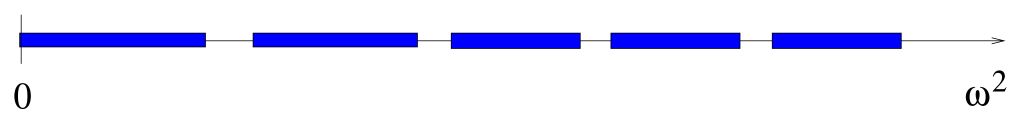
PBG phenomena in a nutshell

Let's look at TE-mode electromagnetic waves in 2D. The periodic medium is described by the dielectric constant $\epsilon_{\mathrm{p}}(x)$; $0 < \epsilon_1 \leq \epsilon_{\mathrm{p}} \leq \epsilon_2 < \infty$.

Consider the eigenvalue problem

$$\Delta u + \omega^2 \epsilon_{\mathrm{p}}(x) u = 0, \quad x \in \mathbb{R}^2,$$

where the spectral parameter ω is frequency. If the medium has a band gap, then the spectrum is continuous but has an interval Γ where u does not exist for $\omega \in \Gamma$.



Band gap calculation

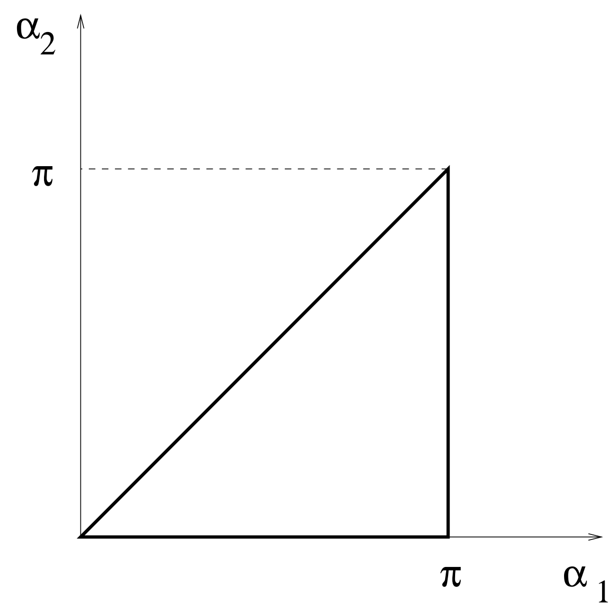
We seek solutions $v(x, \alpha)$ satisfying Helmholtz's equation with boundary condition

$$v(x + e_j, \alpha) = v(x, \alpha)e^{i\alpha_j},$$

where α is a vector in $\mathbb{R}^2$. Because of the periodicity of $\epsilon_{\mathrm{p}}(x)$, $v(x, \alpha)$ will be periodic in α over the cube $P := [0, 2\pi)^2$.

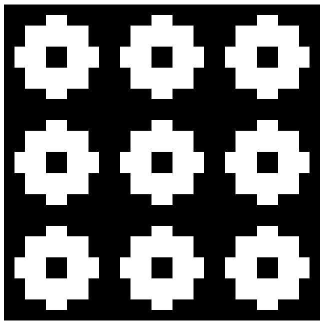
The "wavenumber" parameter α is a 2-D vector. The dispersion relation $\omega_m(\alpha)$ are surfaces. Symmetry of the medium induces symmetry of the dispersion relation. For a periodic cell with diagonal symmetry, we can restrict α to a triangle called the Brioullin zone, given by

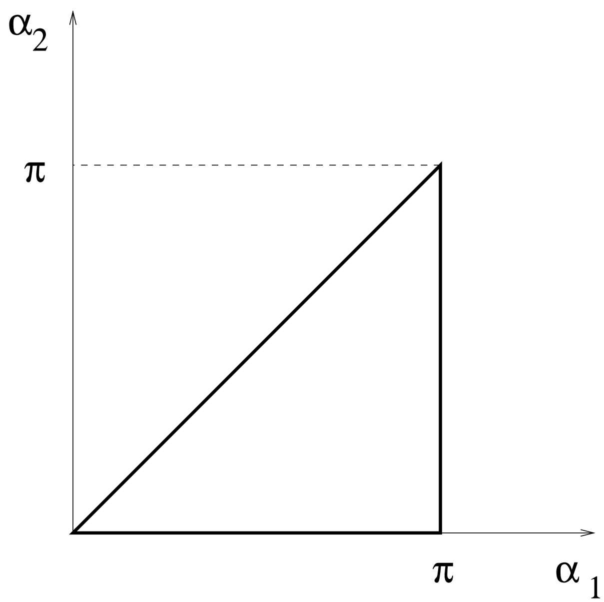
$$B = \{0 \le \alpha_2 \le \alpha_1, 0 \le \alpha_1 \le \pi\}$$

