A computer-assisted Band-Gap Proof for 3D Photonic Crystals

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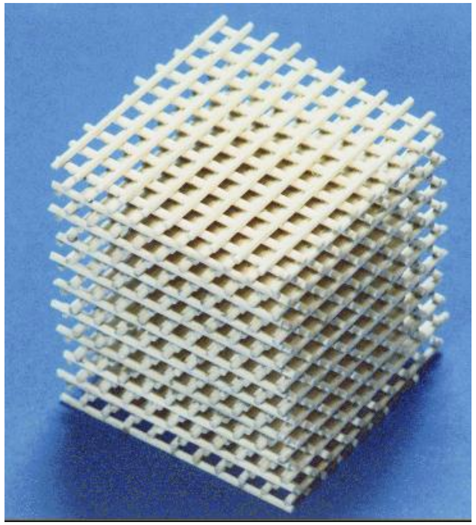
Photonic Crystals

We consider periodic optic media (photonic crystals). In such media light is absorbed for all frequencies which are not within a **band gap**.



(www.cfn.uni-karlsruhe.de)

In nanotechnology, photonic crystals are fabricated and band gaps can be observed.

Photonic crystal: periodic dielectric medium such that electromagnetic waves of certain frequencies *cannot propagate* in it.

Range of the prohibited frequencies: (complete) *band gap*

Physical reason: destructive interference

Practical interest: Design periodic materials which *have* band gaps!

Analytically very difficult!

Here: Computer-assisted proof of band gap.

Physical model: Homogeneous Maxwell's equations ($c = 1$)

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

$$\text{div} B = 0, \quad \text{div} D = 0,$$

together with the constitutive relations

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

(E electric field, H magnetic field, D displacement field, B magnetic induction field)

ε, μ: material tensors. *Isotropic* material: ε, μ scalar real-valued functions, not time-dependent
ε electric permittivity, μ magnetic permeability.

Photonic crystal: non-magnetic, i.e. $\mu \equiv 1$, $B \equiv H$.

Look for *monochromatic* waves:

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

Maxwell's equations give

$$\text{curl}E = -i\omega H, \qquad \text{curl}H = i\omega\varepsilon E, \qquad \text{div}H = 0, \qquad \text{div}(\varepsilon E) = 0.$$

Applying curl to the first two equations gives two decoupled systems:

$$\begin{aligned} \text{curl curl } E &= \omega^2 \varepsilon E \\ \text{div}(\varepsilon E) &= 0 \end{aligned} \qquad \text{and} \qquad \begin{aligned} \text{curl } \frac{1}{\varepsilon} \text{ curl}H &= \omega^2 H \\ \text{div}H &= 0 \end{aligned}$$

Operator theoretical formulation

$$L^2_{\text{div}}(\mathbb{R}^3) := \{u \in L^2(\mathbb{R}^3)^3 : \text{div}\ u = 0\} \quad \begin{cases} \subset L^2(\mathbb{R}^3)^3 \text{ closed} \\ \subset H(\text{div}, \mathbb{R}^3) \end{cases}$$

$$\mathcal{H} := L^2_{\text{div}}(\mathbb{R}^3) \cap H(\text{curl}, \mathbb{R}^3)$$

Maxwell's equation for H-field ($\text{curl}\frac{1}{\varepsilon}\text{curl}H = \omega^2 H,\ \text{div}H = 0$) reads, for $u := H$,

$$u \in \mathcal{H} \setminus \{0\},\ \int_{\mathbb{R}^3} \frac{1}{\varepsilon}(\text{curl}u) \cdot \overline{(\text{curl}v)}dx = \omega^2 \int_{\mathbb{R}^3} u \cdot \bar{v}dx \text{ for each } v \in \mathcal{H}$$

or, using $B[u,v] := \int_{\mathbb{R}^3} \frac{1}{\varepsilon}(\text{curl}u) \cdot \overline{(\text{curl}v)}dx + \int_{\mathbb{R}^3} u \cdot \bar{v}dx \quad (u, v \in \mathcal{H}),\ \lambda := \omega^2 + 1,$

$$\boxed{u \in \mathcal{H} \setminus \{0\},\ B[u,v] = \lambda \int_{\mathbb{R}^3} u \cdot \bar{v}dx \text{ for all } v \in \mathcal{H}} \quad (*)$$

