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A computer-assisted proof for photonic band gaps

Vu Hoang, Michael Plum, and Christian Wieners (March 13, 2008)

ABSTRACT. We investigate photonic crystals, modeled by a spectral problem for Maxwell's equations with periodic electric permittivity. Here, we specialize to a two-dimensional situation and to polarized waves. By Floquet-Bloch theory, the spectrum has band-gap structure, and the bands are characterized by families of eigenvalue problems on a periodicity cell, depending on a parameter k varying in the Brillouin zone K . We propose a computer-assisted method for proving the presence of band gaps: For k in a finite grid in K , we obtain eigenvalue enclosures by variational methods supported by finite element computations, and then capture all $k \in K$ by a perturbation argument.

1. Introduction

A photonic crystal is a material with periodic dielectric structure. It is well known (see [10, 11, 6]) that the propagation of electromagnetic waves in photonic crystals exhibits *band-gap* behavior, i. e., light whose frequency falls into a band-gap cannot propagate inside the material. For applications, it is interesting to design structures having band-gaps; however, the task of predicting and proving the existence of gaps is, from an purely analytical viewpoint, extremely difficult and tedious; see [5]. In this paper, we propose a *computer-assisted* method for proving the existence of band-gaps.

We consider a mathematical model for two-dimensional photonic crystals. This model arises as follows: we start with the homogeneous Maxwell's equations (in dimensionless form)

$$\operatorname{curl} E = -\frac{\partial B}{\partial t}, \quad \operatorname{curl} H = \frac{\partial D}{\partial t}, \quad \operatorname{div} B = 0, \quad \operatorname{div} D = 0,$$

together with the constitutive relations

$$D = \varepsilon E, \quad B = \mu H.$$

Here, E, H, D, B denote the electric field, the magnetic field, the displacement field and the magnetic induction field, respectively. ε is the electric permittivity, and μ the magnetic permeability.

In the context of photonic crystals, we assume $\mu = 1$, and $\varepsilon(x)$ to be a *periodic* function in space, i. e., there exist linearly independent vectors, $a_1, a_2 \in \mathbf{R}^2$ such that $\varepsilon(x + a_j) = \varepsilon(x)$ for $x \in \mathbf{R}^2$, $j = 1, 2$. We will call the parallelogram Ω spanned by a_1, a_2 a *periodicity cell* of ε or of the associated lattice $\mathbf{Z}a_1 + \mathbf{Z}a_2 \subset \mathbf{R}^2$. Furthermore, we assume that $0 < \varepsilon_{\min} \leq \varepsilon(x) \leq \varepsilon_{\max}$ for $x \in \mathbf{R}^2$.

Looking for *monochromatic* waves

$$E(x, t) = e^{i\omega t} E(x), \quad H(x, t) = e^{i\omega t} H(x)$$

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we obtain the time-harmonic Maxwell's equations

$$\operatorname{curl} E = -i\omega H, \quad \frac{1}{\varepsilon} \operatorname{curl} H = i\omega E, \quad \operatorname{div} H = 0, \quad \operatorname{div}(\varepsilon E) = 0,$$

and applying curl to the first two equations gives two decoupled systems:

$$\operatorname{curl} \operatorname{curl} E = \omega^2 \varepsilon E, \quad \operatorname{div}(\varepsilon E) = 0$$

and

$$\operatorname{curl} \frac{1}{\varepsilon} \operatorname{curl} H = \omega^2 H, \quad \operatorname{div} H = 0.$$

Further specializing to a 2D-situation, we suppose $\varepsilon = \varepsilon(x_1, x_2)$, and look for *polarized* waves

$$E = (0, 0, u).$$

The divergence condition on E implies $u = u(x_1, x_2)$; thus, $\operatorname{curl} \operatorname{curl} E = (0, 0, -\Delta u)$, whence the first equation for E reads, with $\lambda = \omega^2$,

$$-\Delta u = \lambda \varepsilon u \text{ on } \mathbf{R}^2.$$

We realize this spectral problem in the Hilbert space $L_2(\mathbf{R}^2)$, with inner product weighted by ε , using the self-adjoint operator A defined by

$$D(A) := H^2(\mathbf{R}^2), \quad Au := -\frac{1}{\varepsilon} \Delta u. \quad (1)$$

Applying *Floquet-Bloch* theory to this operator we obtain the *band-gap* structure of the spectrum $\sigma(A)$ of A . More precisely, we have

$$\sigma(A) = \bigcup_{n \in \mathbf{N}} I_n, \quad (2)$$

where I_n are compact real intervals with $\min I_n \rightarrow \infty$ as $n \rightarrow \infty$. I_n is called the *n*-th *spectral band* [10, 11, 13]. Although “usually” the bands I_n overlap there *might* be gaps between them; these are the band-gaps of prohibited frequencies mentioned earlier. Floquet-Bloch theory further gives

$$I_n = \{\lambda_{k,n} : k \in K\} = [\min_{k \in K} \lambda_{k,n}, \max_{k \in K} \lambda_{k,n}],$$

where K is the *Brillouin zone* (a compact set in \mathbf{R}^2 , determined by Floquet-Bloch theory, and depending only on the periodicity cell Ω of ε), and $\lambda_{k,n}$ is the *n*-th eigenvalue of the problem

$$-(\nabla + ik) \cdot (\nabla + ik)u = \lambda \varepsilon u \text{ on } \Omega, \text{ with periodic boundary conditions on } \partial\Omega. \quad (3)$$

$\lambda_{\cdot,n}$ is called the *n*-th branch of the *dispersion relation*.

In our two-dimensional situation (in contrast to the one-dimensional case), no additional, more direct analytical characterization of I_n is known. Nevertheless, one can try to obtain information about the band structure (for a specific dielectric function ε) simply by choosing a finite grid in the Brillouin zone and then computing $\lambda_{k,1}, \dots, \lambda_{k,N}$ *numerically* for k in the grid. One might then find numerical evidence for a gap. If so, we propose the following strategy for *proving* the existence of a spectral gap by computer-assistance: we compute *verified* eigenvalue enclosures for $\lambda_{k,1}, \dots, \lambda_{k,N}$ (N chosen fixed) for k in the *grid*. Using a perturbation argument we are then able to deduce also enclosures for $\lambda_{k,1}, \dots, \lambda_{k,N}$ for k *between* grid-points. If the grid is sufficiently fine and our eigenvalue enclosures are sufficiently accurate (see below) we can rigorously prove the existence of a gap.

2. Formulation of the spectral problem

For the periodic lattice $\Lambda := \mathbf{Z}a_1 + \mathbf{Z}a_2$ we define the space

$$H^1(\mathbf{R}^2/\Lambda) = \left\{ u \in H^1_{\text{loc}}(\mathbf{R}^2) : u(x+y) = u(x) \text{ for all } y \in \Lambda \text{ and a.e. } x \in \Omega \right\}$$

of periodic H^1 -functions in \mathbf{R}^2 , and for a periodicity cell $\Omega \subset \mathbf{R}^2$ of Λ we consider the space

$$H^1_{\text{per}}(\Omega) = \left\{ u|_{\Omega} : u \in H^1(\mathbf{R}^2/\Lambda) \right\}$$

(containing periodic boundary conditions on $\partial\Omega$). Every function $u \in H^1(\mathbf{R}^2/\Lambda)$ is uniquely defined by its restriction $u|_{\Omega} \in H^1_{\text{per}}(\Omega)$. The corresponding Brillouin zone $K \subset \mathbf{R}^2$ is a periodicity cell of the dual lattice $\Lambda' = \{y' \in \mathbf{R}^2 : y \cdot y' \in 2\pi\mathbf{Z} \text{ for all } y \in \Lambda\}$. More precisely, K is the set of all $y' \in \mathbf{R}^2$ which are closer to zero than to every other point of Λ' .

In order to study the spectrum of the operator A introduced in (1), we are led, by Floquet-Bloch theory, to the family of eigenvalue problems (3), which are realized by the family of operators A_k given by

$$\begin{aligned} D(A_k) &:= H^2(\Omega) \cap H^1_{\text{per}}(\Omega), \\ A_k u &:= -\frac{1}{\varepsilon}(\nabla + ik) \cdot (\nabla + ik)u = \frac{1}{\varepsilon} \left[-\Delta u - 2ik \cdot \nabla u + |k|^2 u \right] \end{aligned}$$

for every $k \in K$. Each A_k is self-adjoint in $L_2(\Omega)$ with respect to the weighted inner product

$$\langle u, v \rangle_{\varepsilon} = \int_{\Omega} \varepsilon u \bar{v} dx$$

with associated norm $\|\cdot\|_{\varepsilon}$. Furthermore, A_k has a compact resolvent and therefore a discrete spectrum

$$\sigma(A_k) = \{\lambda_{k,n} : n \in \mathbf{N}\}.$$

Floquet-Bloch theory further gives (compare (2))

$$\sigma(A) = \bigcup_{k \in K} \sigma(A_k) = \bigcup_{n \in \mathbf{N}} [\lambda_{\min,n}, \lambda_{\max,n}],$$

with $\lambda_{\min,n} = \min_{k \in K} \lambda_{k,n}$, $\lambda_{\max,n} = \max_{k \in K} \lambda_{k,n}$. Our aim is to prove the existence of a spectral gap, i. e., to find some $m \in \mathbf{N}$ such that

$$\lambda_{\max,m-1} < \lambda_{\min,m},$$

by providing guaranteed bounds for $\lambda_{\max,m-1}$ and $\lambda_{\min,m}$.

Mainly for numerical purposes (more precisely, in order to avoid the necessity for numerical basis functions in $H^2(\Omega)$), we also consider the weak formulation of the eigenvalue problem $A_k u = \lambda u$, which reads

$$a_k(u, v) = \lambda \langle u, v \rangle_{\varepsilon}, \quad v \in H^1_{\text{per}}(\Omega), \quad (4)$$

where

$$a_k(u, v) := \int_{\Omega} \nabla_k u \cdot \overline{\nabla_k v} dx \quad (u, v \in H^1_{\text{per}}(\Omega)), \quad \nabla_k u := \nabla u + ik u.$$

The associated energy norm (respectively semi-norm if $k = 0$) is denoted by $\|v\|_k = \sqrt{a_k(u, u)}$.