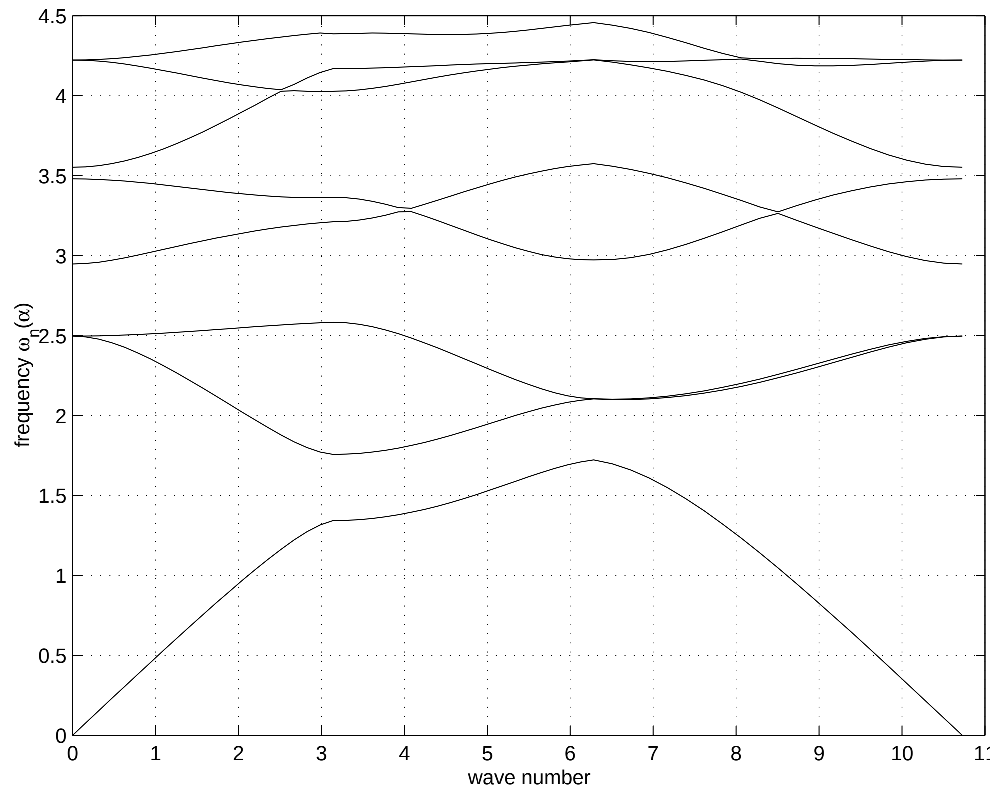


Brioullin zone.

The dispersion relation is now graphed as a function of α restricted to the boundary of the Brioullin zone.







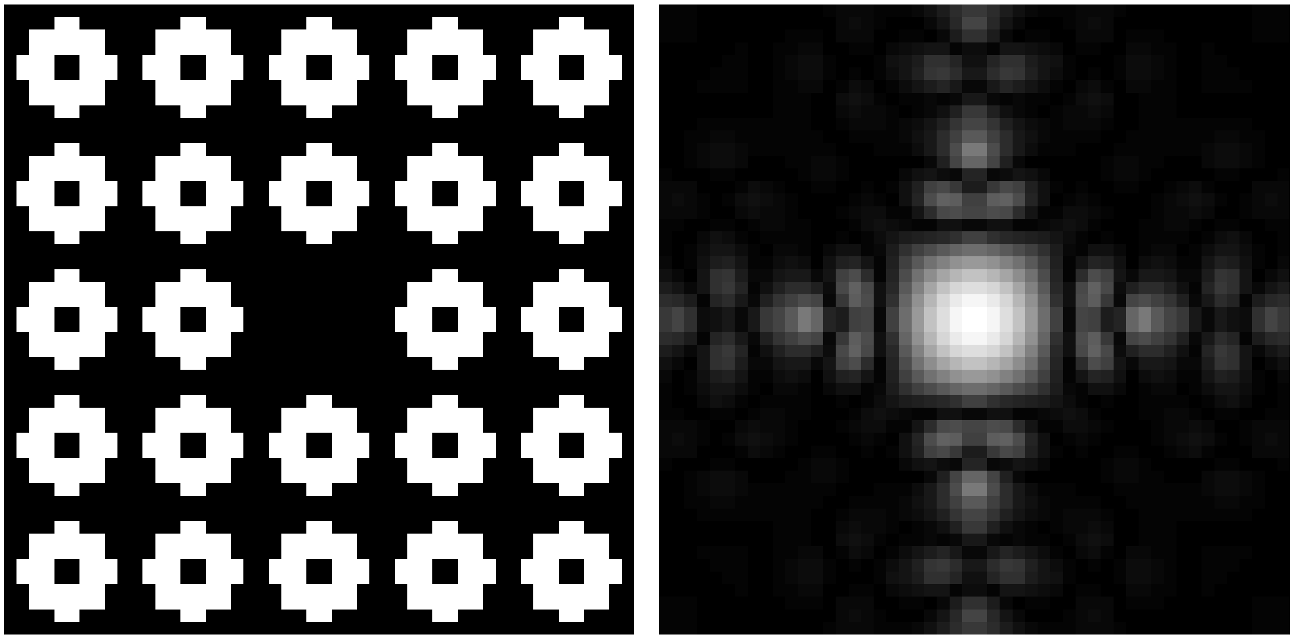
Defect mode

To the periodic medium $\epsilon_{\text{p}}(x)$ introduce a localized perturbation $\eta(x)$ (compactly supported). Now the equation is

$$\Delta u + \omega^2(\epsilon_{\text{p}}(x) + \eta(x))u = 0, \quad x \in \mathbb{R}^2.$$

The spectral stability theorem states that the essential spectrum of the perturbed problem is the same as that of the periodic problem. The only difference will be the creation of a discrete spectrum.

