Photonic Band Gap Computations

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Outline

1. The **Mathematics** of Photonic Band Gaps (revisited)
2. The **Approximation** of Photonic Band Gaps (revisited)
3. The **Computation** of Photonic Band Gaps (state-of-the-art)
4. The **Verification** of Photonic Band Gap (summarized)
5. The **Optimization** of Photonic Band Gap (work in progress)

The numerical results are obtained in cooperation with A. Bulovyatov.

The verification method is developed in cooperation with V. Hoang and M. Plum.

The optimization method is developed in cooperation with M. Richter and W. Dörfler.
The Maxwell Eigenvalue Problem

We consider the Maxwell eigenvalue problem for the magnetic field $H$ for optic waves (where we have $\mu \equiv 1$)

\[ \nabla \times \varepsilon^{-1} \nabla \times H = \lambda H \]  
\[ \nabla \cdot H = 0 \]  
(1a)  
(1b)

in the case that $\varepsilon$ is a periodic function with $\varepsilon(x) = \varepsilon(x + z)$ for all $z \in \mathbb{Z}^3$.

Let $\Omega = (0, 1)^3$ be a fundamental cell, and $K = [-\pi, \pi]^3$ be the Brillouin zone. The ansatz $H(x) = e^{ik \cdot x} \tilde{H}(x)$ with $x \in \Omega$, $k \in K$ and $\tilde{H}$ periodic in $\Omega$ yields

\[ \nabla_k \times \varepsilon^{-1} \nabla_k \times \tilde{H} = \lambda \tilde{H} \]  
\[ \nabla_k \cdot \tilde{H} = 0 \]  
(2a)  
(2b)

in $\Omega$, where $\nabla_k = \nabla + ik$.

The reduced problem for $k \in K$ has a discrete spectrum with eigenvalues

\[ 0 \leq \lambda_{k,1} \leq \lambda_{k,1} \leq \cdots \leq \lambda_{k,N} \leq \cdots \]

**Theorem**  Problem (1) has the spectrum $\sigma = \bigcup_{n \in \mathbb{N}} [\inf_{k \in K} \lambda_{k,n}, \sup_{k \in K} \lambda_{k,n}]$.

(application of the Floquet-Bloch theory)

If $\left( \sup_{k \in K} \lambda_{k,n}, \inf_{k \in K} \lambda_{k,n+1} \right)$ is non-empty for some $n \in \mathbb{N}$, this is a **band gap**.
Approximation of the Maxwell Eigenvalue Problem

Let \( X = H^1_{\text{per}}(\text{curl}; \Omega) \subset H(\text{curl}; \Omega) \) be the subspace of periodic vector fields. For \( u, v \in X \) we define the Hermitian bilinear forms

\[
a_k(u, v) = \int_{\Omega} \epsilon^{-1} \nabla_k \times u \cdot \nabla_k \times v \, dx,
\]

\[
m(u, v) = \int_{\Omega} u \cdot \nu \, dx
\]

Let \( Q = H^1_{\text{per}}(\Omega) \subset H^1(\Omega) \) be the subspace of periodic scalar functions. Let

\[
b_k(v, q) = \int_{\Omega} v \cdot \nabla_k q \, dx,
\]

\[
c_k(p, q) = \int_{\Omega} \nabla_k p \cdot \nabla_k q \, dx,
\]

and \( V_k = \{ v \in X : b_k(v, q) = 0 \text{ for all } q \in Q \} \).

**Weak Form**
Find \((u, \lambda) \in V_k \times \mathbb{R}\) such that

\[
a_k(u, v) = \lambda \ m(u, v) \quad \text{for all} \quad v \in V_k.
\]

**Discrete Approximation**
Let \( X_{h,k} \subset X \) and \( Q_{h,k} \subset Q \) be discrete subspaces.
Set \( V_{h,k} = \{ v_{h,k} \in X_{h,k} : b_k(v_{h,k}, q_{h,k}) = 0 \text{ for all } q_{h,k} \in Q_{h,k} \} \).
Find \((u_{h,k}, \lambda_{h,k}) \in V_{h,k} \times \mathbb{R}\) such that

\[
a_k(u_{h,k}, v_{h,k}) = \lambda_{h,k} \ m(u_{h,k}, v_{h,k}) \quad \text{for all} \quad v_{h,k} \in V_{h,k}.
\]
Lowest order conforming finite elements