3. Eigenvalue bounds

In this section we summarize enclosure results for eigenvalues of A_k (or of the variational problem (4)), where $k \in K$ is *fixed*. The enclosures are obtained by computing approximations and by providing explicit error bounds. We first compute numerical Rayleigh-Ritz approximations $(\tilde{\lambda}_{k,n}, \tilde{u}_{k,n}) \in \mathbf{R} \times \tilde{V}$ (for $n = 1, \dots, N$) of the discrete problem

$$a_k(\tilde{u}, \tilde{v}) = \tilde{\lambda} \langle \tilde{u}, \tilde{v} \rangle_\varepsilon \quad \text{for all } \tilde{v} \in \tilde{V},$$

where $\tilde{V} \subset H_{\text{per}}^1(\Omega)$ is a finite dimensional subspace, $N \in \mathbf{N}$ is chosen fixed, $N \leq \dim \tilde{V}$. We assume that $\tilde{u}_{k,1}, \dots, \tilde{u}_{k,N}$ are linearly independent.

Upper bounds for the first N eigenvalues are directly obtained from the approximations by the Rayleigh-Ritz method based on Poincaré's min-max principle:

THEOREM 1. *Define the hermitian matrices*

$$\mathbf{A} = \left(a_k(\tilde{u}_{k,m}, \tilde{u}_{k,n}) \right)_{m,n=1,\dots,N}, \quad \mathbf{B} = \left(\langle \tilde{u}_{k,m}, \tilde{u}_{k,n} \rangle_\varepsilon \right)_{m,n=1,\dots,N} \in \mathbf{C}^{N,N},$$

and let

$$\Lambda_{k,1} \leq \Lambda_{k,2} \leq \dots \leq \Lambda_{k,N}$$

be the eigenvalues of the matrix eigenvalue problem $\mathbf{A}\mathbf{x} = \Lambda \mathbf{B}\mathbf{x}$. Then,

$$\lambda_{k,n} \leq \Lambda_{k,n}, \quad n = 1, \dots, N.$$

For a proof, see [14].

Lower bounds for eigenvalues can be obtained by a dual approach due to Goerisch, if a certain spectral separation parameter β is known (see the following Theorem 2, and the subsequent remarks), and if dual approximations

$$\tilde{\sigma}_{k,n} \approx \nabla_k \tilde{u}_{k,n}, \quad \tilde{\sigma}_{k,n} \in H(\text{div}_k, \Omega) := \{\tau \in L_2(\Omega)^2 : \nabla_k \cdot \tau \in L_2(\Omega)\}$$

have been computed in addition.

THEOREM 2. *Let $\gamma > 0$ be an arbitrary shift parameter.*

For scaled dual approximations $\hat{\sigma}_{k,n} := \frac{1}{\lambda_{k,n} + \gamma} \tilde{\sigma}_{k,n}$, $n = 1, \dots, N$, define

$$\begin{aligned} \mathbf{S} &:= \left(\langle \hat{\sigma}_{k,m}, \hat{\sigma}_{k,n} \rangle \right)_{m,n=1,\dots,N} \in \mathbf{C}^{N,N}, \\ \mathbf{T} &:= \frac{1}{\gamma} \left(\langle \tilde{u}_{k,m} + \frac{1}{\varepsilon} \nabla_k \cdot \hat{\sigma}_{k,m}, \tilde{u}_{k,n} + \frac{1}{\varepsilon} \nabla_k \cdot \hat{\sigma}_{k,n} \rangle_\varepsilon \right)_{m,n=1,\dots,N} \in \mathbf{C}^{N,N}. \end{aligned}$$

If $\beta \in \mathbf{R}$ satisfies

$$0 < \beta \leq \lambda_{k,N+1} + \gamma, \tag{5}$$

if the matrix $\mathbf{P} := \mathbf{A} + (\gamma - 2\beta)\mathbf{B} + \beta^2(\mathbf{S} + \mathbf{T})$ is positive definite, and if the eigenvalues

$$\theta_1 \geq \theta_2 \geq \dots \geq \theta_N$$

of the eigenvalue problem

$$\left(\mathbf{A} + (\gamma - \beta)\mathbf{B} \right) \mathbf{x} = \theta \mathbf{P}\mathbf{x} \tag{6}$$

are negative, we have the lower eigenvalue bounds

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

PROOF. The result is a direct consequence of the general Goerisch-Theorem on lower eigenvalue bounds (see, e. g., [2, Theorem 5]), applied to the shifted eigenvalue problem

$$a_k(u, v) + \gamma \langle u, v \rangle_\varepsilon = (\lambda + \gamma) \langle u, v \rangle_\varepsilon, \quad v \in H_{\text{per}}^1(\Omega).$$

This theorem requires the choice of a vector space X , a sesquilinear form b on X , and a linear operator $T : H_{\text{per}}^1(\Omega) \rightarrow X$. Here, we use

$$X := L_2(\Omega)^3, \quad b(w, z) := \int_{\Omega} (w_1 \bar{z}_1 + w_2 \bar{z}_2 + \gamma \varepsilon w_3 \bar{z}_3) dx, \quad T(u) := (\nabla_k u, u).$$

Note that, for $n = 1, \dots, N$,

$$w_n := \left(\hat{\sigma}_{k,n}, \frac{1}{\gamma} \left[\tilde{u}_{k,n} + \frac{1}{\varepsilon} \nabla_k \cdot \hat{\sigma}_{k,n} \right] \right) \in X$$

satisfies $b(w_n, T\varphi) = \langle \tilde{u}_{k,n}, \varphi \rangle_\varepsilon$ ($\varphi \in H_{\text{per}}^1(\Omega)$) as needed, and that $(b(w_m, w_n))_{m,n=1,\dots,N} = \mathbf{S} + \mathbf{T}$. \square

REMARK 3. The application of Theorem 2 requires some care; thus we shortly comment on practical aspects for our specific problem.

- a) The choice of a suitable spectral separation parameter β is more problematic than indicated by (5), because in fact we need, much stronger than (5), that

$$\Lambda_{k,N} + \gamma < \beta \leq \lambda_{k,N+1} + \gamma \tag{7}$$

(with $\Lambda_{k,N}$ defined in Theorem 1), in order to obtain *negative* eigenvalues $\theta_1, \dots, \theta_N$ of problem (6) as required. Note that the matrix on the left-hand side of (6) is negative definite if and only if $\Lambda_{k,N} + \gamma < \beta$.

In our application of Theorem 2, however, we check (5) and the negativity of $\theta_1, \dots, \theta_N$, instead of checking (7), in order to avoid the computation of $\Lambda_{k,N}$.

For the construction of β , we use a spectral homotopy method explained in the next section.

- b) The condition of the matrix \mathbf{P} being positive definite (required in Theorem 2) is usually not critical. It is satisfied, for example, if $\beta - \gamma$ is not an eigenvalue of problem (4) (i. e., if equality is avoided in (7)). In numerical practice, positive definiteness of \mathbf{P} is of course checked directly during the verified solution of problem (6).
- c) If N is chosen suitably, we do not need lower bounds for all eigenvalues $\lambda_{k,1}, \dots, \lambda_{k,N}$, but only for $\lambda_{k,N-\ell}, \dots, \lambda_{k,N}$ with some “small” $\ell \in \mathbf{N}_0$, usually even only for $\ell = 0$. For this reduced task, a slightly different application of Goerisch’s general theorem can be used which requires the verified solution of an $(\ell + 1) \times (\ell + 1)$ matrix eigenvalue problem only, rather than the $N \times N$ problem (6). Nevertheless we used the “full” Theorem 2 because the quality of its lower bounds is usually better than for the $(\ell + 1) \times (\ell + 1)$ version, and since N is not too large (≈ 10) anyway in our applications.
- d) In order to obtain close bounds, the dual approximation $\tilde{\sigma}_{k,n} \in H(\text{div}_k, \Omega)$ has to be computed such that both defects, $\nabla_k \tilde{u}_{k,n} - \tilde{\sigma}_{k,n}$ and $\tilde{\lambda}_{k,n} \tilde{u}_{k,n} + \frac{1}{\varepsilon} \nabla_k \cdot \tilde{\sigma}_{k,n}$ are small. Practically we proceed as follows: given $(\tilde{\lambda}_{k,n}, \tilde{u}_{k,n}) \in \mathbf{R} \times \tilde{V}$, we search an approximate minimizer $\tilde{\sigma}_{k,n} \in \tilde{W}$ (with $\tilde{W} \subset H(\text{div}_k, \Omega)$ denoting some suitable finite dimensional approximation subspace) of the functional

$$J_{k,n}(\tilde{\sigma}) = \frac{1}{2} \|\tilde{\sigma} - \nabla_k \tilde{u}_{k,n}\|^2 + \frac{c}{2} \|\tilde{\lambda}_{k,n} \tilde{u}_{k,n} + \frac{1}{\varepsilon} \nabla_k \cdot \tilde{\sigma}\|_\varepsilon^2$$

(with a suitable parameter $c > 0$, and with $\|\cdot\|$ denoting the unweighted L_2 -norm), i. e., we solve the following linear problem for $\tilde{\sigma}_{k,n} \in \tilde{W}$:

$$\int_{\Omega} (\tilde{\sigma}_{n,k} - \nabla_k \tilde{u}_{k,n}) \cdot \tilde{\tau} + c \int_{\Omega} \varepsilon (\tilde{\lambda}_{k,n} \tilde{u}_{k,n} + \frac{1}{\varepsilon} \nabla_k \cdot \tilde{\sigma}_{k,n}) \nabla_k \cdot \tilde{\tau} dx = 0, \quad \tilde{\tau} \in \tilde{W}.$$

- e) The spectral shift $\gamma > 0$ can be chosen arbitrary; an optimal choice is not predictable analytically. We choose γ according to a strategy discussed in [3].
- f) In the computation of the entries of the matrices \mathbf{A} , \mathbf{B} , \mathbf{P} entering problem (6), we have to take care of all possible numerical errors, i. e., rounding errors (by *interval arithmetic*; see e.g. [7, 15]) and possibly also quadrature errors. Therefore, the matrix entries are usually complex *intervals*. For the verified solution of the matrix eigenvalue problem (6) (and also of the Rayleigh-Ritz problem $\mathbf{A}\mathbf{x} = \Lambda\mathbf{B}\mathbf{x}$) we thus need to handle interval matrices. Many approaches to this problem are known in numerical linear algebra (see, e.g., [1]). We use the following Lemma which is very simple in its application.