In particular, if (ω, u) solves the equation with $\omega \in \Gamma$, then $u(x)$ is localized.



A defect mode calculated by the ‘supercell’ method.

Problem: Can we design a structure so that the resulting defect mode has certain desirable properties?

Attributes to design for:

- Localization length
- Frequency

under manufacturing constraints.

Dirichlet problem

A simpler problem, but a good 'demo' problem.

Also, since we will be looking modes that are highly localized, the eigenfunction of the infinite medium will be well approximated by that of the bounded domain.

Consider

$$-\Delta u = \lambda \epsilon(x) u, \quad x \in \Omega,$$

$$u = 0, \quad x \in \partial\Omega.$$

We will design for medium $\epsilon(x)$. Note that we are not assuming a periodic background plus perturbation[a].

[a] we could ...

The domain Ω is a bounded domain in $\mathbb{R}^2$, we normalize the eigenfunction by

$$\int_\Omega \epsilon u^2 = 1.$$

We take dielectric constant from the admissible class

$$\mathcal{A} = \{\epsilon \in L^\infty(\Omega) : 0 < \epsilon_1 \leq \epsilon(x) \leq \epsilon_2, \ \text{ a.e}\}.$$

We know that for $\epsilon \in \mathcal{A}$, there will be an infinite sequence of non-negative, real eigenvalues

$$0 < \lambda_0(\epsilon) \leq \lambda_1(\epsilon) \leq \lambda_2(\epsilon) \leq \cdots,$$

and associated eigenfunctions $u_j(\epsilon)$, $j = 0, 1, 2, \cdots$.

A design problem

Find a dielectric constant $\epsilon \in \mathcal{A}$ such that
a particular eigenfunction $u(\epsilon)$ is most localized at a point.

A model objective function is

$$J(\epsilon, u) = \int_{\Omega} |x|^2 \epsilon u^2.$$

This is not a well-posed problem!

Not even a well-posed question

- We want one eigenfunction to be localized, but which one?
- As we iterate, an eigenvalue may become repeated. How to we follow the 'right' eigenfunction?

Two well-posed formulations.

Global problem

For some $N < \infty$, define

$$\mathcal{E}_N(\epsilon) = \{u \in H_0^1(\Omega) : \quad u \text{ is an eigenfunction associated with some } \lambda_j(\epsilon),\ j \le N, \text{ satisfying } \textstyle\int \epsilon |u|^2 = 1\}.$$

Note that $\mathcal{E}_N(\epsilon)$ is finite-dimensional for each ϵ. The global problem we consider is

$$\inf_{\epsilon \in \mathcal{A}} \min_{u \in \mathcal{E}_N(\epsilon)} J(\epsilon, u) = \int_\Omega w \epsilon |u|^2. \tag{1}$$

Problem (1) admits a solution $\epsilon \in \mathcal{A}$.

Local problem

Choose some $\epsilon_0 \in \mathcal{A}$ which yields an associated eigenvalue $\lambda_k(\epsilon_0)$ such that

$$\min_j |\lambda_k(\epsilon_0) - \lambda_j(\epsilon_0)| \geq 2\delta > 0.$$

In other words, the k-th eigenvalue is unique and separated from the other eigenvalues by 2δ. Then define a new admissible set

$$\mathcal{A}_\delta = \{\epsilon \in \mathcal{A} : \min_j |\lambda_k(\epsilon) - \lambda_j(\epsilon)| \geq \delta\},$$

where it is assumed that the eigenvalues are ordered according to multiplicity. Thus $\mathcal{A}_\delta$ contains a set of material parameters for which the k-th eigenvalue is always distinct and bounded away from all other eigenvalues.

We then formulate the "local problem" of optimizing the k-th eigenfunction

$$\inf_{\epsilon \in \mathcal{A}_\delta} J(\epsilon) = \int_\Omega w\epsilon |u_k|^2, \tag{2}$$

again normalized so that $\int \epsilon |u_k|^2 = 1$.

Problem (2) admits a solution $\epsilon \in \mathcal{A}_\delta$.

Discretized problem

Upon discretization, we end up with the following finite dimensional problem

$$Au = \lambda S(\epsilon)u,$$

where u and ϵ are finite dimensional, and A is a symmetric positive definite matrix representing $-\Delta$, and $S(\epsilon)$ is a diagonal matrix. The objective function is

$$J(\epsilon) = u^t \mathrm{diag}(\epsilon w)u.$$

where w is the weight.

Instead of an infinity of eigenvalues for each ϵ, we now have a finite number.

A computational approach

Let $b = 1/\sqrt{\epsilon}$, and B the diagonal matrix form by b.

Define $v = B^{-1}u$, the eigenproblem with the normalization is

$$BABv - \lambda v = 0, \quad \langle v, v \rangle = 1.$$

The objective can be rewritten as

$$J(b) = \frac{1}{2}\langle v(b), Wv(b) \rangle$$

where W is the matrix representing the weight.

We can compute the gradient of $J(b)$ using the adjoint-state method

$$g = \mathrm{diag}(q)ABv - \mathrm{diag}(v)ABq + 2\langle q, v\rangle \mathrm{diag}(v)ABv,$$

where the adjoint state q solves

$$BABq - \langle v, BABv\rangle q - 2\langle q, v\rangle BABv = Wv.$$

Observation: If we iteratively take steps in the direction of $-g$ starting with $v(b)$ associated with a simple eigenvalue, we are OK as long as the eigenvalues remain simple. But in general, we would expect eigenvalues to cross as we 'crawl' around the design space. We must find a way of continuing along the trajectory of the eigenvector we started with.