Let \( \bar{\Omega} = \bigcup_{c \in \mathcal{C}_h} \bar{\Omega}_c \) be a decomposition into hexahedral cells \( c \in \mathcal{C}_h \), and let \( \phi_c : \hat{\Omega} = [0, 1]^3 \rightarrow \Omega_c \) be the transformation to the reference cell. We define

\[
X_{h,0} = \{ u \in X : D\phi_c^{-1} u \circ \phi_c \in P_{0,1,1} e_x + P_{1,0,1} e_y + P_{1,1,0} e_z \text{ for all } c \in \mathcal{C}_h \},
\]

\[
Q_{h,0} = \{ q \in Q : q \circ \phi_c \in P_{1,1,1} \text{ for all } c \in \mathcal{C}_h \}.
\]

Let \( \mathcal{V}_h \subset \bar{\Omega} \) be the set of all vertices \( z_v \), and let \( \mathcal{E}_h \) be the set of all edges \( e = (x_e, y_e) \) with midpoint \( z_e = 0.5(x_e + y_e) \) and tangent \( t_e = y_e - x_e \).

A nodal basis \( \{ \psi_{e,0} : e \in \mathcal{E}_h \} \subset X_{h,0} \) exists such that for all \( u_{h,0} \in X_{h,0} \)

\[
u_{h,0} = \sum_{e \in \mathcal{E}_h} \langle \psi'_{e,0} , u_{h,0} \rangle \psi_{e,0} , \quad \langle \psi'_{e,0} , u_{h,0} \rangle = \int_{x_e}^{y_e} u_{h,0} \cdot t_e ds ,
\]

and a nodal basis \( \{ \phi_{v,0} : v \in \mathcal{V}_h \} \subset Q_{h,0} \) exists such that for all \( q_{h,0} \in Q_{h,0} \)

\[
q_{h,0} = \sum_{v \in \mathcal{V}_h} \langle \phi'_{e,0} , q_{h,0} \rangle \phi_{v,0} , \quad \langle \phi'_{e,0} , q_{h,0} \rangle = q_{h,0}(z_v) .
\]

(curl conforming elements were introduced by Nédélec)
Conforming Elements with Shifted Basis

For \( k \in K \) we define modified elements with a phase shift

\[
\mathbf{x}_{h,k} = \text{span}\{\psi_{e,k} : e \in \mathcal{E}_h\}, \quad \psi_{e,k}(x) = e^{-ik \cdot (x-z_e)} \psi_{e,0}(x)
\]

\[
Q_{h,k} = \text{span}\{\phi_{v,k} : v \in \mathcal{V}_h\}, \quad \phi_{v,k}(x) = e^{-ik \cdot (x-z_v)} \phi_{v,0}(x)
\]

with

\[
u_{h,k} = \sum_{e \in \mathcal{E}_h} \langle \psi'_{e,k}, u_{h,k} \rangle \psi_{e,k}, \quad \langle \psi'_{e,k}, u_{h,k} \rangle = \int_{x_e} y^e e^{ik \cdot (x-z_e)} u_{h,0} \cdot t_e ds,
\]

\[
q_{h,k} = \sum_{v \in \mathcal{V}_h} \langle \phi'_{e,k}, q_{h,k} \rangle \phi_{v,k}, \quad \langle \phi'_{e,k}, q_{h,k} \rangle = q_{h,k}(z_v).
\]

We have

\[
\nabla_k \phi_{v,k}(x) = e^{-ik \cdot (x-z_v)} \nabla \phi_{v,0}(x)
\]

\[
\nabla_k \times \psi_{e,k}(x) = e^{-ik \cdot (x-z_e)} \nabla \times \psi_{e,0}(x)
\]

\[
\nabla_k \cdot \psi_{e,k}(x) = e^{-ik \cdot (x-z_e)} \nabla \cdot \psi_{e,0}(x)
\]

\[
a_k(\psi_{e1,k}, \psi_{e2,k}) = e^{ik \cdot (z_{e1} - z_{e2})} a_0(\psi_{e1,0}, \psi_{e2,0})
\]