LEMMA 4. *Let $\mathcal{A}, \mathcal{B} \subset \mathbf{C}^{N,N}$ be Hermitian matrices with interval entries, and with \mathbf{B} positive definite for all $\mathbf{B} \in \mathcal{B}$. For some fixed Hermitian $\mathbf{A}_0 \in \mathcal{A}$, $\mathbf{B}_0 \in \mathcal{B}$, let $(\tilde{\lambda}_n, \tilde{\mathbf{x}}_n)$ ($n = 1, \dots, N$) denote approximate eigenpairs of $\mathbf{A}_0\mathbf{x} = \lambda\mathbf{B}_0\mathbf{x}$, with $\tilde{\mathbf{x}}_m^* \mathbf{B}_0 \tilde{\mathbf{x}}_n \approx \delta_{m,n}$. Suppose that, for some $r_0, r_1 > 0$,*

$$\|\mathbf{X}^* \mathbf{A} \mathbf{X} - \mathbf{X}^* \mathbf{B} \mathbf{X} \Lambda\|_{\infty} \leq r_0, \quad \|\mathbf{X}^* \mathbf{B} \mathbf{X} - \mathbf{I}\|_{\infty} \leq r_1, \quad \mathbf{A} \in \mathcal{A}, \mathbf{B} \in \mathcal{B},$$

where $\mathbf{X} = (\tilde{\mathbf{x}}_1, \dots, \tilde{\mathbf{x}}_N)$, $\Lambda = \text{diag}(\tilde{\lambda}_1, \dots, \tilde{\lambda}_N)$. If $r_1 < 1$, we have for all $\mathbf{A} \in \mathcal{A}$, $\mathbf{B} \in \mathcal{B}$ and all eigenvalues λ of $\mathbf{A}\mathbf{x} = \lambda\mathbf{B}\mathbf{x}$

$$\lambda \in \bigcup_{n=1}^N B(\tilde{\lambda}_n, r), \quad \text{where } r = \frac{r_0}{1 - r_1}, \quad \text{and } B(\lambda, r) = \{z \in \mathbf{C} : |z - \lambda| \leq r\}.$$

Moreover, each connected component of this union contains as many eigenvalues as midpoints $\tilde{\lambda}_i$.

PROOF. Since $r_1 < 1$, the matrix $\mathbf{X}^* \mathbf{B} \mathbf{X}$ is regular and we have $\|(\mathbf{X}^* \mathbf{B} \mathbf{X})^{-1}\|_{\infty} \leq \frac{1}{1 - r_1}$. Moreover the eigenvalue problem $\mathbf{A}\mathbf{x} = \lambda\mathbf{B}\mathbf{x}$ is equivalent to

$$\left(\Lambda + (\mathbf{X}^* \mathbf{B} \mathbf{X})^{-1} (\mathbf{X}^* \mathbf{A} \mathbf{X} - \mathbf{X}^* \mathbf{B} \mathbf{X} \Lambda) \right) \mathbf{y} = \lambda \mathbf{y}$$

(where $\mathbf{y} = \mathbf{X}^{-1}\mathbf{x}$), whence Gershgorin's Theorem gives the result. \square

Note that guaranteed bounds r_0 and r_1 can easily be computed (using interval arithmetic).

4. Spectral homotopy

For determining a spectral separation parameter β , as needed in Theorem 2, we consider the functions

$$\varepsilon_s(x) := (1 - s)\varepsilon_{\max} + s\varepsilon(x), \quad x \in \Omega, \quad 0 \leq s \leq 1,$$

and the family of eigenvalue problems

$$a_k(u, v) = \lambda \langle u, v \rangle_{\varepsilon_s}, \quad v \in H_{\text{per}}^1(\Omega), \quad (8)$$

where $0 \leq s \leq 1$, and with $k \in K$ still fixed as in the previous section. For $s \in [0, 1]$, let $(\lambda_n^{(s)})_{n \in \mathbf{N}}$ denote the sequence of eigenvalues of problem (8), ordered by magnitude. We observe the following simple facts:

i) For $s = 0$, problem (8) has constant coefficients. Thus, it is solvable in closed form if the parallelogram Ω is a *rectangle*. E. g., if $\Omega = (0, 1)^2$, as in our numerical example, the solutions are

$$\lambda_{(n_1, n_2)} = \frac{1}{\varepsilon_{\max}} \left((2\pi n_1 + k_1)^2 + (2\pi n_2 + k_2)^2 \right), \quad (9)$$

$$u_{(n_1, n_2)}(x) = \exp \left(2\pi i (n_1 x_1 + n_2 x_2) \right), \quad n_1, n_2 \in \mathbf{Z},$$

and the eigenvalues $\lambda_n^{(0)}$ are obtained from these by ordering according to magnitude.

ii) For $s = 1$, problem (8) coincides with our given problem (4), whence $\lambda_n^{(1)} = \lambda_{k,n}$ ($n \in \mathbf{N}$).
 iii) ε_s is decreasing in s , whence the Rayleigh quotient of problem (8) is increasing in s . Poincaré's min-max principle therefore implies that

$$\text{for each fixed } n \in \mathbf{N}, \lambda_n^{(s)} \text{ is increasing in } s. \quad (10)$$

We perform the following homotopy method along $s \in [0, 1]$, compare also [12, 4]. With $N \in \mathbf{N}$ denoting the number of eigenvalues we wish to enclose, we choose some $M > N$ such that there is a reasonable gap between $\lambda_{M-1}^{(0)}$ and $\lambda_M^{(0)}$. Suppose that for some $s_1 > 0$ approximations $\tilde{\lambda}_1^{(s_1)}, \dots, \tilde{\lambda}_{M-1}^{(s_1)}$ have been computed which *indicate* (not prove!) that

$$\lambda_{M-1}^{(s_1)} < \lambda_M^{(0)}. \quad (11)$$

Then, since $\lambda_M^{(0)} \leq \lambda_M^{(s_1)}$ by (10), we can apply Theorem 2 to problem (8) with $s = s_1$, with $M - 1$ instead of N , and with $\beta := \lambda_M^{(0)} + \gamma$. The conjecture (11) gives rise to the hope that the eigenvalues $\theta_1, \dots, \theta_N$ of the corresponding problem (6) are negative; compare Remark a) after Theorem 2. If they turn out indeed to be negative (according to the verified solution of problem (6)), Theorem 2 gives lower bounds

$$\mu_n^{(s_1)} \leq \lambda_n^{(s_1)}, \quad n = 1, \dots, M - 1. \quad (12)$$

Let s_1 be chosen “almost” maximal with the property that Theorem 2 successfully gives lower bounds $\mu_n^{(s_1)}$ as described above.

Now suppose first that $\mu_{M-2}^{(s_1)}$ and $\mu_{M-1}^{(s_1)}$ are “well separated”. Then we repeat the above procedure with s_1 in place of 0 and $M - 1$ instead of M : For some $s_2 > s_1$ (to be chosen “almost” maximal), we compute approximations $\tilde{\lambda}_1^{(s_2)}, \dots, \tilde{\lambda}_{M-2}^{(s_2)}$ which indicate that $\lambda_{M-2}^{(s_2)} < \mu_{M-1}^{(s_1)}$. Then, since $\mu_{M-1}^{(s_1)} \leq \lambda_{M-1}^{(s_1)} \leq \lambda_{M-1}^{(s_2)}$ by (12) and (10), we can apply Theorem 2 to problem (8) with $s = s_2$, with $M - 2$ instead of N , and with $\beta := \mu_{M-1}^{(s_1)} + \gamma$. If the θ -eigenvalues turn out to be negative (as expected), Theorem 2 gives lower bounds

$$\mu_n^{(s_2)} \leq \lambda_n^{(s_2)}, \quad n = 1, \dots, M - 2.$$

If $\mu_{M-2}^{(s_1)}$ and $\mu_{M-1}^{(s_1)}$ are *not* “well separated”, i. e., if they belong to a *cluster* $\mu_{M-L}^{(s_1)}, \dots, \mu_{M-1}^{(s_1)}$, but $\mu_{M-L-1}^{(s_1)}$ and $\mu_{M-L}^{(s_1)}$ are “well separated”, we choose $s_2 > s_1$ (“almost” maximal) and compute approximations $\tilde{\lambda}_1^{(s_2)}, \dots, \tilde{\lambda}_{M-L-1}^{(s_2)}$ indicating that $\lambda_{M-L-1}^{(s_2)} < \mu_{M-L}^{(s_1)}$. We apply Theorem 2 with $s = s_2$, $M - L - 1$ instead of N , and $\beta := \mu_{M-L}^{(s_1)} + \gamma$. In the successful case we obtain lower bounds

$$\mu_n^{(s_2)} \leq \lambda_n^{(s_2)}, \quad n = 1, \dots, M - L - 1.$$

We go on with this algorithm until $s_r = 1$ for some $r \in \mathbf{N}$ (or until the algorithm breaks down since no eigenvalue is left to continue with). With R denoting the total number of eigenvalues which had to be “dropped” during the algorithm according to the above description, we finally

obtain lower bounds

$$\mu_{k,n} = \mu_n^{(1)} \leq \lambda_n^{(1)} = \lambda_{k,n}, \quad n = 1, \dots, M - R,$$

and we are done if $M - R \geq N$.