Tracking an eigenfunction

We will be updating matrix B

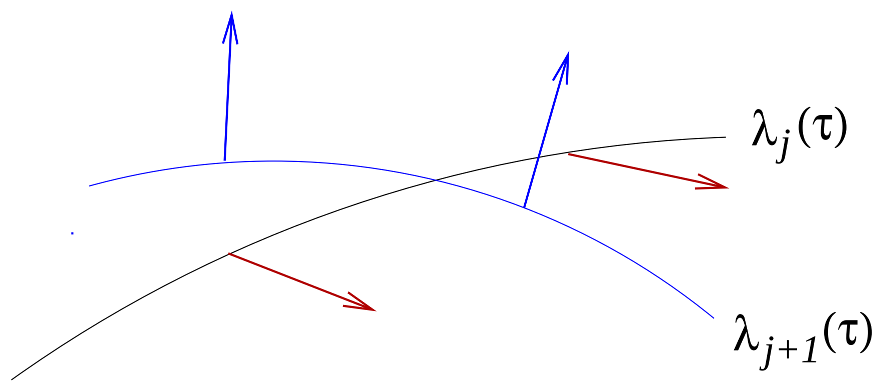
$$B_+ = B - \tau \text{diag}(g)$$

where τ is the step size in the negative gradient direction. The eigenvalue problem after the update is

$$B_+ A B_+ v = \lambda v.$$

The matrix B_+ is an analytic function of τ.

Tracking is possible due to a theorem by Kato which states that the eigenvectors v are are holomorphic functions of τ.



Thus we can identify an eigenfunction after an update with the one it comes from for sufficiently small τ.

Algorithm

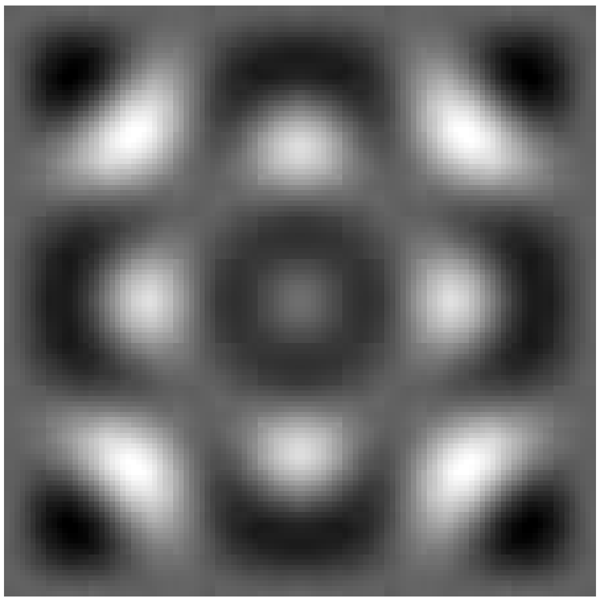
1. Set $n = 0$. Choose an initial design b_0 and a distinct eigenvalue $\lambda_k(b_0)$, with associated eigenvector v_0.
2. Compute the gradient g of $J(b_n)$, associated with the distinct eigenvector v_n.
3. Find eigenvectors of

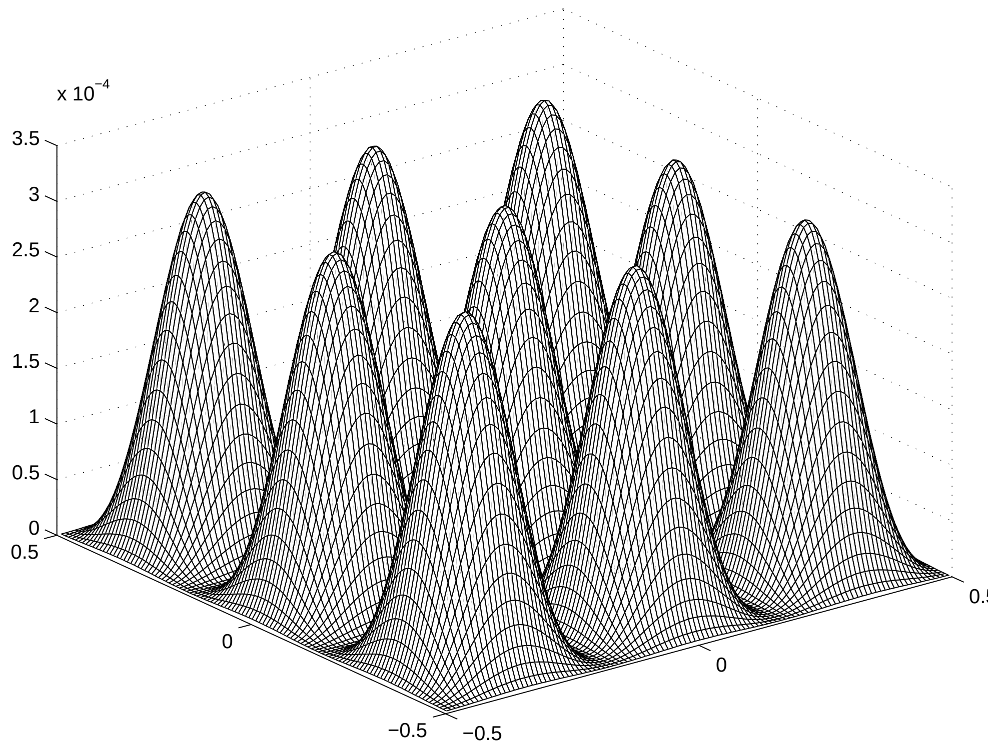
$$\mathtt{diag}(b_n - \tau g) A \, \mathtt{diag}(b_n - \tau g).$$