\[
m(\psi_{e1,k}, \psi_{e2,k}) = e^{ik \cdot (z_{e1} - z_{e2})} m(\psi_{e1,0}, \psi_{e2,0})
\]

\[
b_k(\psi_{e,k}, \phi_{v,k}) = e^{ik \cdot (z_{e} - z_{v})} b_0(\psi_{e,0}, \phi_{v,0})
\]

\[
c_k(\phi_{v1,k}, \phi_{v2,k}) = e^{ik \cdot (z_{v1} - z_{v2})} c_0(\phi_{v1,0}, \phi_{v2,0})
\]
Finite Element Convergence

The finite element spaces $X_{h,k}$, $Q_{h,k}$, and $V_{h,k}$ satisfy

- **Ellipticity on $V_{h,k}$**
  There exists $C > 0$ s.t.
  \[
  a_k(u_{h,k}, u_{h,k}) \geq C \|u_{h,k}\|_{L^2}^2 \quad \text{for all } u_{h,k} \in V_{h,k}.
  \]

- **Weak approximability of $Q$**
  There exists $\rho_1(h) > 0$, tending to zero as $h$ goes to zero such that
  \[
  \sup_{v_{h,k} \in V_{h,k}} \frac{b_k(v_{h,k}, q)}{\|v_{h,k}\|_{\text{curl}}} \leq \rho_1(h) \|q\|_{H^1} \quad \text{for all } q \in Q.
  \]

- **Strong approximability of $V$**
  For some $r > 0$ there exists $\rho_2(h) > 0$, tending to zero as $h$ goes to zero such that for any $u \in V \cap H^{1+r}(\Omega, \mathbb{C}^3)$ there exists $u_{h,k} \in V_{h,k}$ satisfying
  \[
  \|u - u_{h,k}\|_{\text{curl}} \leq \rho_2(h) \|u\|_{H^{1+r}}.
  \]

**Theorem** Let $(u, \lambda)$ a solution of the continuous eigenvalue problem, and let $(u_{h,k}, \lambda_{h,k})$ be the corresponding discrete solution. Then, we have

\[
(u_{h,k}, \lambda_{h,k}) \rightarrow (u, \lambda) \quad \text{for} \quad h \rightarrow 0.
\]

(Boffi-Conforti-Gastaldi 2006)
The Projection

For $u_{h,k} \in X_{h,k}$ we construct $p_{h,k} \in Q_{h,k}$ such that $u_{h,k} - \nabla_k p_{h,k} \in V_{h,k}$, i.e.,

$$0 = b_k(u_{h,k} - \nabla_k p_{h,k}, q_{h,k})$$
$$= b_k(u_{h,k}, q_{h,k}) - c_k(p_{h,k}, q_{h,k})$$

for all $q_{h,k} \in Q_{h,k}$

Thus, we have $B_{h,k} u_{h,k} = C_{h,k} p_{h,k}$ and $u_{h,k} = S_{h,k} p_{h,k}$ with operators

- "div": $B_{h,k} : X_{h,k} \rightarrow Q'_{h,k}$ is defined by
  $$\langle B_{h,k} v_{h,k}, \phi_{v,k} \rangle = b_k(v_{h,k}, \phi_{v,k}), \quad v \in V_h$$

- "Laplace": $C_{h,k} : Q_{h,k} \rightarrow Q'_{h,k}$ is defined by
  $$\langle C_{h,k} q_{h,k}, \phi_{v,k} \rangle = c_k(q_{h,k}, \phi_{v,k}), \quad v \in V_h$$

- "grad": $S_{h,k} : Q_{h,k} \rightarrow X_{h,k}$ is given by nodal evaluation

$$S_{h,k} q_{h,k} = \sum_{e=(x_e,y_e) \in E_h} (q_{h,k}(y_e)e^{i k \cdot (y_e - z_e)} - q_{h,k}(x_e)e^{i k \cdot (x_e - z_e)}) \psi_{e,k}.$$  

This defines a projection

$$P_{h,k} = \text{id} - S_{h,k} \circ C_{h,k}^{-1} \circ B_{h,k} : X_{h,k} \rightarrow V_{h,k}.$$  

(special care is required for $k = 0$)
Modified LOBPCG Method (including projection)

Let $T_{h,k} : X'_{h,k} \longrightarrow X_{h,k}$ be a preconditioner for $A^\delta_{h,k} = A_{h,k} + \delta M_{h,k} : X_{h,k} \longrightarrow X'_{h,k}$.