Lax-Milgram yields selfadjoint operator $T : L^2_{\text{div}}(\mathbb{R}^3) \to \mathcal{H} \subset L^2_{\text{div}}(\mathbb{R}^3)$,

$$B[Tr, v] = \int_{\mathbb{R}^3} r \cdot \bar{v}dx \quad (r \in L^2_{\text{div}}(\mathbb{R}^3), v \in \mathcal{H}),$$

$D(A) := \text{range}(T) \subset \mathcal{H},\ A := T^{-1}$ selfadjoint. $(*) \Leftrightarrow \boxed{u \in D(A) \setminus \{0\},\ Au = \lambda u}$

Now let $\varepsilon \in L^\infty(\mathbb{R}^3)$ (with $\varepsilon \geq \varepsilon_{\mathsf{min}} > 0$) be periodic with periodicity cell $\Omega \subset \mathbb{R}^3$ (bounded parallelogram). Standard crystal: $\Omega = (0,1)^3$

Floquet-Bloch theory gives: The *spectrum* σ of $(*)$ has *band-gap* structure; more precisely:

$$\sigma = \bigcup_{n\in\mathbb{N}} I_n,$$

where I_n are compact real intervals with $\min I_n \to \infty$ as $n \to \infty$.

I_n is called the n-th *spectral band*.

"Usually", the bands I_n overlap. But there *might* be gaps between them.

These are the band-gaps of prohibited frequencies mentioned earlier.

Floquet-Bloch theory tells further:

$$I_n = \{\lambda_{k,n} : k \in K\}$$

where K is the *Brillouin zone* (compact set in $\mathbb{R}^3$, determined by $\Omega, K = [-\pi,\pi]^3$ if $\Omega = (0,1)^3$), and $\lambda_{k,n}$ n-th eigenvalue of (written formally)

$$\boxed{\text{curl}\left(\frac{1}{\varepsilon}\text{curl}u\right) + u = \lambda u \text{ on } \Omega, \text{div}u = 0 \text{ on } \Omega,\ e^{-ik\cdot x}u(x) \text{ satisfies periodic b.c. on } \partial\Omega}$$

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

Precise formulation of (k-dependent) problem on Ω:

(Problem with periodic boundary condition: trace of $u \in \mathcal{H}$ only in $H^{-\frac{1}{2}}(\partial\Omega)$.)

G discrete lattice associated with Ω ($G = \mathbb{Z}^3$ if $\Omega = (0,1)^3$).

Extension operator $E : L^2(\Omega)^3 \to L^2_{\text{loc}}(\mathbb{R}^3)^3$, $(Ev)(x+g) := v(x)$ $(x \in \Omega,\ g \in G)$.

Then boundary condition ($e^{-ik\cdot x}u(x)$ periodic) together with the required smoothness on Ω reads:

$$E(e^{-ik\cdot}u) \in H_{\text{loc}}(\text{curl}, \mathbb{R}^3) \cap H_{\text{loc}}(\text{div}, \mathbb{R}^3)$$

Let

$$\mathcal{H}_k := \{u \in L^2(\Omega)^3 : \text{div}u = 0,\ E(e^{-ik\cdot}u) \in H_{\text{loc}}(\text{curl}, \mathbb{R}^3) \cap H_{\text{loc}}(\text{div}, \mathbb{R}^3)\}$$