   Of these, identify eigenvector u which is closest to v_n.
4. If $J(u) < J(v_n)$ then

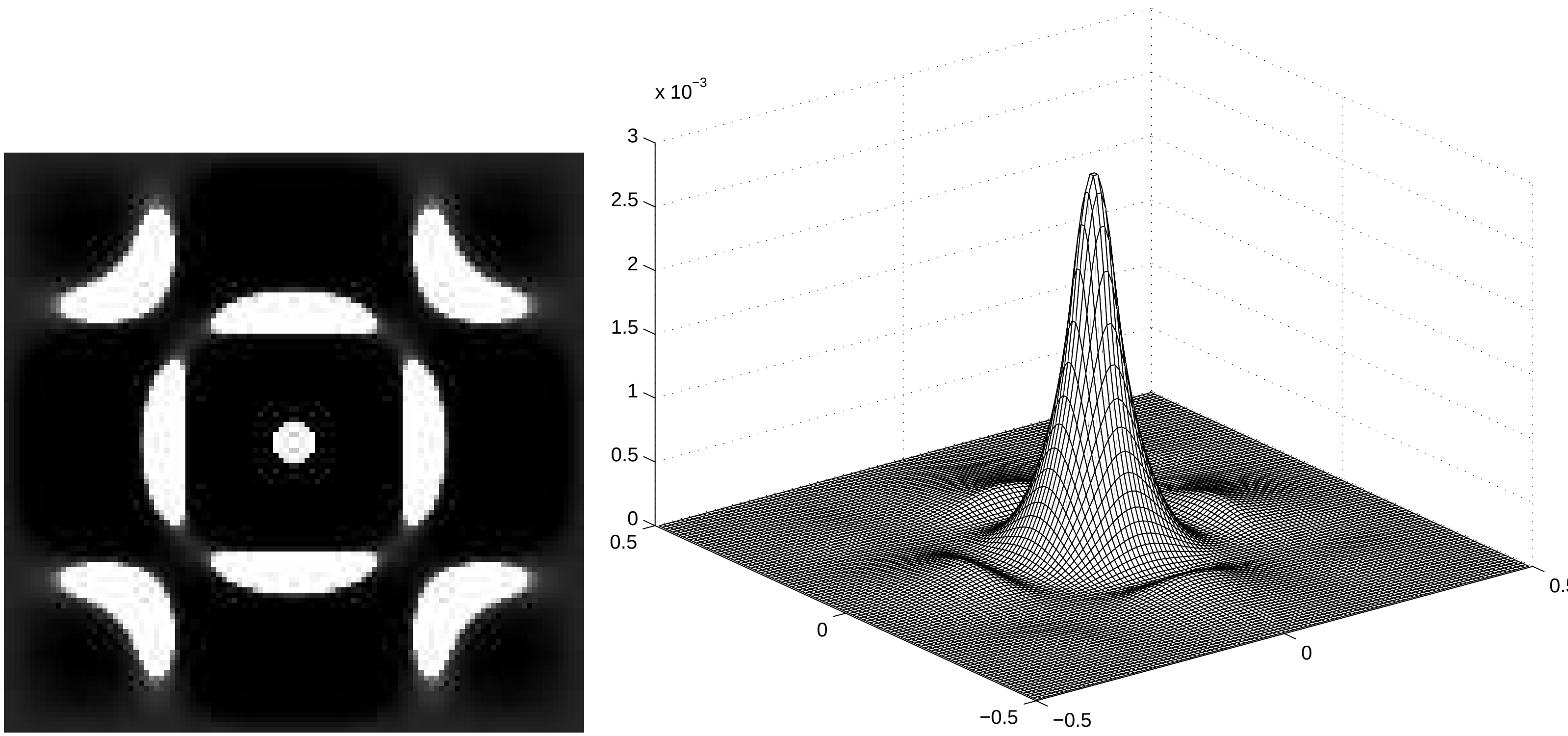
$$v_{n+1} = u, \; b_{n+1} = P(b_n - \tau g),$$

   else reduce τ and go back to step 3.
5. Set $n = n + 1$, continue with step 2.