In addition, we compute upper bounds $\Lambda_{k,1}, \dots, \Lambda_{k,N}$ by Theorem 1 (directly for problem (4), i. e., without any homotopy algorithm).

The condition $M - R \geq N$ is very likely to be satisfied if M is chosen such that $\lambda_M^{(0)} > \Lambda_{k,N}$ (with not too small gap between them). If it is not satisfied, the algorithm has to be re-started with some larger M .

The homotopy algorithm is illustrated in Figure 1 for the specific example investigated in Section 6, and for some particular choice of $k \in K$.

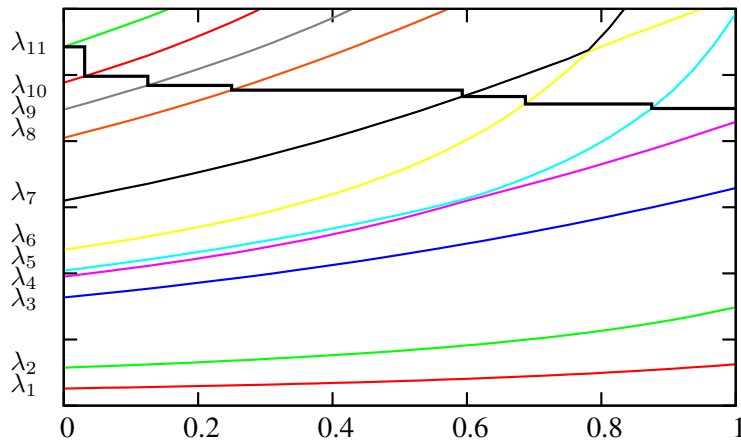


Figure 1: Illustration of the homotopy for the example of Section 6, and for $k = (2.5130, 0.4046)$: we choose $M = 11$, $N = 4$, $s_1 = 1/32$, $s_2 = 4/32$, $s_3 = 8/32$, $s_4 = 19/32$, $s_5 = 22/32$, $s_6 = 28/32$, $s_7 = 1$. By (9), we have $\lambda_{11}^0 \geq 28.21$, and by Theorem 2 we compute lower bounds $\mu_{10}^{(s_1)} = 27.13$, $\mu_9^{(s_2)} = 24.90$, $\mu_8^{(s_3)} = 23.85$, $\mu_7^{(s_4)} = 23.37$, $\mu_6^{(s_5)} = 22.81$, $\mu_5^{(s_6)} = 22.47$, $\mu_4^{(1)} = \mu_{k,4} = 21.42$.

5. A perturbation argument

Eigenvalue bounds (obtained according to the previous sections) for k in a finite set $\mathcal{K} \subset K$ guarantee, in the case $\Lambda_{k,m-1} < \mu_{k,m}$, that the intervals $(\Lambda_{k,m-1}, \mu_{k,m})$ are in the resolvent set of the operator A_k for the corresponding $k \in \mathcal{K}$. Assume $\lambda_{\text{gap}} \in (\Lambda_{k,m-1}, \mu_{k,m})$ for all $k \in \mathcal{K}$ (and some m). We now consider the perturbation of the eigenvalues of A_k when the parameter k is subjected to a small change. If the set $\mathcal{K} \subset K$ is sufficiently dense, and λ_{gap} has some distance from the spectra of A_k for all $k \in \mathcal{K}$, the following perturbation argument will guarantee that λ_{gap} is in the resolvent set for all $k \in K$, which gives the desired proof of a spectral gap. Of course, we need to quantify the expressions “sufficiently dense” and “some distance”.

First we write, for $u, v \in H_{\text{per}}^1(\Omega)$,

$$\begin{aligned} a_{k+h}(u, v) &= \int_{\Omega} (\nabla_k + i h)u \cdot \overline{(\nabla_k + i h)v} \, dx \\ &= \int_{\Omega} (\nabla_k u \cdot \overline{\nabla_k v} - 2i h \cdot (\nabla_k u)\bar{v} + |h|^2 u \bar{v}) \, dx \\ &= a_k(u, v) + s_{kh}(u, v) \end{aligned} \tag{13}$$

(using integration by parts), where

$$s_{kh}(u, v) := \int_{\Omega} \left(-2i h \cdot (\nabla_k u)\bar{v} + |h|^2 u \bar{v} \right) \, dx .$$

Applying the Cauchy-Schwarz inequality for $u \in H_{\text{per}}^1(\Omega)$, $v \in L_2(\Omega)$ yields

$$\begin{aligned} |s_{kh}(u, v)| &\leq 2 \left| \int_{\Omega} \sqrt{\frac{\varepsilon}{\varepsilon_{\min}}} h \cdot (\nabla_k u)\bar{v} \, dx \right| + |h|^2 \left| \int_{\Omega} \frac{\varepsilon}{\varepsilon_{\min}} u \bar{v} \, dx \right| \\ &\leq \frac{2|h|}{\sqrt{\varepsilon_{\min}}} \|u\|_k \|v\|_{\varepsilon} + \frac{|h|^2}{\varepsilon_{\min}} \|u\|_{\varepsilon} \|v\|_{\varepsilon} . \end{aligned} \tag{14}$$

Since the domain $D(A_k) = H^2(\Omega) \cap H_{\text{per}}^1(\Omega)$ of A_k is independent of k , we conclude from (13) that

$$A_{k+h} = A_k + S_{kh}$$

holds, where the operator $S_{kh}: D(A_k) \rightarrow L_2(\Omega)$ is defined by $s_{kh}(u, v) =: \langle S_{kh}u, v \rangle_{\varepsilon}$ for all $v \in L_2(\Omega)$.

Let $R(A_k, \lambda) = (\lambda \text{id} - A_k)^{-1} : L_2(\Omega) \rightarrow D(A_k)$ be the resolvent of A_k for $\lambda \in \mathbf{C} \setminus \sigma(A_k)$.

LEMMA 5. *Let λ be in the resolvent set of A_k and $\|S_{kh}R(A_k, \lambda)\|_{\varepsilon} < 1$. Then λ also belongs to the resolvent set of A_{k+h} .*

PROOF. We have $A_{k+h} - \lambda \text{id} = A_k + S_{kh} - \lambda \text{id} = \left(\text{id} + S_{kh}(A_k - \lambda \text{id})^{-1} \right) (A_k - \lambda \text{id})$, so $(\lambda \text{id} - A_{k+h})^{-1}$ exists since $\text{id} - S_{kh}R(A_k, \lambda)$ has a bounded inverse by our assumption (implying that the inverse can be represented by a convergent Neumann series). \square

Provided we know that λ does not belong to the spectrum of A_k , this lemma gives a sufficient condition for λ *not* belonging to the spectrum of A_{k+h} .

For practical use, we need to rewrite the assumption of Lemma 5 with *computable* terms:

LEMMA 6. *Let $\lambda \in [\Lambda_{k,m-1} + \delta, \mu_{k,m} - \delta]$ for some $\delta > 0$ and some $m \in \mathbf{N}$. Then*

$$\|S_{kh}R(A_k, \lambda)\|_{\varepsilon} \leq \frac{1}{\delta} \left(2|h| \sqrt{\frac{\mu_{k,m}}{\varepsilon_{\min}}} + \frac{|h|^2}{\varepsilon_{\min}} \right) .$$

PROOF. For $u \in H_{\text{per}}^1(\Omega)$ we obtain from (14) that

$$\begin{aligned} \|S_{kh}R(A_k, \lambda)u\|_{\varepsilon}^2 &= \langle S_{kh}R(A_k, \lambda)u, S_{kh}R(A_k, \lambda)u \rangle_{\varepsilon} \\ &= s_{kh}(R(A_k, \lambda)u, S_{kh}R(A_k, \lambda)u) \\ &\leq \left(\frac{2|h|}{\sqrt{\varepsilon_{\min}}} \|R(A_k, \lambda)u\|_k + \frac{|h|^2}{\varepsilon_{\min}} \|R(A_k, \lambda)u\|_{\varepsilon} \right) \|S_{kh}R(A_k, \lambda)u\|_{\varepsilon} \end{aligned}$$

and thus $\|S_{kh}R(A_k, \lambda)u\|_\varepsilon \leq \frac{2|h|}{\sqrt{\varepsilon_{\min}}} \|R(A_k, \lambda)u\|_k + \frac{|h|^2}{\varepsilon_{\min}} \|R(A_k, \lambda)u\|_\varepsilon$. Expanding u with respect to a complete orthonormal system of eigenfunctions $\{u_{k,n}\}_{n \in \mathbf{N}}$ of A_k we can estimate

$$\|R(A_k, \lambda)u\|_\varepsilon^2 = \sum_{n \in \mathbf{N}} \frac{1}{(\lambda_{k,n} - \lambda)^2} |\langle u, u_{k,n} \rangle_\varepsilon|^2 \leq \frac{1}{\delta^2} \|u\|_\varepsilon^2$$

and

$$\begin{aligned} \|R(A_k, \lambda)u\|_k^2 &= \langle A_k R(A_k, \lambda)u, R(A_k, \lambda)u \rangle_\varepsilon \\ &= \sum_{n \in \mathbf{N}} \frac{\lambda_{k,n}}{(\lambda_{k,n} - \lambda)^2} |\langle u, u_{k,n} \rangle_\varepsilon|^2 \leq \frac{\mu_{k,m}}{\delta^2} \|u\|_\varepsilon^2, \end{aligned}$$

using $\frac{\lambda_{k,n}}{(\lambda_{k,n} - \lambda)^2} = \frac{1}{\lambda_{k,n} - \lambda} + \frac{\lambda}{(\lambda_{k,n} - \lambda)^2} \leq \frac{1}{\delta} + \frac{\lambda}{\delta^2} = \frac{\delta + \lambda}{\delta^2} \leq \frac{\mu_{k,m}}{\delta^2}$. The desired inequality follows. \square

Lemmata 5 and 6 together give the following

THEOREM 7. *For $k \in \mathcal{K}$, choose $\delta_k > 0$ and suppose that, for some $m \in \mathbf{N}$ and some interval I ,*

- a) $I \subset [\Lambda_{k,m-1} + \delta_k, \mu_{k,m} - \delta_k]$ for all $k \in \mathcal{K}$,
- b) $K \subset \bigcup_{k \in \mathcal{K}} B(k, r_k)$, where $r_k = \sqrt{\varepsilon_{\min}} \left(\sqrt{\mu_{k,m} + \delta_k} - \sqrt{\mu_{k,m}} \right)$ and $B(k, r_k) = \{k' \in \mathbf{R}^2 : |k' - k| < r_k\}$.