S0) Choose randomly $u^1_{h,k}, \ldots, u^N_{h,k} \in X_{h,k}$. Compute $v^n_{h,k} = P_{h,k} u^n_{h,k} \in V_{h,k}$.

S1) Ritz-step: Set up Hermitian matrices

$$\hat{A} = \left( a_k(v^m_{h,k}, v^n_{h,k}) \right)_{m,n=1,\ldots,N}, \quad \hat{M} = \left( m(v^m_{h,k}, v^n_{h,k}) \right)_{m,n=1,\ldots,N} \in \mathbb{C}^{N \times N}$$

and solve the matrix eigenvalue problem $\hat{A} \hat{z}^n = \lambda^n \hat{M} \hat{z}^n$.

S2) Compute $y^n_{h,k} = \sum_{n=1}^{N} \hat{z}^n_m v^n_{h,k} \in V_{h,k}$.

S3) Compute $r^n_{h,k} = A_{h,k} y^n_{h,k} - \lambda^n M_{h,k} y^n_{h,k} \in X'_{h,k}$, check for convergence.

S4) Compute $u^n_{h,k} := T_{h,k} r^n_{h,k} \in X_{h,k}$ and $w^n_{h,k} = P_{h,k} u^n_{h,k} \in V_{h,k}$.

S5) Perform Ritz-step for $\{v^1_{h,k}, \ldots, v^N_{h,k}, w^1_{h,k}, \ldots, w^N_{h,k} \} \subset V_{h,k}$ of size $2N$.

S6) Go to step S2).

The full algorithm uses orthogonalization, new random vectors, and a Ritz-step of size $3N$.

(the LOBPCG method was introduced by Knyazev 2001)
Multigrid Preconditioner for the Maxwell Operator

Let $X_{0,k} \subset X_{1,k} \subset \cdots \subset X_{J,k}$ be finite element space of mesh size $h_j = 2^{-j} h_0$. The multigrid preconditioner $T_{j,k} : X'_{j,k} \rightarrow X_{j,k}$ is defined recursively:

For $j = 0$, define $T_{0,k} = \left( A_0^\delta \right)^{-1}$.

For $j > 0$, the definition of $T_{j,k}$ requires:

1) a prolongation operator $I_{j,k} : X_{j-1,k} \rightarrow X_{j,k}$;
2) the adjoint operator $I'_{j,k} : X'_{j,k} \rightarrow X'_{j-1,k}$;
3) a smoother $R_{j,k} : X'_{j,k} \rightarrow X_{j,k}$ for $A_{j,k}$;
4) a smoother $D_{j,k} : Q'_{j,k} \rightarrow Q_{j,k}$ for $C_{j,k}$;
5) a transfer operator $S_{j,k} : Q_{j,k} \rightarrow X_{j,k}$;
6) the adjoint transfer operator $S'_{j,k} : X'_{j,k} \rightarrow Q'_{j,k}$.

Now, define $T_{j,k}$ by

$$\text{id} - A_j^\delta T_{j,k} = \left( \text{id} - A_j^\delta I_{j,k} T_{j-1,k} I'_{j,k} \right) \left( \text{id} - \delta^{-1} A_j^\delta S_{j,k} D_{j-1,k} S'_{j,k} \right) \left( \text{id} - A_j^\delta R_{j,k} \right).$$

(this multigrid variant was introduced and analyzed by Hiptmair 1998)
Eigenvalue Computation for a Photonic Crystal

We compute Block-Floquet modes for $\mathbf{k} = (3, 1, -1)$ in the unit cube $\Omega = (0, 1)^3$ with periodic boundary conditions

$$\nabla_k \times \varepsilon^{-1} \nabla_k \times \widetilde{H} = \lambda \widetilde{H}, \quad \nabla_k \cdot \widetilde{H} = 0.$$ 

Band structure of a photonic crystal

Eigenfunction – (Bloch-Floquet mode)

Calculation of the first 7 eigenvalues (≈ 1 million d.o.f.)