Eigenvalue problem generated by Floquet-Bloch theory

(curl($\frac{1}{\varepsilon}$curl$u$) $+ u = \lambda u$ on Ω, div$u = 0$ on Ω, $e^{-ik\cdot x}u(x)$ satisfies periodic b.c. on $\partial\Omega$) now reads:

$$u \in \mathcal{H}_k \setminus \{0\}, \quad \underbrace{\int_\Omega \frac{1}{\varepsilon}(\text{curl}u) \cdot \overline{(\text{curl}v)}dx + \int_\Omega u \cdot \bar{v}dx}_{=:B_\Omega(u,v)} = \lambda \int_\Omega u \cdot \bar{v}dx \quad (EWP_k)$$

$$\text{for all } v \in \mathcal{H}_k$$

Strategy for proving gap:

1) Choose finitely many *grid points* in K

2) Compute verified eigenvalue enclosures for $\lambda_{k,1}, \ldots, \lambda_{k,N}$ (N chosen fixed) for k in the *grid*

3) Use perturbation type argument to deduce from 2) also enclosures for $\lambda_{k,1}, \ldots, \lambda_{k,N}$ for k *between* grid-points

Together enclosure for $\lambda_{k,1}, \ldots, \lambda_{k,N}$ for *all* $k \in K$
$\longrightarrow$ enclosures for the bands $I_1, \ldots, I_N$
$\longrightarrow$ If a gap in these enclosures occurs: *proof of gap*

Perturbation argument:

Let $\mathcal{H}_k^0 \supset \mathcal{H}_k$ be given by omitting the condition div$u = 0$ in $\mathcal{H}_k$, i.e.

$$\mathcal{H}_k^0 := \{u \in L^2(\Omega)^3 : E(e^{-ik\cdot}u) \in H_{\text{loc}}(\text{curl}, \mathbb{R}^3) \cap H_{\text{loc}}(\text{div}, \mathbb{R}^3)\}$$

and consider, besides (EWP_k), the problem with $\mathcal{H}_k^0$ instead of $\mathcal{H}_k$:

$$u \in \mathcal{H}_k^0 \setminus \{0\},$$

$$\int_\Omega \frac{1}{\varepsilon}(\text{curl}u)\cdot\overline{(\text{curl}v)}dx + \int_\Omega u\cdot\bar{v}dx = \lambda \int_\Omega u\cdot\bar{v}dx \quad \text{for all} \quad v \in \mathcal{H}_k^0 \quad (\text{EWP}_\text{k}^0)$$

$\lambda = 1$ is an eigenvalue of infinite multiplicity of (EWP_k^0). (For each $\varphi \in H^2(\Omega)$ s.t. $e^{-ik\cdot x}\nabla\varphi(x)$ satisfies periodic b.c., $\nabla\varphi$ is an eigenfunction.)

This is the *only* difference between the spectra of (EWP_k) and (EWP_k^0)!

Defining $w(x) := e^{-ik\cdot x}u(x)$, we obtain the equivalent problem

$$\boxed{\begin{array}{l} w \in \mathcal{H}^0 \setminus \{0\}, \\ \int\limits_\Omega \frac{1}{\varepsilon}[\text{curl} w + ik \times w] \cdot \overline{[\text{curl} v + ik \times v]} dx + \int\limits_\Omega w \cdot \bar{v} dx = \lambda \int\limits_\Omega w \cdot \bar{v} dx \\ \hfill \text{for all } v \in \mathcal{H}^0 \end{array}} \quad (\widetilde{EWP_k^0})$$

where

$$\mathcal{H}^0 := \{w \in L^2(\Omega)^3 : Ew \in H_{\text{loc}}(\text{curl}, \mathbb{R}^3) \cap H_{\text{loc}}(\text{div}, \mathbb{R}^3)\}$$

(independent of k !)

Let k be one of the *gridpoints* (to be) chosen in the Brillouin zone K; consider perturbation $k+h$ of k.