Then, I is contained in a spectral gap, i. e., $I \subset (\lambda_{k,m-1}, \lambda_{k,m})$ for all $k \in K$.

PROOF. For $k' \in K$ find some $k \in \mathcal{K}$ with $|h| < r_k$ for $h = k' - k$, which is possible by assumption b). Then, we have $|h| + \sqrt{\varepsilon_{\min}} \sqrt{\mu_{k,m}} < \sqrt{\varepsilon_{\min}} \sqrt{\mu_{k,m} + \delta_k}$ and thus

$$\frac{1}{\varepsilon_{\min} \delta_k} \left(|h|^2 + 2|h| \sqrt{\varepsilon_{\min}} \sqrt{\mu_{k,m}} \right) < 1.$$

Then, assumption a) and Lemmata 5 and 6 imply $I \subset (\lambda_{k+h,m-1}, \lambda_{k+h,m}) = (\lambda_{k',m-1}, \lambda_{k',m})$. \square

6. A numerical example

The numerical tests are realized in the finite element code M++ [16] supporting periodic boundary conditions. We use bi-quadratic finite elements on quadrilaterals, and the matrix eigenvalue problems are solved approximately by a preconditioned subspace iteration with Ritz projections [8]. Finally, for obtaining reliable results, all bounds are calculated with the interval library of C-XSC [7] (version 2.0 [9]). Within this software, all integrals, and other expressions involved in the inclusion algorithm, are evaluated by interval arithmetic guaranteeing a full rounding error control.

6.1. A Candidate. Let $\Lambda = \mathbb{Z}^2$, $\Omega = (0, 1)^2$, whence $K = [-\pi, \pi]^2$. Let $\varepsilon(x) = 1$ for $x \in [1/16, 15/16]^2$ and $\varepsilon(x) = 5$ else. By symmetry we have the same spectrum for $k = (k_1, k_2)$, $(-k_1, k_2)$, $(k_1, -k_2)$, (k_2, k_1) , so that the computations can be reduced to $K_0 \subset K$, see Fig. 2: the symmetry of the material distribution transfers to corresponding symmetry properties of the eigenfunctions (e. g., $u_{(k_1, k_2), n}(x, y) = u_{(-k_1, k_2), n}(1 - x, y)$), and thus, to a corresponding coincidence of the eigenvalues, i. e., we have $\{\lambda_{k, n} : k \in K\} = \{\lambda_{k, n} : k \in K_0\}$.

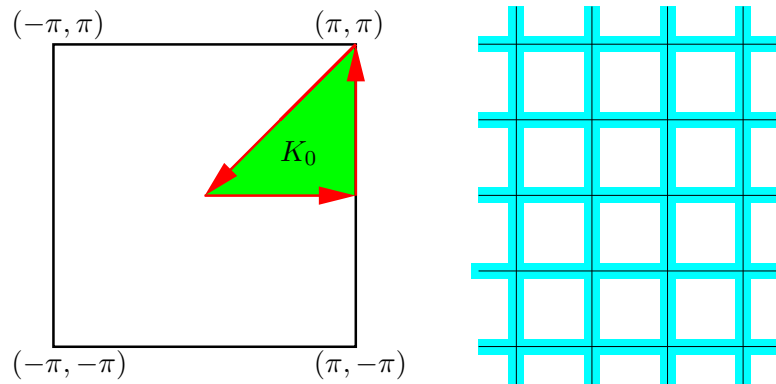


Figure 2: Illustration of the Brillouin zone K (left) and the periodic material distribution ε (right).

By first numerical tests along $k \in \partial K_0$ we observe a candidate for a spectral gap between $\lambda_{k,3}$ and $\lambda_{k,4}$, see Fig. 3.

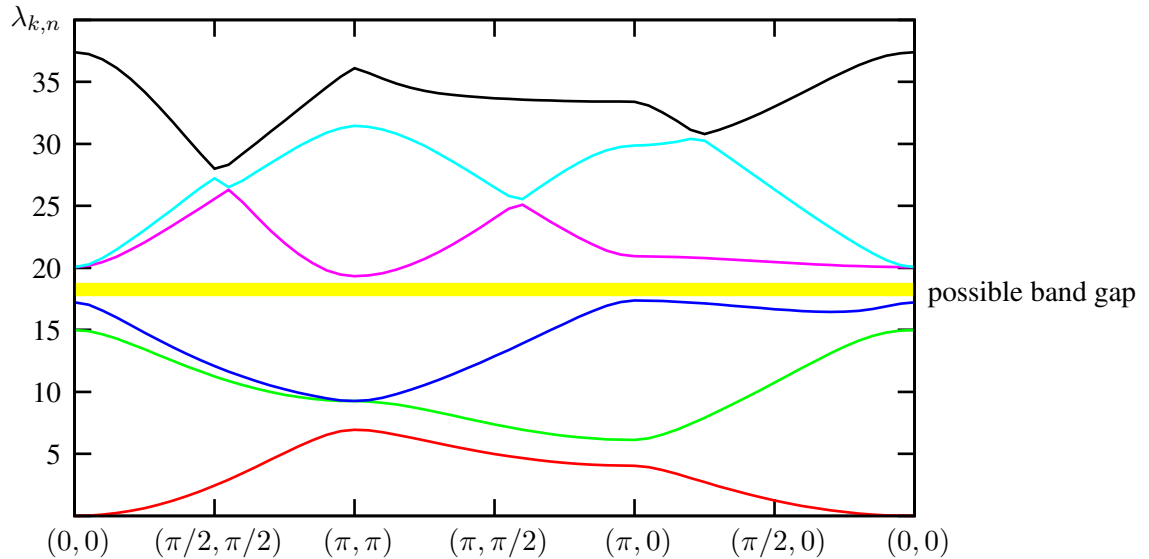


Figure 3: Illustration of the eigenvalue distribution $\{\lambda_{k, n} : k \in \partial K_0\}$ for $n = 1, 2, 3, 4, 5, 6$.

In a second numerical test, $\lambda_{k,1}, \dots, \lambda_{k,4}$ are computed for k in a grid in K , and again we observe the same possible gap, see Fig. 4.

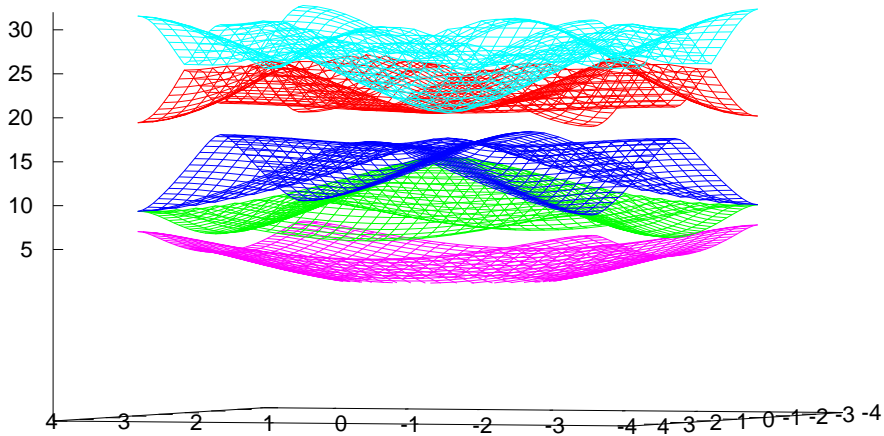


Figure 4: Illustration of the eigenvalue distribution of $\lambda_{k,n}$ for $n = 1, 2, 3, 4, 5$ for k in a grid in K .

6.2. The band gap verification. Verifying the existence of a band gap for this example consists of the following steps:

- The numerical approximation indicates a possible band gap interval $(\tilde{\lambda}_{\max,3}, \tilde{\lambda}_{\min,4}) = (17.26, 19.19)$;
- We select a suitable finite subset $\mathcal{K} \subset K_0$. For each $k \in \mathcal{K}$ we compute an upper eigenvalue bound $\Lambda_{k,3}$ and a lower eigenvalue bound $\mu_{k,4}$ (see Tab. 1); Tab. 2 illustrates the corresponding homotopies needed for Theorem 2, as explained in Section 4.
- For each $k \in \mathcal{K}$ we compute

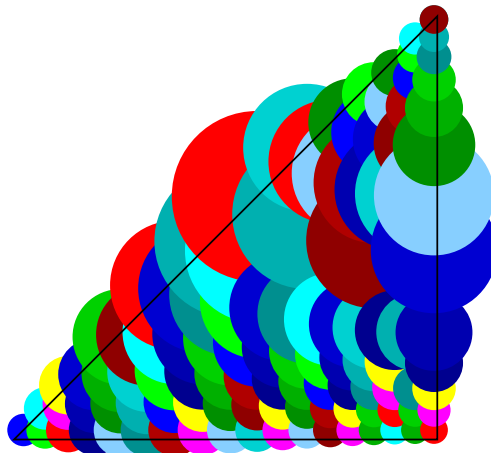
$$\delta_k \leq \min\{18.2 - \Lambda_{k,3}, \mu_{k,4} - 18.25\}, \quad r_k = \sqrt{\varepsilon_{\min}} \left(\sqrt{\mu_{k,4} + \delta_k} - \sqrt{\mu_{k,4}} \right).$$

- We check

$$K_0 \subset \bigcup_{k \in \mathcal{K}} B(k, r_k) \quad (\text{see Fig. 5}).$$

Theorem 7 proves the existence of a spectral gap containing the interval $I = (18.2, 18.25)$.