<table>
<thead>
<tr>
<th>N processor kernels</th>
<th>Total time</th>
<th>Speed up factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>32</td>
<td>5:11 min.</td>
<td>1.79</td>
</tr>
<tr>
<td>64</td>
<td>2:53 min.</td>
<td>1.85</td>
</tr>
<tr>
<td>128</td>
<td>1:33 min.</td>
<td>1.42</td>
</tr>
<tr>
<td>256</td>
<td>1:05 min.</td>
<td>1.39</td>
</tr>
<tr>
<td>512</td>
<td>0:47 min.</td>
<td></td>
</tr>
</tbody>
</table>

Calculation of the first 7 eigenvalues on 512 processor kernels

<table>
<thead>
<tr>
<th>Refinement level</th>
<th>d.o.f.</th>
<th>Total time</th>
<th>Scale up factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>( j = 4 )</td>
<td>13 872</td>
<td>00:18 min.</td>
<td>1.32</td>
</tr>
<tr>
<td>( j = 5 )</td>
<td>104 544</td>
<td>00:24 min.</td>
<td>1.91</td>
</tr>
<tr>
<td>( j = 6 )</td>
<td>811 200</td>
<td>00:47 min.</td>
<td>3.98</td>
</tr>
<tr>
<td>( j = 7 )</td>
<td>6 390 144</td>
<td>03:08 min.</td>
<td>6.85</td>
</tr>
<tr>
<td>( j = 8 )</td>
<td>50 725 632</td>
<td>21:31 min.</td>
<td></td>
</tr>
</tbody>
</table>

(every refinement level increases the problem size by a factor of 8)
Photonic Crystals: Eigenvalue Convergence

Calculation of the first 7 eigenfunctions (up to $\approx 50$ million d.o.f.)

<table>
<thead>
<tr>
<th>$j$</th>
<th>$\lambda_1^j$</th>
<th>$\lambda_2^j$</th>
<th>$\lambda_3^j$</th>
<th>$\lambda_4^j$</th>
<th>$\lambda_5^j$</th>
<th>$\lambda_6^j$</th>
<th>$\lambda_7^j$</th>
</tr>
</thead>
</table>

Convergence of the first 7 eigenfunctions measured by $\frac{|\lambda_{n+1}^j - \lambda_n^j|}{|\lambda_n^j - \lambda_{n-1}^j|}$

| $\lambda_n^4 - \lambda_n^3$ | 0.0369 0.0361 0.4587 0.5177 1.0338 0.9227 0.9192 |
|-----------------------------|---------|---------|---------|---------|---------|---------|---------|
| $\lambda_n^5 - \lambda_n^4$ | 0.0139 0.0139 0.1288 0.1459 0.3534 0.2115 0.2108 |
| $\lambda_n^6 - \lambda_n^5$ | 0.0052 0.0052 0.0384 0.0435 0.1049 0.0620 0.0566 |
| $\lambda_n^7 - \lambda_n^6$ | 0.0019 0.0019 0.0120 0.0137 0.0330 0.0183 0.0162 |
| $\lambda_n^8 - \lambda_n^7$ | 0.0007 0.0006 0.0038 0.0044 0.0109 0.0056 0.0049 |
Photonic Crystals: Eigenmodes

Illustration of an isosurface of the field intensity and the field directions.
Band Gap Verification

Analytically, it can be shown that photonic crystals with band gaps exist (by asymptotic investigations).

Numerically, one can check a given photonic crystals for band gap candidates.

Our aim is—combining analysis and numerics—to provide a rigorous proof for the existence of a band gap for a specific test configuration.

