Numerical modeling and design optimization of periodic dielectric structures

IMA Hot Topics Workshop:
Modeling and Analysis of Optical Devices
September 9–10, 1999

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Research supported by:
AFOSR, Sloan Foundation.

Outline:

- Photonic bandgap structures
- 3D numerical methods
  (with J. Pasciak, J. Gopalakrishnan)
- Design optimization in 2D
  (with S. Cox)
- Conclusions

Also relevant:

- Modeling and design optimization of grating structures...

Photonic bandgap structures

Structures are “artificial crystals” constructed from dielectric materials.

Behave in some sense as optical analogues of electronic semiconductor materials.

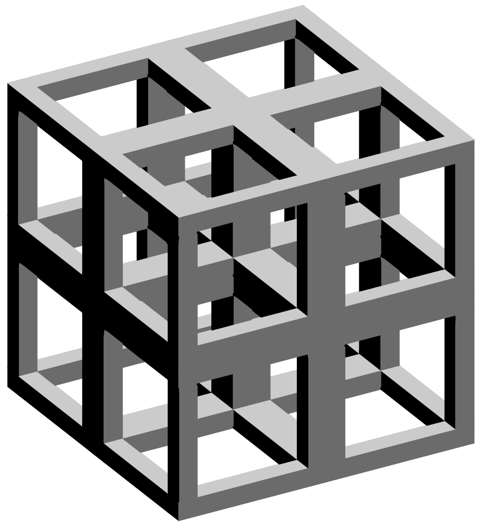
For certain arrangements of materials, electromagnetic wave propagation is prohibited in specific frequency ranges.

Potential photonics applications:

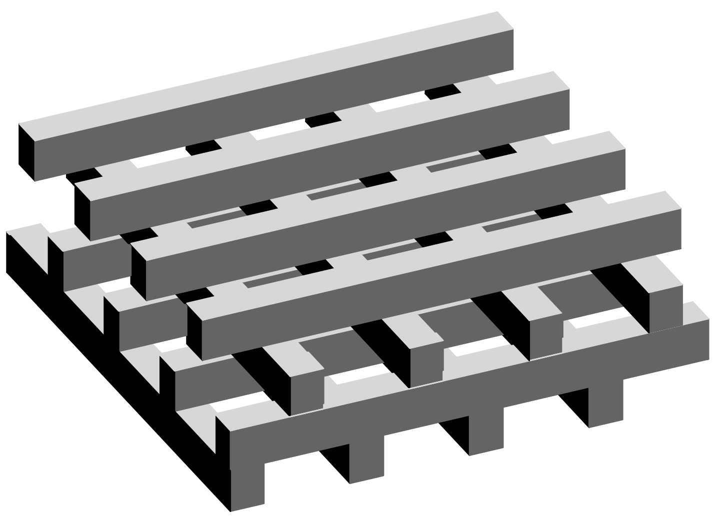
- integrated optical waveguides,
- fast single mode light emitting diodes,
- optical filters and transducers,
- high speed photonic switches,

Similar applications in microwaves, ultrasound.

Examples



Scaffold structure
after *H.S. Sözüer and J.W. Haus*.



Silicon bars, 4.2μm spacing,
after *S.Y. Lin, et al, Nature, July 1998.*

Direct problem

Classical electromagnetic waves in $\mathbb{R}^3$

$$\begin{aligned} \nabla \times E - i\omega\mu H &= 0, \\ \nabla \times H + i\omega\epsilon E &= 0, \end{aligned}$$

where μ is constant and ϵ is periodic:

$$\epsilon(x+n) = \epsilon(x), \quad \text{for } x \in \mathbb{R}^3 \text{ and } n \in \Lambda.$$

Here $\Lambda = Z^3$ is the integer lattice.

Setting $\gamma = (\mu\epsilon)^{-1}$, it follows that

$$\begin{aligned} \nabla \times \gamma \nabla \times H &= \omega^2 H, \\ \nabla \cdot H &= 0. \end{aligned}$$

Define the periodic domain $\Omega = \mathbb{R}^3/\Lambda$
and the first Brillouin zone $K = [-\pi, \pi]^3$.

We wish to find *Bloch eigenfunctions* H satisfying Maxwell's equations such that

$$H(x) = e^{i\alpha\cdot x} H_\alpha(x),$$

where H_α is periodic in x, and $\alpha \in K$.
For each $\alpha \in K$, it follows that

$$\begin{aligned} \nabla_\alpha \times \gamma \nabla_\alpha \times H_\alpha &= \omega^2 H_\alpha, \quad \text{in } \Omega, \\ \nabla_\alpha \cdot H_\alpha &= 0, \qquad\quad \text{in } \Omega, \end{aligned}$$

where $\nabla_\alpha = (\nabla + i\alpha)$. We henceforth drop the subscript α when referring to H_α.

Standard approach to solving this system is by *truncated plane wave decomposition* (PWD).

PWD is very natural, has fast convergence for media with smooth spatial variation.

Gibbs-type phenomena can lead to slow convergence in media with jump discontinuities.