Figure 5: Illustration of the covering $\bigcup B(k, r_k)$ of K_0 by 95 balls. The approximate eigenfunctions $\tilde{u}_{k,n}$ are computed in a finite element space \tilde{V} with $\dim \tilde{V} = 12290$, for the dual approximations $\tilde{W} = \tilde{V} \times \tilde{V}$ is used. The full verification process required 52 h computing time.



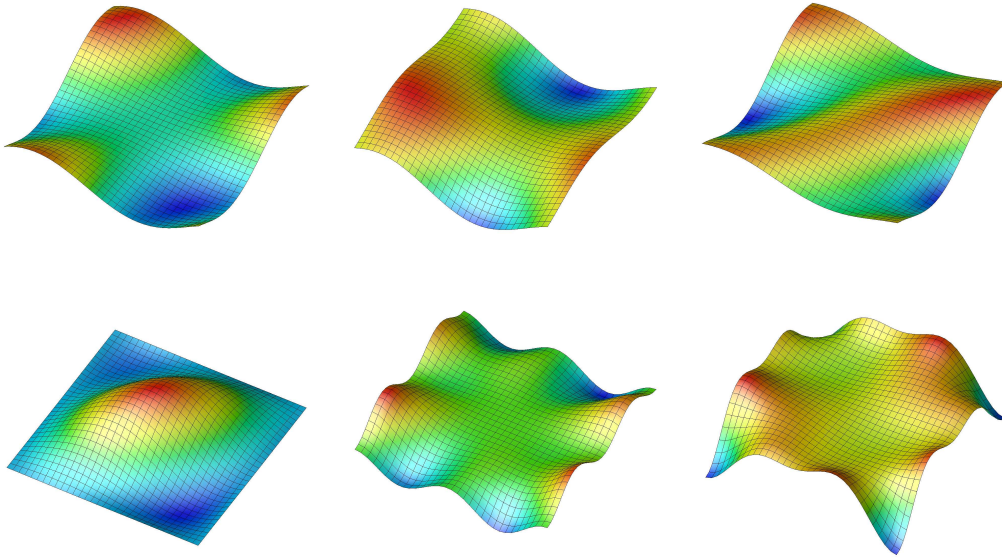
k	$\Lambda_{k,1}$	$\Lambda_{k,2}$	$\Lambda_{k,3}$	$\mu_{k,4}$	δ_k	k	$\Lambda_{k,1}$	$\Lambda_{k,2}$	$\Lambda_{k,3}$	$\mu_{k,4}$	δ_k
(0.0000,0.0000)	0.000	14.907	17.148	19.915	0.115	(2.4544,0.0982)	2.934	7.545	17.047	20.654	0.124
(0.0982,0.0000)	0.005	14.890	17.109	19.908	0.120	(2.4544,0.2945)	2.969	7.581	16.710	21.072	0.158
(0.0982,0.0982)	0.011	14.873	17.069	19.976	0.124	(2.4544,0.5890)	3.087	7.700	15.858	22.046	0.242
(0.1963,0.0000)	0.020	14.835	17.004	19.939	0.131	(2.4544,0.8836)	3.282	7.896	14.857	23.167	0.334
(0.1963,0.1963)	0.040	14.772	16.857	20.099	0.146	(2.5525,0.0000)	3.139	7.237	17.138	20.705	0.114
(0.2945,0.0982)	0.050	14.727	16.824	19.991	0.150	(2.5525,0.0982)	3.143	7.242	17.091	20.754	0.119
(0.3927,0.0000)	0.080	14.598	16.723	19.974	0.161	(2.5525,0.3927)	3.208	7.310	16.503	21.394	0.179
(0.3927,0.2945)	0.125	14.502	16.396	20.321	0.195	(2.6507,0.0000)	3.346	6.950	17.176	20.725	0.110
(0.4909,0.0982)	0.130	14.401	16.553	20.012	0.179	(2.6507,0.0982)	3.351	6.954	17.130	20.773	0.115
(0.5890,0.0000)	0.179	14.171	16.502	19.937	0.184	(2.6507,0.2945)	3.384	6.992	16.796	21.046	0.149
(0.5890,0.1963)	0.199	14.156	16.323	20.203	0.203	(2.6507,2.4544)	5.730	9.267	10.012	20.791	0.270
(0.5890,0.3927)	0.258	14.093	15.905	20.647	0.245	(2.7489,0.0000)	3.546	6.685	17.209	20.740	0.107
(0.6872,0.0982)	0.248	13.893	16.387	20.073	0.197	(2.7489,0.0982)	3.550	6.689	17.162	20.787	0.111
(0.7854,0.5890)	0.495	13.532	15.184	21.380	0.314	(2.7489,0.1963)	3.562	6.704	17.030	20.913	0.125
(0.8836,0.0982)	0.406	13.254	16.329	20.076	0.198	(2.7489,0.5890)	3.693	6.856	15.988	22.090	0.229
(0.8836,0.2945)	0.446	13.261	15.975	20.496	0.238	(2.7489,1.5708)	4.567	7.839	12.675	24.122	0.532
(0.9817,0.0982)	0.499	12.906	16.330	20.162	0.203	(2.7489,2.7489)	6.315	9.318	9.503	19.911	0.181
(1.0799,0.0982)	0.602	12.546	16.345	20.188	0.201	(2.8471,0.0000)	3.728	6.451	17.235	20.751	0.104
(1.1781,0.1963)	0.729	12.187	16.228	20.323	0.212	(2.8471,0.0982)	3.732	6.455	17.189	20.797	0.109
(1.1781,0.3927)	0.788	12.218	15.743	20.860	0.260	(2.8471,0.1963)	3.744	6.470	17.057	20.914	0.122
(1.1781,0.8836)	1.102	12.338	14.089	22.679	0.412	(2.8471,0.3927)	3.792	6.529	16.606	21.429	0.168
(1.2763,0.0000)	0.832	11.804	16.455	20.180	0.189	(2.8471,1.1781)	4.296	7.139	14.029	24.552	0.403
(1.3744,0.1963)	0.982	11.443	16.305	20.447	0.204	(2.8471,1.9635)	5.251	8.211	11.490	22.228	0.404
(1.5708,0.0000)	1.251	10.683	16.594	20.336	0.174	(2.9452,0.0000)	3.881	6.261	17.254	20.759	0.102
(1.5708,0.1963)	1.270	10.697	16.405	20.520	0.193	(2.9452,0.0982)	3.885	6.266	17.207	20.803	0.106
(1.5708,0.4909)	1.370	10.769	15.623	21.367	0.270	(2.9452,0.2945)	3.916	6.307	16.876	21.182	0.141
(1.5708,1.1781)	1.932	11.133	13.170	24.078	0.487	(2.9452,0.8836)	4.193	6.665	15.060	23.297	0.314
(1.6690,0.0000)	1.408	10.312	16.649	20.374	0.168	(2.9452,2.2580)	5.803	8.511	10.689	20.988	0.289
(1.7671,0.0000)	1.574	9.945	16.706	20.395	0.161	(2.9452,2.7489)	6.531	9.110	9.545	19.648	0.154
(1.7671,0.1963)	1.593	9.960	16.518	20.620	0.180	(2.9452,2.8471)	6.648	9.185	9.385	19.489	0.137
(1.8653,0.0000)	1.748	9.582	16.764	20.464	0.155	(2.9452,2.9452)	6.741	9.221	9.279	19.377	0.125
(1.8653,0.2945)	1.790	9.616	16.368	20.889	0.195	(3.0434,0.0000)	3.987	6.134	17.265	20.763	0.100
(1.8653,0.6872)	1.977	9.767	15.147	22.218	0.312	(3.0434,0.0982)	3.990	6.139	17.219	20.806	0.105
(1.9635,0.0000)	1.929	9.223	16.823	20.494	0.149	(3.0434,0.1963)	4.002	6.154	17.087	20.900	0.119
(1.9635,0.1963)	1.948	9.239	16.637	20.639	0.168	(3.0434,0.2945)	4.021	6.180	16.888	21.188	0.139
(1.9635,1.4726)	2.953	10.039	12.405	25.532	0.543	(3.0434,0.4909)	4.081	6.263	16.356	21.786	0.192
(2.0617,0.0000)	2.118	8.871	16.881	20.509	0.142	(3.0434,0.6872)	4.171	6.385	15.734	22.509	0.252
(2.0617,0.2945)	2.160	8.907	16.489	20.939	0.182	(3.0434,2.4544)	6.172	8.702	10.209	20.288	0.220
(2.1598,0.0000)	2.313	8.525	16.938	20.580	0.136	(3.0434,2.6507)	6.461	8.937	9.764	19.778	0.168
(2.1598,0.1963)	2.332	8.542	16.755	20.764	0.155	(3.0434,3.0434)	6.863	9.197	9.212	19.238	0.110
(2.1598,0.3927)	2.386	8.592	16.291	21.269	0.201	(3.1416,0.0000)	4.024	6.088	17.269	20.764	0.100
(2.1598,0.7854)	2.604	8.787	15.009	22.683	0.323	(3.1416,0.0982)	4.028	6.094	17.223	20.807	0.105
(2.2580,0.0000)	2.514	8.187	16.993	20.608	0.130	(3.1416,0.1963)	4.039	6.109	17.091	20.896	0.118
(2.2580,0.4909)	2.627	8.293	16.058	21.634	0.224	(3.1416,0.3927)	4.084	6.172	16.643	21.433	0.164
(2.3562,0.0000)	2.720	7.859	17.046	20.629	0.124	(3.1416,2.8471)	6.731	9.084	9.422	19.400	0.128
(2.3562,0.1963)	2.738	7.876	16.864	20.845	0.143	(3.1416,3.0434)	6.884	9.177	9.216	19.216	0.108
(2.3562,1.9635)	4.412	9.383	11.133	23.201	0.488	(3.1416,3.1416)	6.905	9.189	9.189	19.193	0.105
(2.4544,0.0000)	2.929	7.541	17.094	20.632	0.119						

Table 1: Eigenvalue bounds for $k \in \mathcal{K}$, obtained by Theorems 1 and 2. For the lower bounds $\mu_{k,4}$ the spectral homotopy method described in Section 4 is used; see Table 2.