Theorem: Let $[a,b] \subset \mathbb{R}$ be an interval such that, for some $n \in \mathbb{N}$,

$$(1<)\lambda_{k,n} < a < b < \lambda_{k,n+1}$$

(whence $[a,b] \subset$ resolvent set of unperturbed problem (EWP_k^0)), and let $|h| < \delta_k$, where $\delta_k > 0$ is such that

$$\delta_k \cdot \max\left\{1, \frac{1}{\varepsilon_{\min}} + \delta_k\right\} \cdot \max\left\{\frac{\lambda_{k,n}}{a-\lambda_{k,n}}, \frac{\lambda_{k,n+1}}{\lambda_{k,n+1}-b}\right\} \leq 1.$$

Then, $[a,b]$ is contained in the resolvent set of the perturbed problem (EWP_{k+h}^0).

Corollary: Let the assumptions of the Theorem hold for *all* gridpoints k in K, and suppose that

$$\bigcup_{\text{gridpoints } k \in K} \text{Ball}(k, \delta_k) \supset K.$$

Then, $[a,b]$ is contained in a spectral band-gap.

Remaining task: Compute enclosures for eigenvalues $\lambda_{k,1}, \ldots, \lambda_{k,N}$ of (EWP_k) for all *gridpoints* k; $N \in \mathbb{N}$ chosen fixed.
Let $k \in K$ denote a fixed gridpoint now.

First step: Compute *approximate* eigenpairs to

$$u \in \mathcal{H}_k \setminus \{0\}, \quad \underbrace{\int_\Omega \frac{1}{\varepsilon}(\text{curl}\, u) \cdot \overline{(\text{curl}\, v)} dx + \int_\Omega u \cdot \bar{v} dx}_{=: B_\Omega(u,v)} = \lambda \int_\Omega u \cdot \bar{v} dx \quad \text{for all } v \in \mathcal{H}_k \qquad (EWP_k)$$

by Ritz method with appropriate basis functions in $\mathcal{H}_k$

Second step: Upper eigenvalue bounds by Rayleigh-Ritz method (with approximate eigenfunctions as basis functions)

Third step: Lower eigenvalue bounds by Lehmann-Goerisch method

Rayleigh-Ritz-Method (upper bounds)

Fix k in the grid.

Theorem. Let $\tilde{u}_{k,1}, \dots, \tilde{u}_{k,N} \in \mathcal{H}_k$ be linearly independent (approximate eigenfunctions),

$$\begin{aligned} \mathbf{A} &= \Big(B_\Omega(\tilde{u}_{k,n}, \tilde{u}_{k,m})\Big)_{n,m=1,\dots,N} \\ \mathbf{B} &= \Big(\langle \tilde{u}_{k,n}, \tilde{u}_{k,m} \rangle_{L^2}\Big)_{n,m=1,\dots,N} \end{aligned}$$

and let $\Lambda_{k,1} \leq \cdots \leq \Lambda_{k,N}$ be the eigenvalues of

$$\mathbf{Ax} = \mathbf{\Lambda Bx}.$$

Then

$$\lambda_{k,n} \leq \Lambda_{k,n} \qquad (n = 1, \dots, N).$$

Lehmann-Goerisch-Method

for *lower* eigenvalue bounds (k in the grid still fixed):

Choose a fixed shift parameter $\gamma > -1$. Compute additional approximations $\tilde{\sigma}_{k,n}$ satisfying, for $n = 1, \ldots, N$,

$$\frac{1}{\varepsilon}\tilde{\sigma}_{k,n} \in H(\mathsf{curl}, \Omega), \quad E\left(e^{-ik\cdot}\frac{1}{\varepsilon}\tilde{\sigma}_{k,n}\right) \in H_{\mathsf{loc}}(\mathsf{curl}, \mathbb{R}^3),$$
$$\tilde{\sigma}_{k,n} \approx \frac{1}{\tilde{\lambda}_{k,n} + \gamma}\mathsf{curl}\tilde{u}_{k,n}$$