Weak formulation

For $F, G \in V$, define the hermitian forms

$$\begin{aligned} a(F,G) &= \int_\Omega \gamma(\nabla_\alpha \times F) \cdot \overline{(\nabla_\alpha \times G)}, \\ c(F,G) &= \int_\Omega F \cdot \overline{G}. \end{aligned}$$

Introduce the spaces

$$\begin{aligned} V &= \{F \in L^2(\Omega)^3 : \nabla \times F \in (L^2(\Omega))^3\}, \\ V^{0,\alpha} &= \{F \in V : \ \nabla_\alpha \cdot F = 0 \text{ in } \Omega\}. \end{aligned}$$

Weak formulation:
find $\omega \in \mathbb{R}$ and $H \in V^{0,\alpha}$ satisfying

$$a(H,F) = \omega^2 c(H,F) \quad \text{for all } F \in V^{0,\alpha}.$$

Mixed reformulation

Enforce the div constraint variationally. Let

$$W = \{g \in L^2(\Omega) : \nabla g \in (L^2(\Omega))^3\}.$$

For $\rho \in W$ and $F \in V$, define

$$b(\rho, F) = \int_\Omega \nabla_\alpha \rho \cdot \overline{F}.$$

Mixed form:
find $\omega \in \mathbb{R}$ and $(H, \rho) \in V \times W$ such that

$$\begin{aligned} a(H, F) + b(\rho, F) &= \omega^2 c(H, F), \text{ all } F \in V, \\ \overline{b(g, H)} &= 0, \qquad\qquad \text{all } g \in W. \end{aligned}$$

Stability of mixed reformulation and equivalence with non-mixed problem requires

(1) LBB (inf-sup) condition,

$$\|w\|_W \le C \sup_{X \in V} \frac{(X, \nabla_\alpha w)}{\|X\|_V}, \quad \text{for all } w \in W.$$

(2) Coercivity of $a(\cdot,\cdot)$ on $V^{0,\alpha}$.

Mixed method discretization

To get stable approximations, finite element spaces $V_h \subset V$ and $W_h \subset W$ should satisfy discrete LBB and coercivity conditions.

We construct special finite element spaces to get stable pairs V_h^α, W_h^α by augmenting nodal and Nedelec edge elements by phase factors $e^{-i\alpha\cdot(x-y_j)}$.

Discrete LBB and coercivity conditions hold for these spaces. Additional conditions may be necessary to prove convergence of eigenvalues.

Augmented elements are not piecewise polynomial. Nevertheless, FEM matrix entries are easy to compute.

Preconditioner

It is natural to develop a preconditioned iterative scheme for the non-mixed formulation on the subspace $V_h^{0,\alpha}$.

To construct a preconditioner, start by defining $a_0(\cdot,\cdot)$ on $V \times V$ to be equal to $a(\cdot,\cdot)$ with γ replaced by a constant.

Given a functional G on $V_h^{0,\alpha}$, the preconditioner involves finding $D_h \in V_h^{0,\alpha}$ such that

$$a_0(D_h, F) = G(F), \qquad \text{for all } F \in V_h^{0,\alpha}.$$

The difficulty is that we have no explicit basis for $V_h^{0,\alpha}$. To compute the preconditioner without a basis for $V_h^{0,\alpha}$, we recast the problem in mixed form.

Since a_0, b, c have constant coefficients, the matrix problem corresponding to the mixed form preconditioner

$$\begin{pmatrix} A_0 & B^* \\ B & 0 \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \begin{pmatrix} G \\ 0 \end{pmatrix}$$

transforms via fast Fourier transform (FFT) to a problem of the form

$$\widehat{M}\hat{Q} = \hat{R}.$$

where $\widehat{M}$ is block diagonal, each block consisting of a 4×4 matrix.

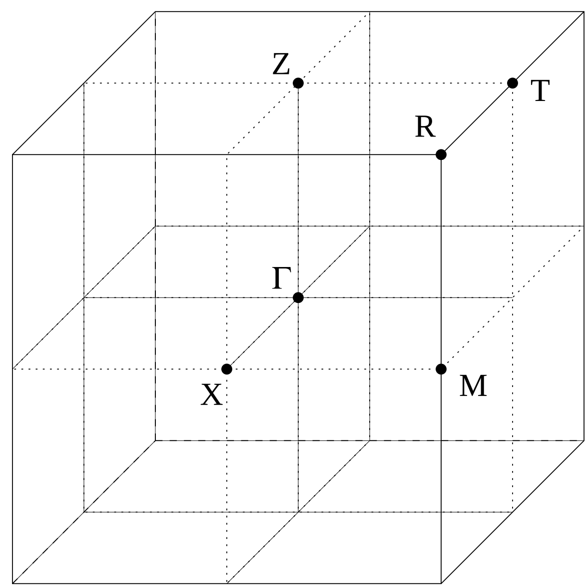
Total work to solve the system is $O(N^3 \log N)$ on an $N \times N \times N$ grid.

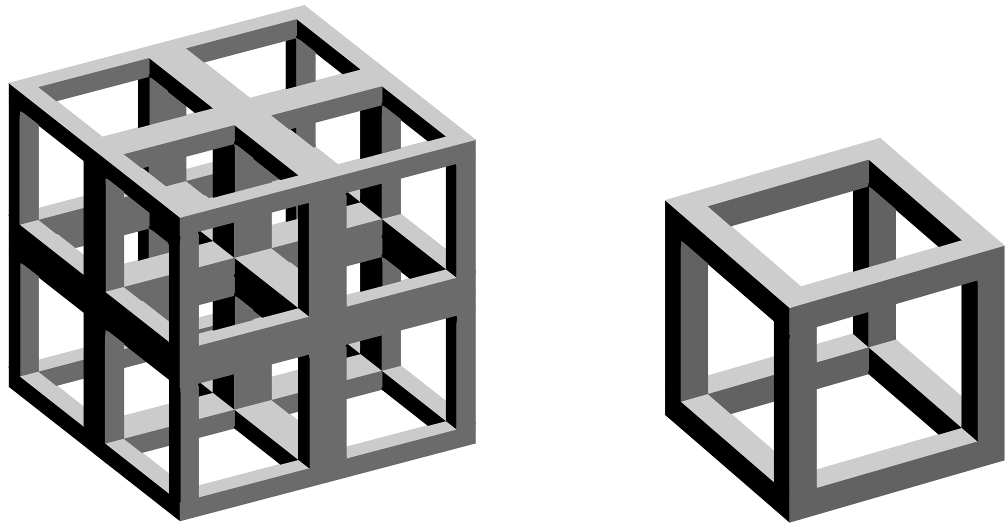
The preconditioner projects into $V_h^{0,\alpha}$.