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(0.0000,0.0000)	$\mu_5^{32/32} \geq 19.915,$ $\lambda_{10}^0 \geq 31.582$	$\mu_6^{15/32} \geq 20.313,$	$\mu_7^{13/32} \geq 21.007,$	$\mu_8^{13/32} \geq 21.007,$	$\mu_9^{11/32} \geq 21.570,$
(0.5890,0.3927)	$\mu_5^{31/32} \geq 20.988,$ $\lambda_{10}^0 \geq 28.722$	$\mu_6^{21/32} \geq 21.677,$	$\mu_7^{16/32} \geq 22.475,$	$\mu_8^{15/32} \geq 22.976,$	$\mu_9^{11/32} \geq 23.694,$
(1.2763,0.0000)	$\mu_5^{25/32} \geq 20.531,$ $\lambda_{10}^0 \geq 25.493$	$\mu_6^{22/32} \geq 20.878,$	$\mu_7^{18/32} \geq 21.239,$	$\mu_8^{6/32} \geq 21.493,$	$\mu_9^{6/32} \geq 22.222,$
(1.5708,0.1963)	$\mu_5^{24/32} \geq 21.023,$ $\lambda_{10}^0 \geq 24.188$	$\mu_6^{24/32} \geq 21.691,$	$\mu_7^{20/32} \geq 22.318,$	$\mu_8^{7/32} \geq 22.669,$	$\mu_9^{5/32} \geq 23.020,$
(2.0617,0.2945)	$\mu_5^{26/32} \geq 21.47,$ $\mu_{10}^{3/32} \geq 23.97,$	$\mu_6^{21/32} \geq 22.18,$ $\lambda_{11}^0 \geq 29.242$	$\mu_7^{21/32} \geq 22.32,$	$\mu_8^{4/32} \geq 22.81,$	$\mu_9^{3/32} \geq 23.42,$
(2.3562,0.0000)	$\mu_5^{26/32} \geq 21.18,$ $\mu_{10}^{2/32} \geq 23.85,$	$\mu_6^{22/32} \geq 22.26,$ $\lambda_{11}^0 \geq 28.745$	$\mu_7^{19/32} \geq 22.55,$	$\mu_8^{5/32} \geq 23.01,$	$\mu_9^{2/32} \geq 23.61,$
(2.6507,2.4544)	$\mu_5^{13/32} \geq 21.360,$ $\mu_{10}^{5/32} \geq 24.017,$	$\mu_6^{12/32} \geq 21.803,$ $\mu_{11}^{4/32} \geq 24.515,$	$\mu_7^{10/32} \geq 22.403,$ $\mu_{12}^{4/32} \geq 25.067,$	$\mu_8^{9/32} \geq 22.950,$ $\lambda_{13}^0 \geq 31.231$	$\mu_9^{6/32} \geq 23.427,$
(2.8471,0.0982)	$\mu_5^{27/32} \geq 21.473,$	$\mu_6^{23/32} \geq 22.865,$	$\mu_7^{16/32} \geq 23.249,$	$\mu_8^{11/32} \geq 23.817,$	$\lambda_9^0 \geq 24.323$
(2.9452,0.0000)	$\mu_5^{27/32} \geq 21.448,$	$\mu_6^{23/32} \geq 22.748,$	$\mu_7^{15/32} \geq 23.116,$	$\mu_8^{11/32} \geq 23.413,$	$\lambda_9^0 \geq 24.928$
(3.0434,0.0000)	$\mu_5^{27/32} \geq 21.408,$	$\mu_6^{23/32} \geq 22.708,$	$\mu_7^{14/32} \geq 22.961,$	$\mu_8^{12/32} \geq 23.624,$	$\lambda_9^0 \geq 25.292$
(3.0434,0.0982)	$\mu_5^{27/32} \geq 21.366,$	$\mu_6^{23/32} \geq 22.762,$	$\mu_7^{14/32} \geq 22.963,$	$\mu_8^{12/32} \geq 23.625,$	$\lambda_9^0 \geq 25.047$
(3.1416,3.1416)	$\lambda_5^0 \geq 19.739$				

Table 2: Spectral homotopy for some sample points $k \in \mathcal{K}$ (for a full list see Tab. 3 and 4).Figure 6: Illustration of the real part of the eigenfunctions $u_{k,1}, \dots, u_{k,6}$ for $k = (\pi, \pi)$.