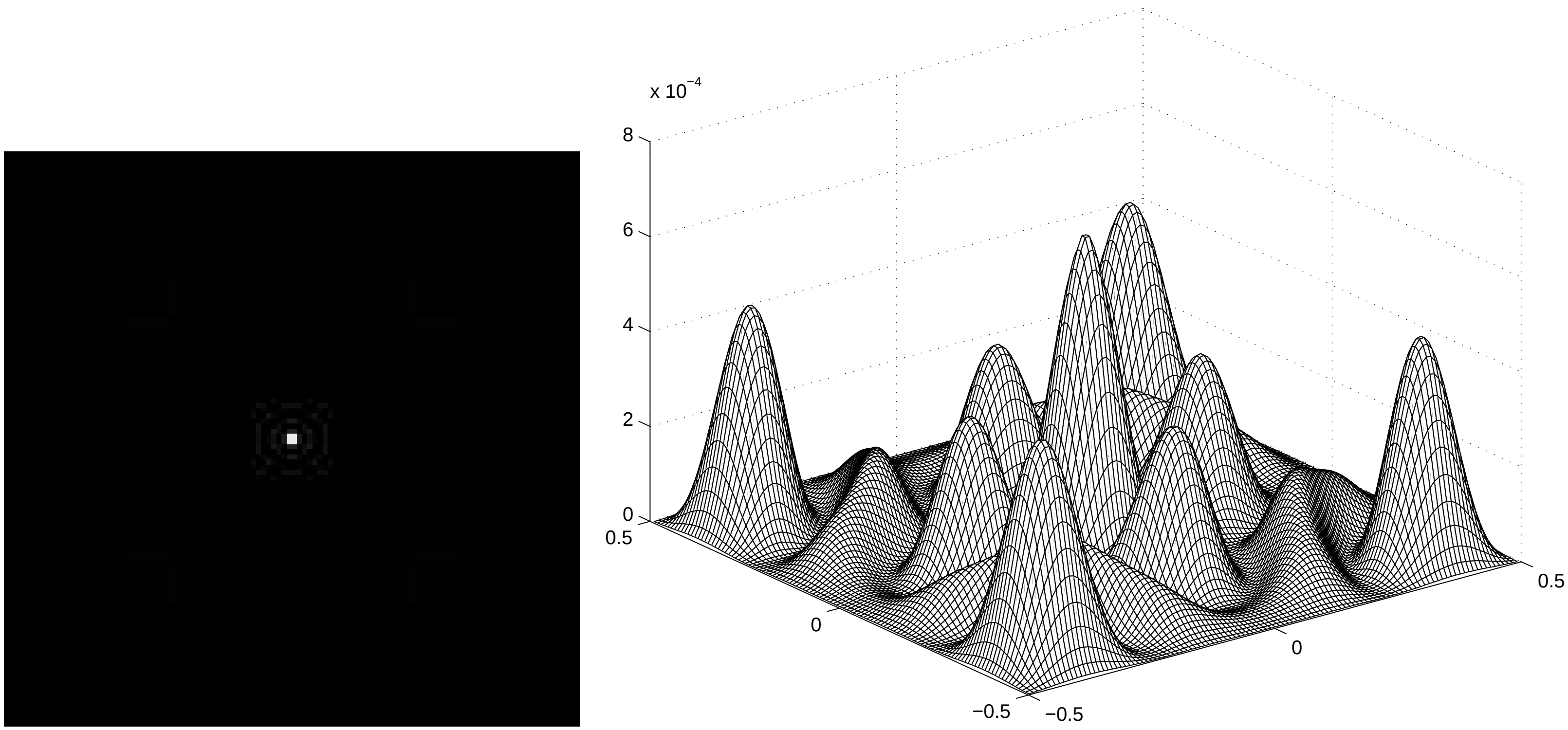




Initial medium and eigenmode.



Optimized medium and eigenmode.