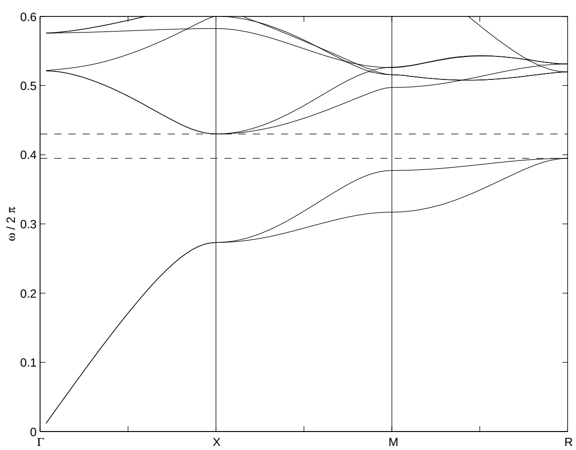
Eigenvalue approximation algorithm

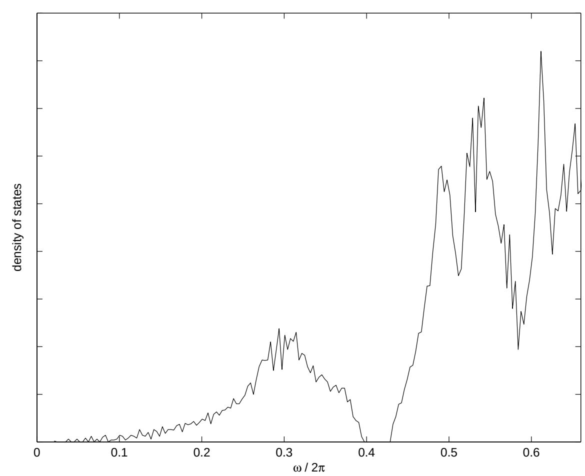
- Eigenvalues are found by a *subspace preconditioning method*.
- The method iteratively locates the first s eigenvalues of a Hermitian operator.
- Under certain assumptions on the preconditioner, convergence rate is *independent* of h.
- Well suited for computing continuously varying families of eigenvalues.

Examples









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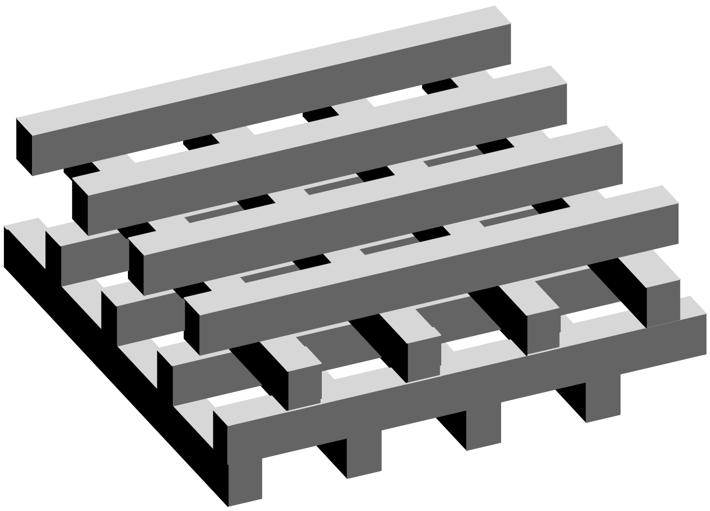