Moreover, suppose that $\beta \in \mathbb{R}$ is known such that

$$\boxed{\Lambda_{k,N} < \beta - \gamma \leq \lambda_{k,N+1}}$$

Theorem (Goerisch). Define

$$\begin{aligned}
\mathbf{A} &= \Big(B_\Omega(\tilde{u}_{k,m}, \tilde{u}_{k,n})\Big)_{m,n=1,\dots,N} \in \mathbb{C}^{N,N}, \\
\mathbf{B} &= \Big(\langle \tilde{u}_{k,m}, \tilde{u}_{k,n}\rangle_{L^2}\Big)_{m,n=1,\dots,N} \in \mathbb{C}^{N,N}, \\
\mathbf{S} &= \Big(\langle \frac{1}{\varepsilon}\tilde{\sigma}_{k,m}, \tilde{\sigma}_{k,n}\rangle_{L^2}\Big)_{m,n=1,\dots,N} \in \mathbb{C}^{N,N}, \\
\mathbf{T} &= \frac{1}{\gamma+1}\Big(\langle \tilde{u}_{k,m} - \mathrm{curl}\left(\frac{1}{\varepsilon}\tilde{\sigma}_{k,m}\right), \tilde{u}_{k,n} - \mathrm{curl}\left(\frac{1}{\varepsilon}\tilde{\sigma}_{k,n}\right)\rangle_{L^2}\Big)_{m,n=1,\dots,N} \in \mathbb{C}^{N,N}.
\end{aligned}$$

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

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

of the eigenvalue problem

$$\Big(\mathbf{A} + (\gamma - \beta)\mathbf{B}\Big)\mathbf{x} = \theta\mathbf{N}\mathbf{x}$$

are negative, we have $\beta - \gamma - \frac{\beta}{1-\theta_n} \leq \lambda_{n,k}$ for $n = 1, \cdots N$.

Spectral Homotopy

For determining β such that $\Lambda_{k,N} < \beta - \gamma \leq \lambda_{k,N+1}$, let

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

and consider the family of eigenvalue problems

$$u \in \mathcal{H}_k \setminus \{0\},\ \int_\Omega \frac{1}{\varepsilon_s(x)}(\mathrm{curl}u) \cdot \overline{(\mathrm{curl}v)}dx + \int_\Omega u \cdot \bar{v} dx = \lambda^{(s)} \int_\Omega u \cdot \bar{v} dx$$

$$\text{for all} \quad v \in \mathcal{H}_k,$$

$0 \leq s \leq 1$, k still fixed in the grid. Eigenvalues $(\lambda_n^{(s)})_{n\in\mathbb{N}}$.

For $\mathbf{s = 0}$: eigenvalues $\lambda_n^{(0)}$ are *known*

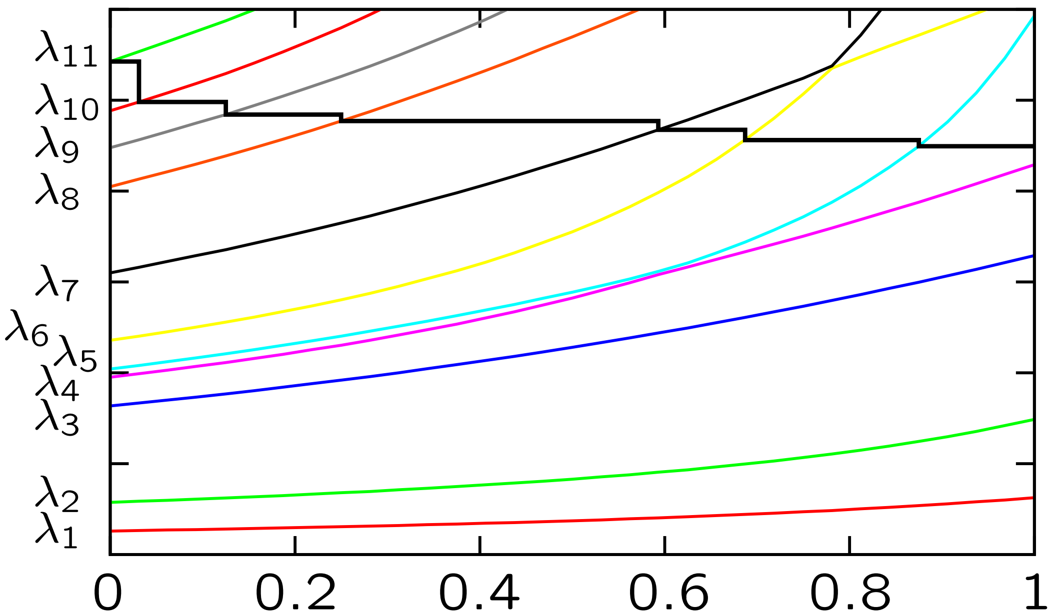
For $\mathbf{s = 1}$: $\lambda_n^{(1)} = \lambda_{k,n}$ $(n \in \mathbb{N})$.