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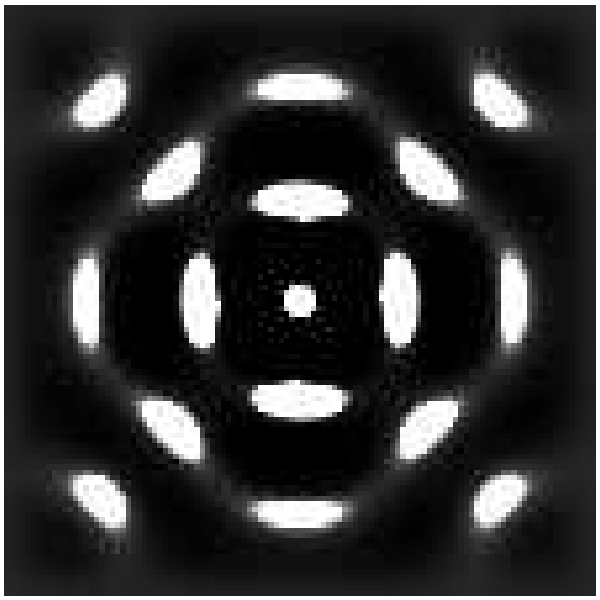
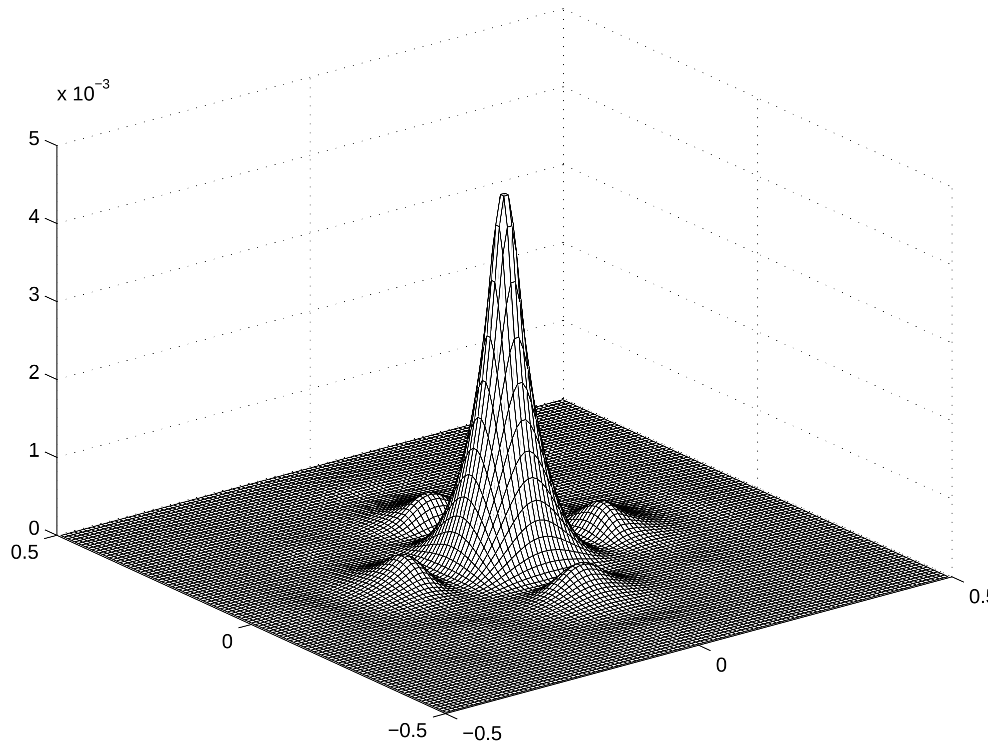
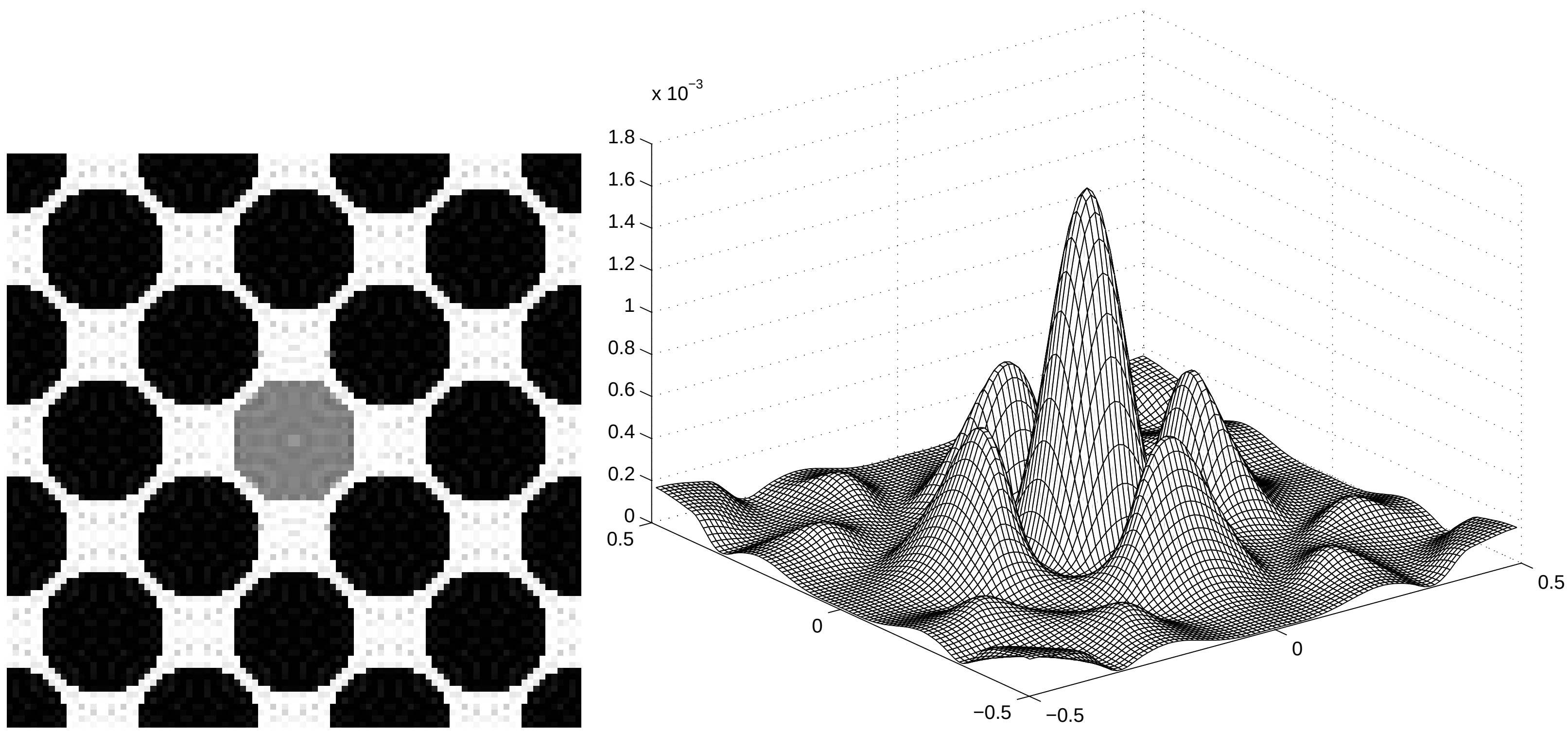
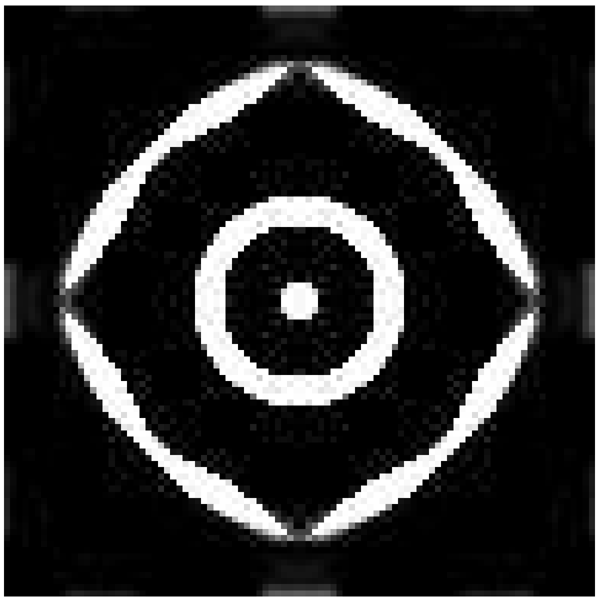