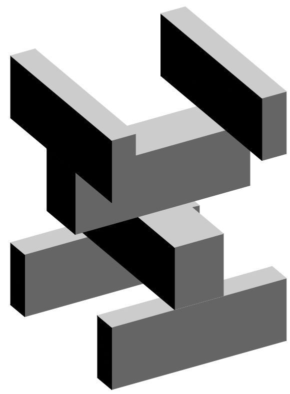

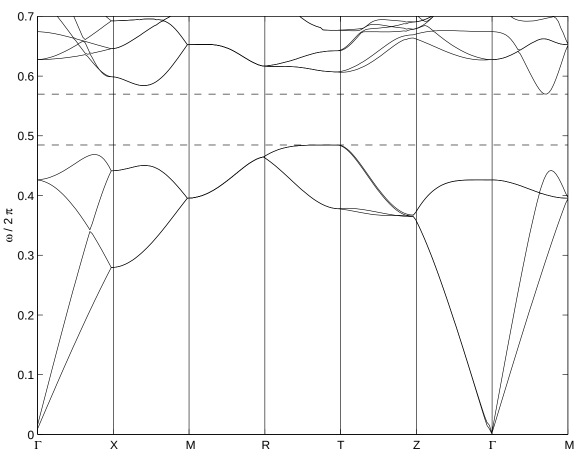

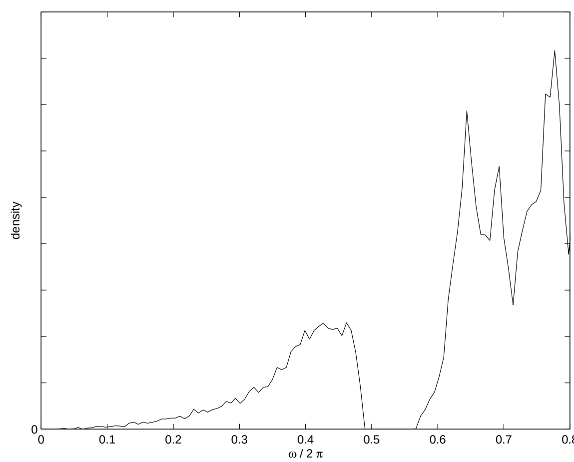

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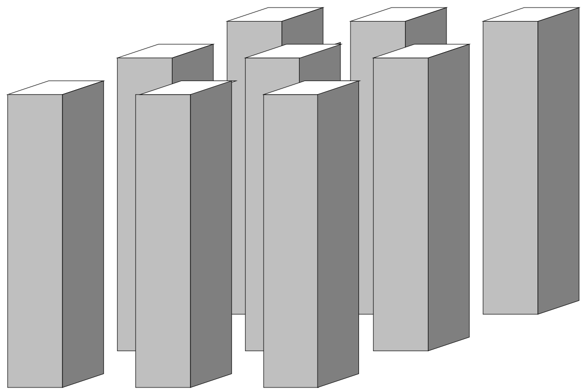
Two-dimensional case



In E-parallel polarization: $E = (0, 0, u)$.
Maxwell's equations become

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

where $\rho(x_1, x_2)$ is the dielectric coefficient.

For H-parallel polarization: $H = (0, 0, u)$.
The analogous eigenvalue problem is

$$-\nabla \cdot \frac{1}{\rho} \nabla u = \omega^2 u, \quad \text{in } \mathbb{R}^2.$$

Obviously, computations are easier in 2D.

Band gaps

Again looking at Bloch modes, the spectrum is a sequence of real eigenvalues

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

where $\alpha \in K = [-\pi, \pi]^2$, and $\lambda_k = \omega_k^2$.

Bloch spectrum

$$\mathcal{B}(\rho) = \{\lambda_j(\rho, \alpha) : \;\; \alpha \in K, \;\; j = 1, 2, 3, \ldots\}.$$

Structure has a band gap if there is a positive interval (a, b) which does not intersect $\mathcal{B}(\rho)$.

How can we find ρ which maximizes $b - a$?

Optimal design

We wish to find structures with maximal gaps.

Assume that we have a structure ρ_0 which has a band gap around some fixed ω_0^2,

$$\lambda_j(\rho_0, \alpha) < \omega_0^2 < \lambda_{j+1}(\rho_0, \alpha), \quad \text{for all } \alpha \in K.$$

Define the gap function

$$G(\rho) = \inf_{\alpha \in K} \left(\min\{\lambda_{j+1}(\rho, \alpha) - \omega_0^2, \omega_0^2 - \lambda_j(\rho, \alpha)\} \right).$$

We would like to maximize $G(\rho)$ over the admissible class

$$ad = \{\rho \in L^\infty(\Omega) : 0 < a_0 \leq \rho(x) \leq a_1\}.$$

$G(\rho)$ is not smooth due to eigenvalue multiplicities and $\inf_\alpha$, $\min_k$ appearing in the definition.

Characterization of generalized gradient

In E-parallel case, we find

$$\partial G(\rho) \subset$$

$$\overline{\text{co}}^{*}\{\text{co}\,\{\text{co}\,\{-\lambda_{j+1}(\rho,\alpha)|v|^2 : v \in \mathcal{E}^1_{j+1}(\rho,\alpha)\}, \text{co}\,\{\lambda_j(\rho,\alpha)|v|^2 : v \in \mathcal{E}^1_j(\rho,\alpha)\}\} : \alpha \in \text{Argmin}\, g(\rho,\cdot)\},$$

where $\mathcal{E}^1_j(\rho,\alpha)$ denotes the eigenspace associated with $\lambda_j(\rho,\alpha)$ with elements v normalized $\int_\Omega \rho|v|^2 = 1$.

Notes:

- All one needs to calculate $\partial G(\rho)$ are the eigenfunctions associated with eigenvalues where the $\inf_\alpha$ is attained.
- Evaluating $\partial G(\rho)$ is essentially no more expensive than evaluating $G(\rho)$.
- $\partial G(\rho)$ is never $\{0\}$.

Optimization scheme

Many general purpose nondifferentiable optimization schemes are applicable.

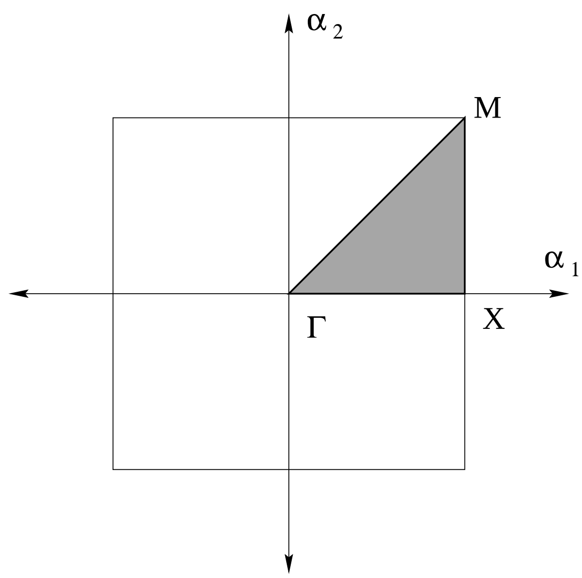
We use a simple projected (generalized) gradient descent method.