This requires the following techniques:

- Close finite element approximations of eigenmodes.
- Upper spectral bounds (Rayleigh-Ritz).
- Lower spectral bounds (Weinstein, Lehmann/Goerisch).
- Spectral exclosure for perturbed operators (Hoang, Plum).
- Spectral homotopy (Goerisch, Plum).
Polarized Waves in 2D

Now, we consider the Maxwell eigenvalue problem for the electric field $E$

$$\nabla \times \nabla \times E = \lambda \varepsilon E, \quad \nabla \cdot \varepsilon E = 0$$

in special case that $\varepsilon$ is periodic in $x_1$ and $x_2$, constant in $x_3$ and that the wave $E = (0, 0, u)$ is polarized, which leads to the Helmholtz problem

$$-\Delta u = \lambda \varepsilon u.$$

We compute in the periodicity cell $\Omega$ for finitely many $k$ in the Brillouin zone

$$(u_{k,n}, \lambda_{k,n}) \in H_{\text{per}}^1(\Omega) \times \mathbb{R} : \int_{\Omega} \nabla_k u_{k,n} \cdot \nabla \bar{v} \, dx = \lambda_{k,n} \int_{\Omega} \varepsilon u_{k,n} \bar{v} \, dx, \quad v \in H_{\text{per}}^1(\Omega)$$

($n = 1, \ldots, N$) with guaranteed accuracy.
A Candidate

We set \( \epsilon(x) = 1 \) for \( x \in [1/16, 15/16]^2 \) and \( \epsilon(x) = 5 \) else. By symmetry we have the same spectrum for \( \mathbf{k} = (k_1, k_2), (\pi - k_1, k_2), (k_1, \pi - k_2), \ldots \).
A Candidate

\[ \lambda_{k,n}(\pi/2, \pi/2), (\pi, \pi), (\pi, \pi/2), (\pi, 0), (\pi/2, 0), (0, 0) \]

The diagram shows the eigenvalues \( \lambda_{k,1}, \ldots, \lambda_{k,6} \) along the test path \( k \in P \subset K \). The band gap is indicated by the yellow horizontal line.
A Candidate

eigenvalue $\lambda_{k,3}$ for all $k \in K$
A Candidate

eigenvalue $\lambda_{k,4}$ for all $k \in K$
eigenvalues $\lambda_{k,1}, \ldots, \lambda_{k,5}$ for all $k \in K$
A Candidate

Bloch modes \( u_{k,1}, \ldots, u_{k,6} \) for \( k = (\pi, \pi) \)
Upper Spectral Bounds (Ritz-Galerkin)

Theorem

For eigenfunction approximations $\tilde{u}_{k,1}, \ldots, \tilde{u}_{k,N} \in H^1(\Omega/\Lambda, \mathbb{C})$ define

$$A = \left( a_k(\tilde{u}_{k,m}, \tilde{u}_{k,n}) \right)_{m,n=1,\ldots,N},$$

$$B = \left( \langle \tilde{u}_{k,m}, \tilde{u}_{k,n} \rangle_\rho \right)_{m,n=1,\ldots,N} \in \mathbb{C}^{N,N}$$

and let

$$\psi_{k,1} \leq \psi_{k,2} \leq \cdots \leq \psi_{k,N}$$

be the eigenvalues of the problem $A x = \psi B x$. Then we have

$$\lambda_{k,n} \leq \psi_{k,n}, \quad n = 1, \ldots, N.$$
Lower Spectral Bounds (Lehmann-Goerisch)

**Theorem**

Let $\gamma > 0$. For eigenfunction approximations $\tilde{u}_{k,n} \in V$ and scaled dual approximations $\hat{\sigma}_{k,n} \approx \frac{1}{\gamma + \lambda_{k,n}} \nabla_k \tilde{u}_{k,n} \in W$ define

$$
\begin{align*}
S &= \left( \left\langle \hat{\sigma}_{k,m}, \hat{\sigma}_{k,n} \right\rangle \right)_{m,n=1,...,N}, \\
T &= \frac{1}{\gamma} \left( \left\langle \tilde{u}_{k,m} + \frac{1}{\rho} \nabla_k \cdot \hat{\sigma}_{k,m}, \tilde{u}_{k,n} + \frac{1}{\rho} \nabla_k \cdot \hat{\sigma}_{k,n} \right\rangle \right)_{m,n=1,...,N}.
\end{align*}
$$

If $\beta > \gamma$ satisfies $\beta - \gamma \leq \lambda_{k,N+1}$, if $N = A + (\gamma - 2\beta)B + \beta^2(S + T)$ is positive definite, and if the eigenvalues

$$
\theta_1 \geq \theta_2 \geq \cdots \geq \theta_N
$$

of the eigenvalue problem

$$
\left( A + (\gamma - \beta)B \right) x = \theta \, N \, x
$$

are negative, we have the lower eigenvalue bound

$$
\beta - \gamma - \beta \frac{1}{1 - \theta_n} \leq \lambda_{n,k}, \quad n = 1, \ldots, N.
$$