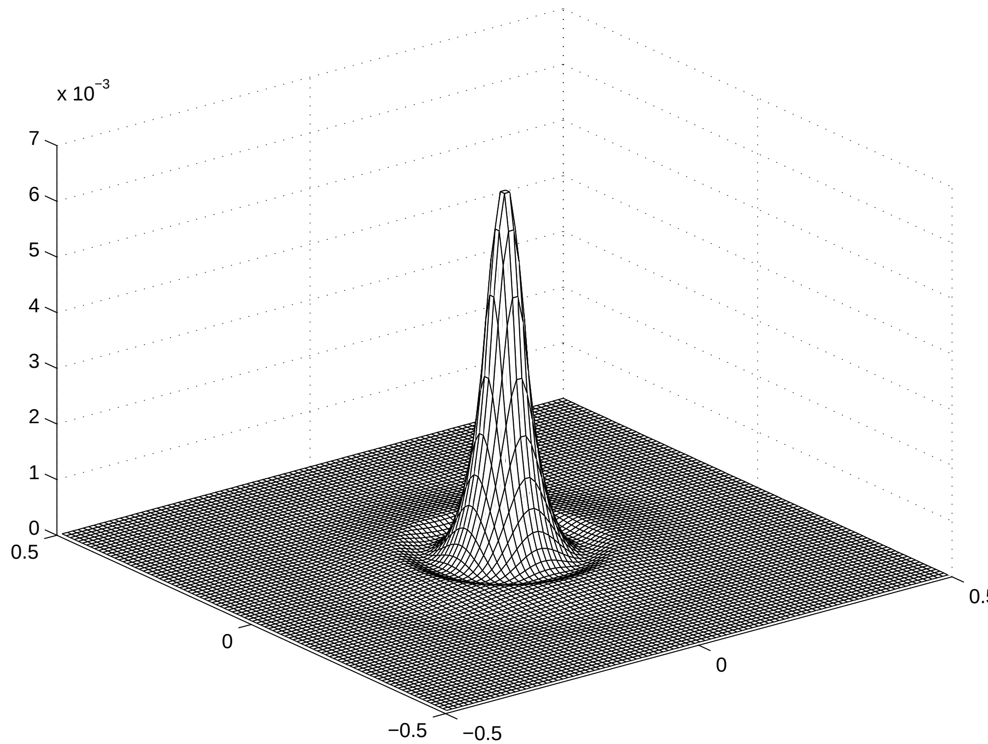


Optimized medium and eigenmode.



Initial medium and eigenmode.





Optimized medium and eigenmode.

Discussion

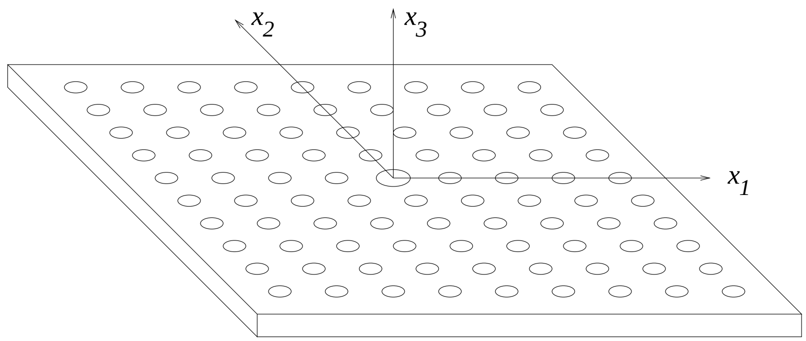
We have presented an approach for optimal design of defect modes in a simple toy problem. We showed

- Wellposed formulations
- A trajectory tracking algorithm
- Numerical results

It can be used to guide design of defects in photonic band gap structures.

Optimizing a membrane structure

(the whole enchilada)



A 'defect mode' in such a structure is known to be lossy. Thus it would be interesting to find arrangement of air holes so that the defect mode

- has minimum loss and is highly localized;
- has desired frequency and satisfies manufacturing constraints.