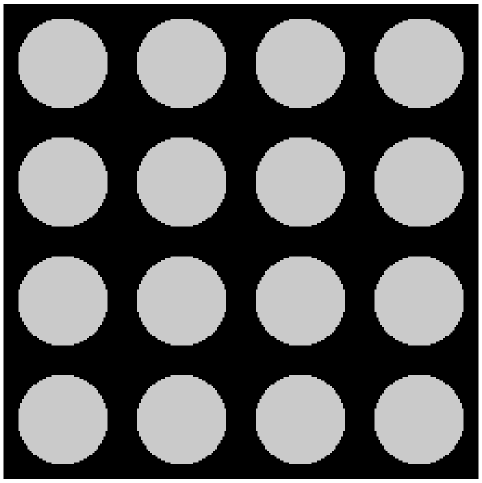
- The method chooses ascent directions from ∂G by solving a low-dimensional linear sub-problem with linear programming.
- Approximate eigenfunctions from current step are used to initialize subspace preconditioning algorithm for next step.

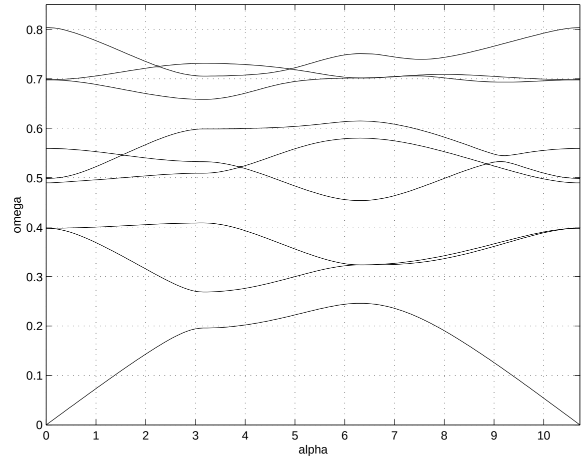
Numerical Experiments

Experiments done with $a_0 = 1$, $a_1 = 9$, large contrast dielectric materials in optical range.

Experiments with higher contrast materials have yielded designs with much larger gaps.



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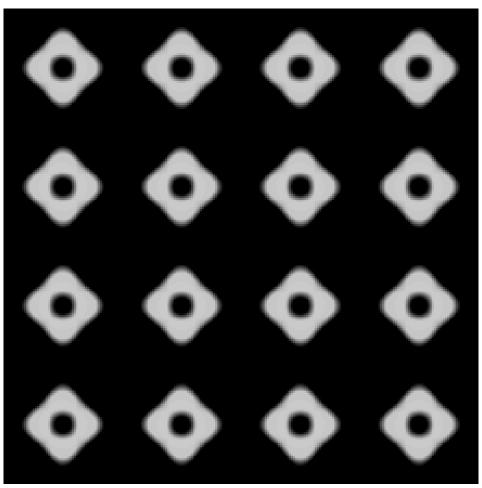

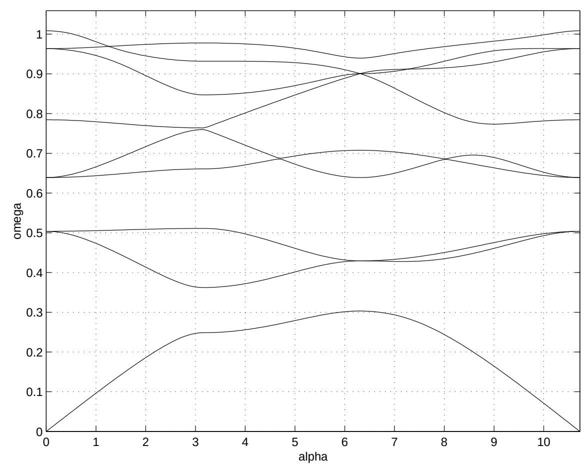
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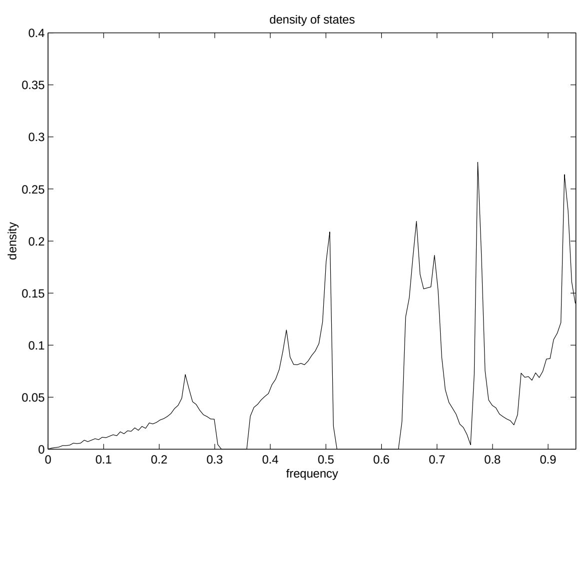
density of states
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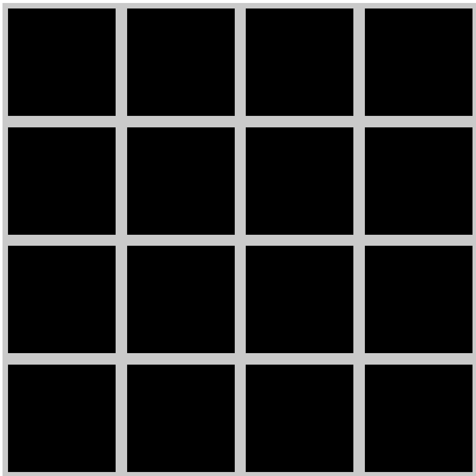