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(2.5525,0.0982)	$\mu_5^{27/32} \geq 21.81, \mu_6^{23/32} \geq 23.19, (1, \mu_7^{19/32}) \geq 23.49, \mu_8^{9/32} \geq 24.10, (1, \mu_9^{3/32}) \geq 24.61, \mu_{10}^{3/32} \geq 25.26, \lambda_{11}^0 \geq 27.706$
(2.5525,0.3927)	$\mu_5^{28/32} \geq 22.417, \mu_6^{22/32} \geq 22.707, \mu_7^{18/32} \geq 22.998, \mu_8^{8/32} \geq 23.583, \mu_9^{3/32} \geq 23.909, \lambda_{10}^0 \geq 24.527$
(2.6507,0.0000)	$\mu_5^{27/32} \geq 21.71, \mu_6^{23/32} \geq 23.00, (1, \mu_7^{18/32}) \geq 23.38, \mu_8^{9/32} \geq 23.65, (1, \mu_9^{1/32}) \geq 24.26, \mu_{10}^{1/32} \geq 24.38, \lambda_{11}^0 \geq 27.559$
(2.6507,0.0982)	$\mu_5^{27/32} \geq 21.67, \mu_6^{23/32} \geq 23.06, (1, \mu_7^{18/32}) \geq 23.38, \mu_8^{9/32} \geq 23.64, (1, \mu_9^{1/32}) \geq 24.06, \mu_{10}^{1/32} \geq 24.58, \lambda_{11}^0 \geq 27.314$
(2.6507,0.2945)	$\mu_5^{27/32} \geq 21.371, \mu_6^{22/32} \geq 22.268, \mu_7^{17/32} \geq 22.886, \mu_8^{8/32} \geq 23.146, \mu_9^{1/32} \geq 23.584, \lambda_{10}^0 \geq 24.616$
(2.6507,2.4544)	$\mu_5^{13/32} \geq 21.360, \mu_6^{12/32} \geq 21.803, \mu_7^{10/32} \geq 22.403, \mu_8^{9/32} \geq 22.950, \mu_9^{6/32} \geq 23.427, \mu_{10}^{5/32} \geq 24.017$
	$\mu_{11}^{4/32} \geq 24.515, \mu_{12}^{4/32} \geq 25.067, \lambda_{13}^0 \geq 31.231$
(2.7489,0.0000)	$\mu_5^{27/32} \geq 21.604, \mu_6^{23/32} \geq 22.899, \mu_7^{17/32} \geq 23.328, \mu_8^{10/32} \geq 23.721, \lambda_9^0 \geq 24.211$
(2.7489,0.0982)	$\mu_5^{27/32} \geq 21.564, \mu_6^{23/32} \geq 22.952, \mu_7^{17/32} \geq 23.328, \mu_8^{10/32} \geq 23.695, \lambda_9^0 \geq 23.966$
(2.7489,0.1963)	$\mu_5^{27/32} \geq 21.440, \mu_6^{22/32} \geq 21.910, \mu_7^{15/32} \geq 22.322, \mu_8^{8/32} \geq 22.713, \lambda_9^0 \geq 23.725$
(2.7489,0.5890)	$\mu_5^{29/32} \geq 22.879, \mu_6^{22/32} \geq 23.242, \mu_7^{18/32} \geq 23.920, \mu_8^{11/32} \geq 24.275, \mu_9^{4/32} \geq 24.663, \lambda_{10}^0 \geq 25.761$
(2.7489,1.5708)	$\mu_5^{29/32} \geq 24.726, \mu_6^{20/32} \geq 25.442, \mu_7^{20/32} \geq 25.946, \mu_8^{14/32} \geq 26.402, \mu_9^{12/32} \geq 26.931, \mu_{10}^{7/32} \geq 27.402$
	$\mu_{11}^{4/32} \geq 27.664, \mu_{12}^{3/32} \geq 28.281, \lambda_{13}^0 \geq 28.652$
(2.7489,2.7489)	$\mu_5^{7/32} \geq 20.25, \mu_6^{7/32} \geq 20.47, (1, \mu_7^{5/32}) \geq 20.84, \mu_8^{5/32} \geq 20.88, \mu_9^{1/32} (1, \mu_{10}^{1/32}) \geq 21.15, \mu_{10}^{1/32} \geq 21.16, \lambda_{11}^0 \geq 21.774$
(2.8471,0.0000)	$\mu_5^{27/32} \geq 21.513, \mu_6^{23/32} \geq 22.812, \mu_7^{16/32} \geq 23.247, \mu_8^{11/32} \geq 23.824, \lambda_9^0 \geq 24.568$
(2.8471,0.0982)	$\mu_5^{27/32} \geq 21.473, \mu_6^{23/32} \geq 22.865, \mu_7^{16/32} \geq 23.249, \mu_8^{11/32} \geq 23.817, \lambda_9^0 \geq 24.323$
(2.8471,0.1963)	$\mu_5^{27/32} \geq 21.348, \mu_6^{22/32} \geq 21.821, \mu_7^{14/32} \geq 22.259, \mu_8^{9/32} \geq 22.782, \lambda_9^0 \geq 24.082$
(2.8471,0.3927)	$\mu_5^{28/32} \geq 22.069, \mu_6^{22/32} \geq 22.386, \mu_7^{15/32} \geq 22.776, \mu_8^{10/32} \geq 23.273, \lambda_9^0 \geq 23.611$
(2.8471,1.1781)	$\mu_5^{32/32} \geq 25.926, \mu_6^{23/32} \geq 27.236, \mu_7^{23/32} \geq 27.225, \mu_8^{17/32} \geq 27.583, \mu_9^{12/32} \geq 28.238, \mu_{10}^{8/32} \geq 28.566$
	$\mu_{11}^{3/32} \geq 29.114, \mu_{12}^{3/32} \geq 29.488, \mu_{13}^{3/32} \geq 30.046, \mu_{14}^{1/32} \geq 30.615, \lambda_{15}^0 \geq 39.403$
(2.8471,1.9635)	$\mu_5^{21/32} \geq 22.756, \mu_6^{15/32} \geq 23.320, \mu_7^{15/32} \geq 23.582, \mu_8^{10/32} \geq 24.074, \mu_9^{9/32} \geq 24.646, \mu_{10}^{5/32} \geq 25.042$
	$\mu_{11}^{3/32} \geq 25.443, \mu_{12}^{2/32} \geq 25.855, \lambda_{13}^0 \geq 30.274$
(2.9452,0.0000)	$\mu_5^{27/32} \geq 21.448, \mu_6^{23/32} \geq 22.748, \mu_7^{15/32} \geq 23.116, \mu_8^{11/32} \geq 23.413, \lambda_9^0 \geq 24.928$
(2.9452,0.0982)	$\mu_5^{27/32} \geq 21.406, \mu_6^{23/32} \geq 22.802, \mu_7^{15/32} \geq 23.118, \mu_8^{11/32} \geq 23.413, \lambda_9^0 \geq 24.683$
(2.9452,0.2945)	$\mu_5^{28/32} \geq 22.258, \mu_6^{23/32} \geq 23.207, \mu_7^{16/32} \geq 23.627, \mu_8^{12/32} \geq 23.917, \lambda_9^0 \geq 24.205$
(2.9452,0.8836)	$\mu_5^{31/32} \geq 24.968, \mu_6^{23/32} \geq 25.703, \mu_7^{20/32} \geq 25.879, \mu_8^{16/32} \geq 26.386, \mu_9^{8/32} \geq 26.844, \mu_{10}^{6/32} \geq 27.534$
	$\mu_{11}^{1/32} \geq 27.836, \lambda_{12}^0 \geq 28.785$
(2.9452,2.2580)	$\mu_5^{15/32} \geq 21.524, \mu_6^{11/32} \geq 21.853, \mu_7^{11/32} \geq 22.369, \mu_8^{8/32} \geq 22.909, \mu_9^{7/32} \geq 23.391, \mu_{10}^{4/32} \geq 23.557$
	$\mu_{11}^{2/32} \geq 23.865, \mu_{12}^{2/32} \geq 24.447, \lambda_{13}^0 \geq 31.623$
(2.9452,2.7489)	$\mu_5^{6/32} \geq 20.138, \mu_6^{5/32} \geq 20.386, \mu_7^{5/32} \geq 20.624, \mu_8^{4/32} \geq 21.168, \mu_9^{4/32} \geq 21.605, \mu_{10}^{3/32} \geq 22.223$
	$\mu_{11}^{3/32} \geq 22.340, \mu_{12}^{3/32} \geq 22.885, \lambda_{13}^0 \geq 33.348$
(2.9452,2.8471)	$\mu_5^{4/32} \geq 19.809, \mu_6^{4/32} \geq 20.116, \mu_7^{4/32} \geq 20.540, \mu_8^{4/32} \geq 21.040, \mu_9^{3/32} \geq 21.323, \mu_{10}^{3/32} \geq 21.825$
	$\mu_{11}^{3/32} \geq 22.202, \mu_{12}^{3/32} \geq 22.479, \lambda_{13}^0 \geq 33.704$
(2.9452,2.9452)	$\mu_5^{3/32} \geq 19.803, \mu_6^{3/32} \geq 19.884, \mu_7^{3/32} \geq 20.461, \mu_8^{3/32} \geq 20.481, \mu_9^{2/32} \geq 21.011, \mu_{10}^{2/32} \geq 21.048$
	$\mu_{11}^{2/32} \geq 21.589, \mu_{12}^{2/32} \geq 21.607, \lambda_{13}^0 \geq 34.065$
(3.0434,0.0000)	$\mu_5^{27/32} \geq 21.408, \mu_6^{23/32} \geq 22.708, \mu_7^{14/32} \geq 22.961, \mu_8^{12/32} \geq 23.624, \lambda_9^0 \geq 25.292$
(3.0434,0.0982)	$\mu_5^{27/32} \geq 21.366, \mu_6^{23/32} \geq 22.762, \mu_7^{14/32} \geq 22.963, \mu_8^{12/32} \geq 23.625, \lambda_9^0 \geq 25.047$
(3.0434,0.1963)	$\mu_5^{27/32} \geq 21.242, \mu_6^{22/32} \geq 21.718, \mu_7^{12/32} \geq 22.039, \mu_8^{10/32} \geq 22.525, \lambda_9^0 \geq 24.807$
(3.0434,0.2945)	$\mu_5^{28/32} \geq 22.218, \mu_6^{23/32} \geq 23.168, \mu_7^{15/32} \geq 23.462, \mu_8^{13/32} \geq 24.186, \lambda_9^0 \geq 24.569$
(3.0434,0.4909)	$\mu_5^{29/32} \geq 23.01, \mu_6^{23/32} \geq 23.85, (2, \mu_7^{17/32}) \geq 24.46, \mu_8^{14/32} \geq 24.83, (2, \mu_9^{3/32}) \geq 25.52, \mu_{10}^{2/32} \geq 25.83, \lambda_{11}^0 \geq 26.574$
(3.0434,0.6872)	$\mu_5^{30/32} \geq 23.88, \mu_6^{23/32} \geq 24.71, (2, \mu_7^{18/32}) \geq 25.02, \mu_8^{15/32} \geq 25.47, (2, \mu_9^{5/32}) \geq 26.04, \mu_{10}^{4/32} \geq 26.46, \lambda_{11}^0 \geq 27.114$
(3.0434,2.4544)	$\mu_5^{11/32} \geq 20.828, \mu_6^{9/32} \geq 21.453, \mu_7^{9/32} \geq 22.024, \mu_8^{7/32} \geq 22.266, \mu_9^{6/32} \geq 22.918, \mu_{10}^{5/32} \geq 23.413$
	$\mu_{11}^{4/32} \geq 23.963, \mu_{12}^{4/32} \geq 24.610, \lambda_{13}^0 \geq 32.666$
(3.0434,2.6507)	$\mu_5^{7/32} \geq 20.167, \mu_6^{6/32} \geq 20.646, \mu_7^{6/32} \geq 21.039, \mu_8^{5/32} \geq 21.561, \mu_9^{5/32} \geq 22.141, \mu_{10}^{4/32} \geq 22.595$
	$\mu_{11}^{4/32} \geq 23.126, \mu_{12}^{4/32} \geq 23.753, \lambda_{13}^0 \geq 33.359$
(3.0434,3.0434)	$\mu_5^{1/32} \geq 19.600, \mu_6^{1/32} \geq 19.622, \mu_7^{1/32} \geq 19.880, \mu_8^{1/32} \geq 19.888, \mu_9^{1/32} \geq 20.359, \mu_{10}^{1/32} \geq 20.377$
	$\mu_{11}^{1/32} \geq 20.640, \mu_{12}^{1/32} \geq 20.649, \lambda_{13}^0 \geq 34.794$
(3.1416,0.0000)	$\mu_5^{27/32} \geq 21.394, \mu_6^{23/32} \geq 22.697, \mu_7^{14/32} \geq 23.079, \mu_8^{12/32} \geq 23.473, \lambda_9^0 \geq 25.660$
(3.1416,0.0982)	$\mu_5^{27/32} \geq 21.353, \mu_6^{23/32} \geq 22.751, \mu_7^{14/32} \geq 23.080, \mu_8^{12/32} \geq 23.474, \lambda_9^0 \geq 25.416$
(3.1416,0.1963)	$\mu_5^{27/32} \geq 21.228, \mu_6^{22/32} \geq 21.706, \mu_7^{12/32} \geq 22.188, \mu_8^{11/32} \geq 22.909, \lambda_9^0 \geq 25.175$
(3.1416,0.3927)	$\mu_5^{28/32} \geq 21.948, \mu_6^{22/32} \geq 22.273, \mu_7^{13/32} \geq 22.628, \mu_8^{11/32} \geq 22.933, \lambda_9^0 \geq 24.704$
(3.1416,2.8471)	$\mu_5^{4/32} \geq 19.927, \mu_6^{4/32} \geq 20.412, \mu_7^{4/32} \geq 20.745, \mu_8^{4/32} \geq 21.086, \mu_9^{4/32} \geq 21.651, \mu_{10}^{4/32} \geq 22.082$
	$\mu_{11}^{4/32} \geq 22.335, \mu_{12}^{4/32} \geq 22.885, \lambda_{13}^0 \geq 34.437$
(3.1416,3.0434)	$\mu_5^{1/32} \geq 19.690, \mu_6^{1/32} \geq 19.798, \mu_7^{1/32} \geq 19.947, \mu_8^{1/32} \geq 20.028, \mu_9^{1/32} \geq 20.215, \mu_{10}^{1/32} \geq 20.308$
	$\mu_{11}^{1/32} \geq 20.448, \mu_{12}^{1/32} \geq 20.561, \lambda_{13}^0 \geq 35.162$
(3.1416,3.1416)	$\lambda_5^0 \geq 19.739$

Table 4: Eigenvalue homotopy (second part).

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