Remark: A suitable $\beta$ is obtained by a spectral homotopy.
**Eigenvalue Exclosure by Perturbation Analysis**

**Theorem**
For some \( \lambda_{\text{gap}} \), \( n > 1 \), and \( k \in K \) assume that \( \delta > 0 \) exits such that

\[
\lambda_{k,n-1} + \delta < \lambda_{\text{gap}} < \lambda_{k,n} - \delta.
\]

Then we have

\[
\lambda_{k+h,n-1} < \lambda_{\text{gap}} < \lambda_{k+h,n}
\]

for all \( h \in \mathbb{R}^2 \) with

\[
|h| < \sqrt{\min_{x \in \Omega} \varepsilon(x)} \left( \sqrt{\lambda_{k,n} + \delta} - \sqrt{\lambda_{k,n}} \right).
\]

For the application we compute a guaranteed lower bound \( \lambda_{k,n,\inf} \leq \lambda_{k,n} \) and upper bounds \( \lambda_{k,n-1,\sup} \geq \lambda_{k,n-1}, \lambda_{k,n,\sup} \geq \lambda_{k,n} \), and

\[
r_k = \sqrt{\min_{x \in \Omega} \varepsilon(x)} \left( \sqrt{\lambda_{k,n,\sup} + \delta} - \sqrt{\lambda_{k,n,\sup}} \right).
\]

This ensures that the interval \((\lambda_{k,n-1,\sup} + \delta, \lambda_{k,n,\inf} - \delta)\) is contained in the resolvent set of the elliptic operator associated to the eigenvalue problem for all \( k' \in \text{Ball}(k, r_k) \).
This figure illustrates Brillouin vectors

\[ \mathbf{k}' \in \bigcup_{\mathbf{k} \in \mathcal{K}} \text{Ball} (\mathbf{k}, r_{\mathbf{k}}) \]

where \( \lambda_{\text{gap}} \in (18.2, 18.25) \) is not a spectral value.

By symmetry this proves that for all \( \mathbf{k} \in K \) the existence of a band gap

\[ (18.2, 18.25) \subset (\lambda_{\text{max},3}, \lambda_{\text{min},4}) \]

for the eigenvalue problem \(-\Delta u = \lambda \varepsilon u \) in \( \mathbb{R}^2 \).

The proof requires the close approximation of more than 5000 eigenvalues and eigenfunctions (for 100 vectors \( k \in \mathcal{K} \) and for a homotopy to bound the rest of the spectrum) and takes about 90 h computing time.
Towards the Optimal Design of Photonic Crystals

Assume that for a given periodic electric permittivity $\varepsilon^0$ a band gap exists, i.e., for some $\lambda_{\text{gap}} \in \mathbb{R}$ and some $n > 1$ we have

$$\lambda_{n-1,k}(\varepsilon^0) < \lambda_{\text{gap}} < \lambda_{n,k}(\varepsilon^0), \quad k \in K.$$ 

The purpose is to find a material distribution $\varepsilon_0 \leq \varepsilon(x) \leq \varepsilon_1$ such that

$$g(\varepsilon) = \min_{k \in K} \{\lambda_{\text{gap}} - \lambda_{n-1,k}(\varepsilon), \lambda_{n,k}(\varepsilon) - \lambda_{\text{gap}}\}$$

is maximal.

Numerically, this can be approximated by a subgradient method defining $\varepsilon^1, \varepsilon^2, \varepsilon^3, \ldots$ by

$$0 \in g(\varepsilon^{m-1}) + \langle \partial g(\varepsilon^{m-1}), \varepsilon^m - \varepsilon^{m-1} \rangle, \quad m = 1, 2, 3, \ldots$$

Here, $\partial g(\varepsilon)$ can be evaluated explicitly by the computation of eigenmodes.

(Realized in 2-d by Cox/Dobson 1999)
Towards the Optimal Design of Photonic Crystals

initial band gap: 0.0444

result after 1150 optimization steps (subgradient method)

optimized band gap: 0.0444