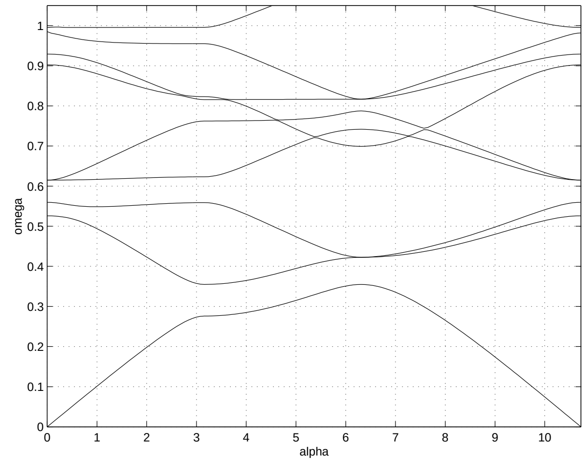
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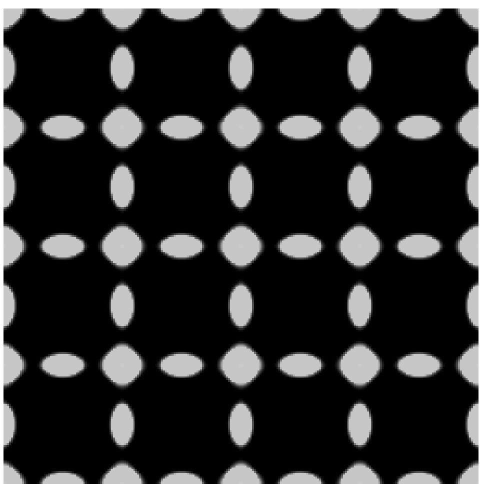

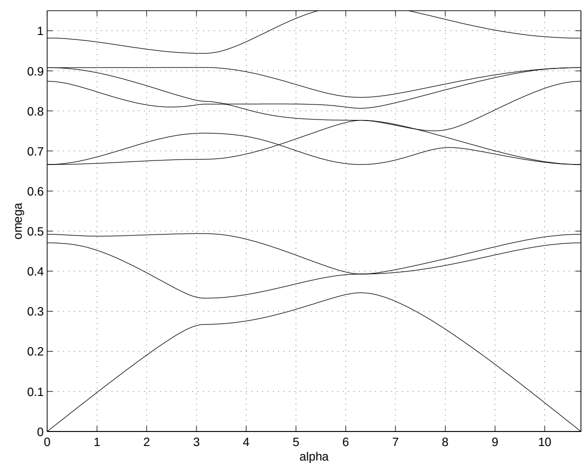
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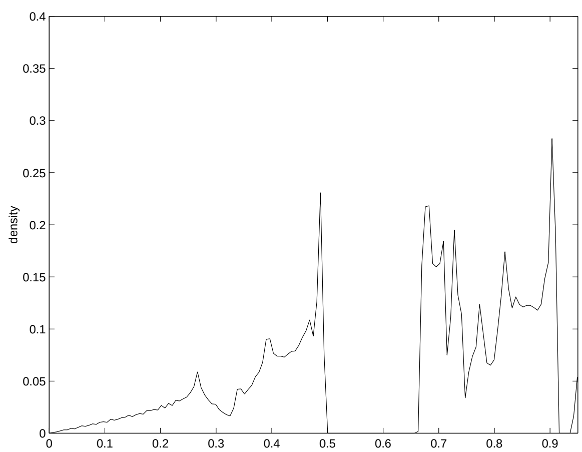
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H-parallel case

Basic design approach of E-parallel case applies, but with difficulties:

- Admissible design set includes anisotropic materials,
- Well-posedness more difficult to establish,
- Numerical difficulties due to decreased regularity of gradient.

If design class is taken to be isotropic, then

$$\partial G(\rho) \subset$$

$$\overline{\text{co}}^{*}\{\text{co}\,\{\text{co}\,\{-|\nabla_\alpha v|^2 : v \in \mathcal{E}^1_{j+1}(\rho,\alpha)\}, \text{co}\,\{|\nabla_\alpha v|^2 : v \in \mathcal{E}^1_{j}(\rho,\alpha)\}\} : \alpha \in \text{Argmin}\, g(\rho,\cdot)\}.$$

Evolution strategy

Choose function $q_0(\alpha)$ which lies between two bands. Choose a target $q_1(\alpha)$.

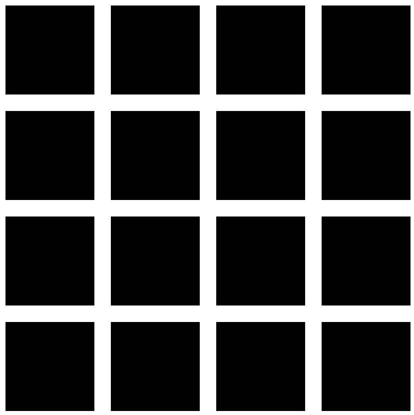
Define $q_t(\alpha) = (1 - t)q_0(\alpha) + tq_0(\alpha)$, and

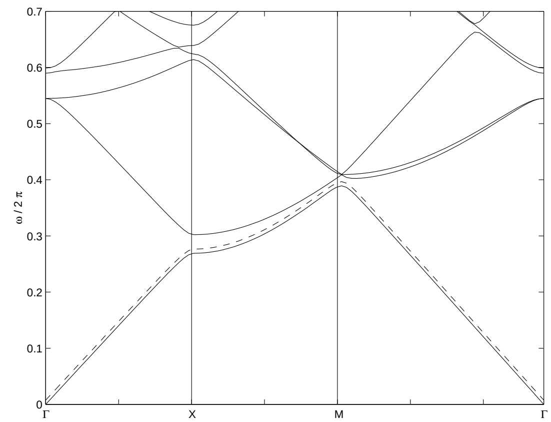
$G(\rho, q_t) = \inf_{\alpha \in K}(\min_k |\lambda_k(\rho, \alpha) - q_t(\alpha)|)$.

Wish to continuously deform initial q_0 into desired target q_1, then maximize gap around q_1.

Evolution algorithm consists of an outer loop which moves q_t toward q_1, and an inner loop which increases $G(\rho, q_t)$ by gradient ascent.

When q_1 is reached, gradient ascent continues until convergence.

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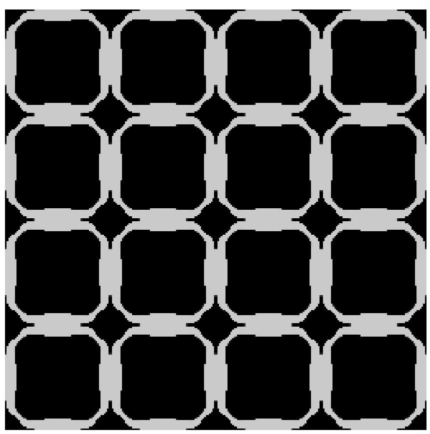

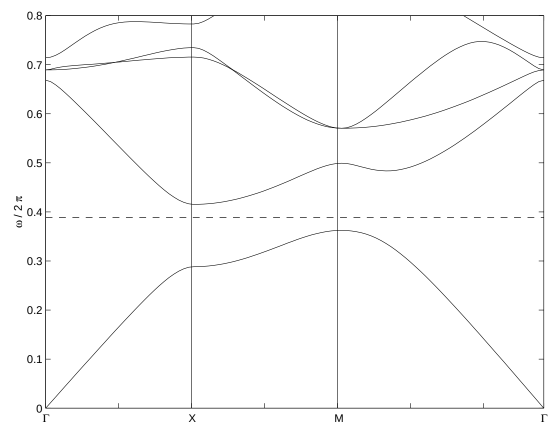
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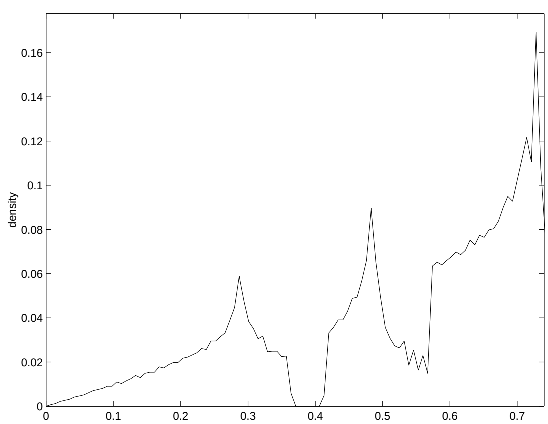
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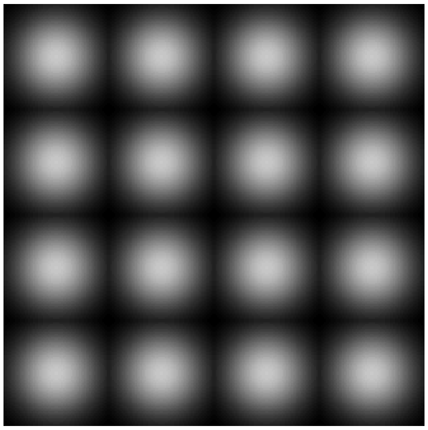

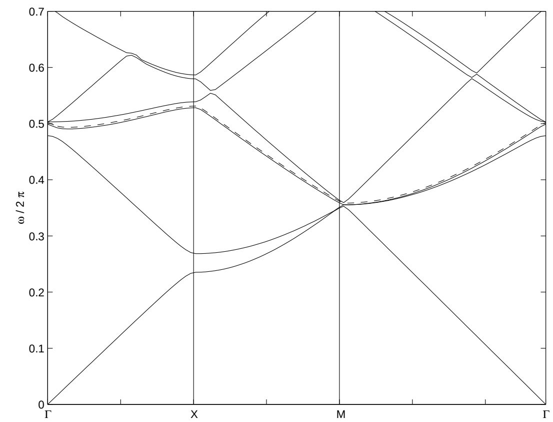
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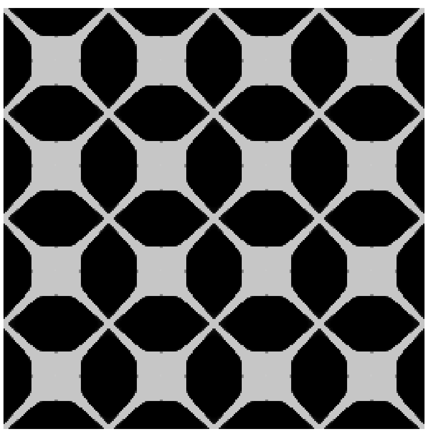

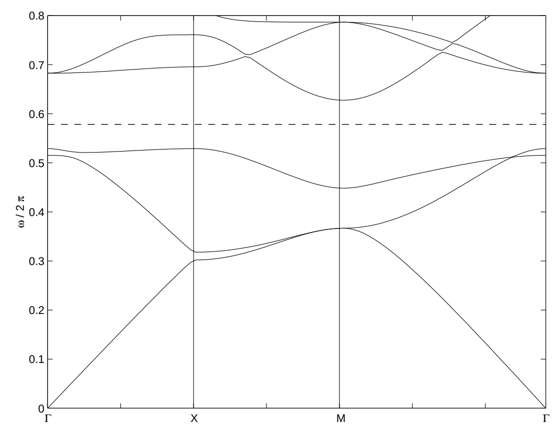
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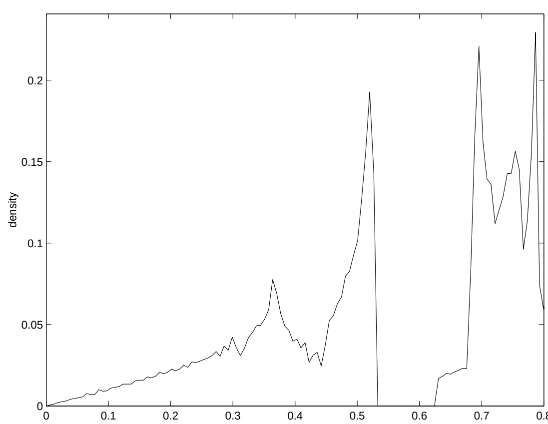
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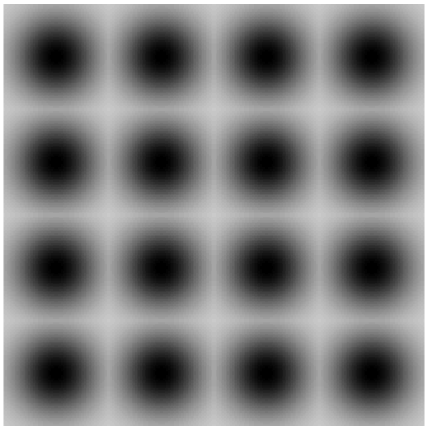

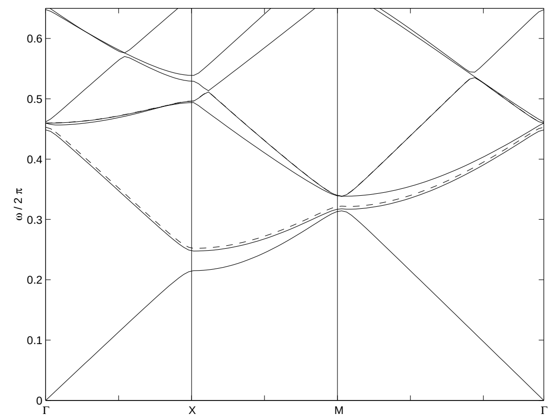

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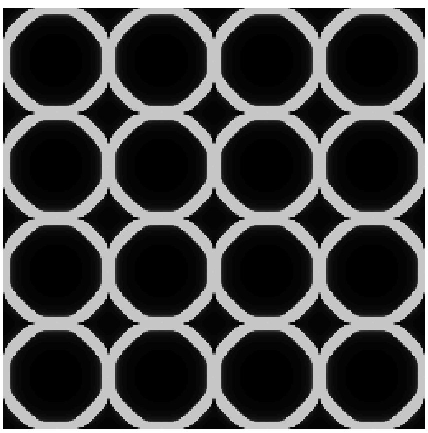

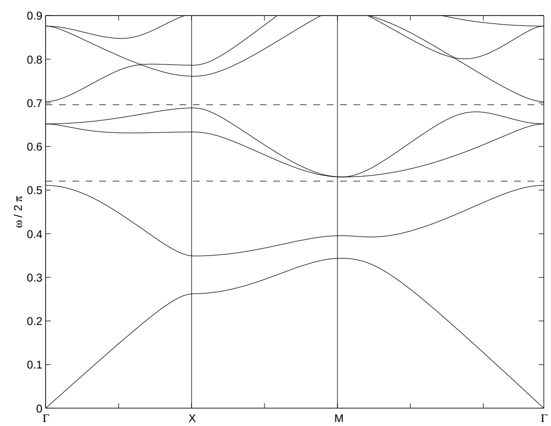

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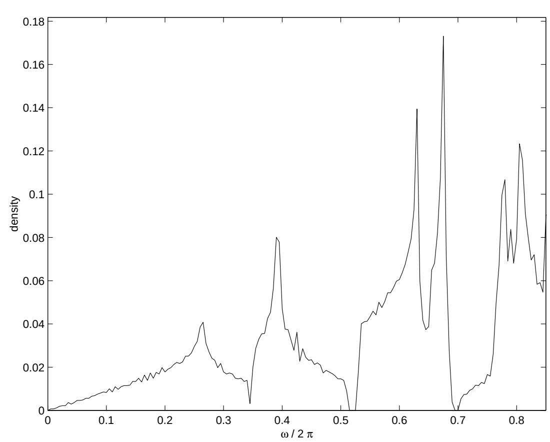

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Conclusions

- Iterative PDE solution techniques coupled with simple optimization strategies make large optimal design problems feasible.

- This technology has great potential in industry for design of gratings, bandgap structures. Can extend to other photonics problems.