Lemma. For each fixed $n \in \mathbb{N}$,

$$\lambda_n^{(s)} \leq \lambda_n^{(t)} \qquad \text{for } 0 \leq s \leq t \leq 1.$$

(Proof by Poincaré's min-max principle.)

Spectral Homotopy



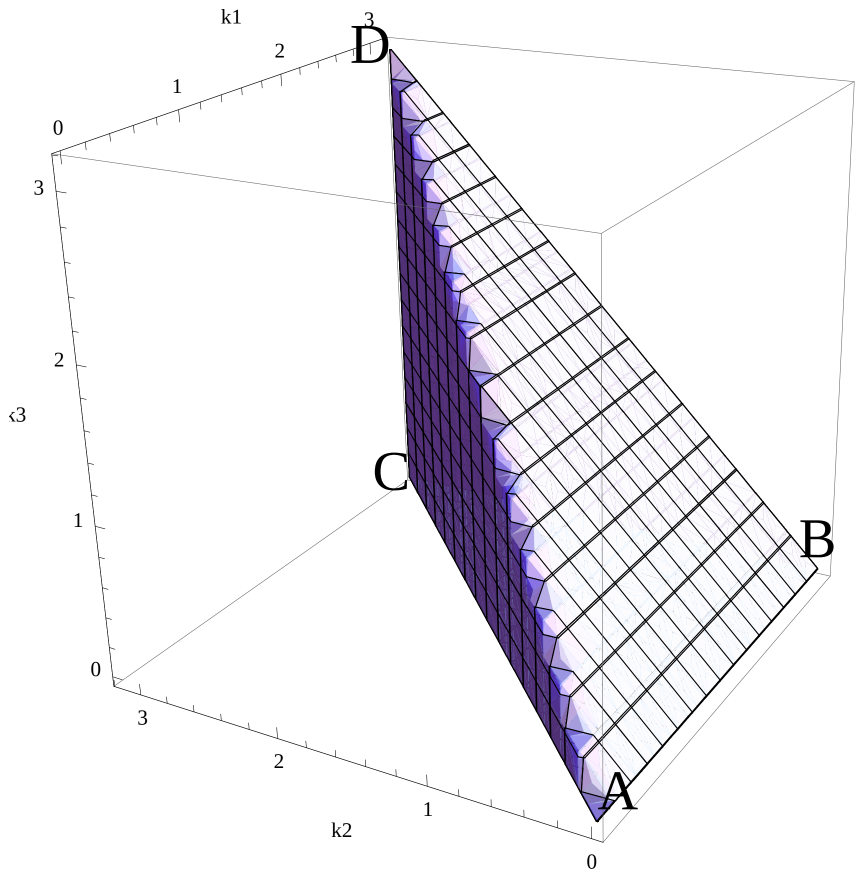
Concrete case: $\Omega = (0,1)^3$, $\varepsilon(x) := \begin{cases} 1 & \text{if } \left|x - \left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)\right| < \frac{1}{2} \\ 25 & \text{otherwise} \end{cases}$

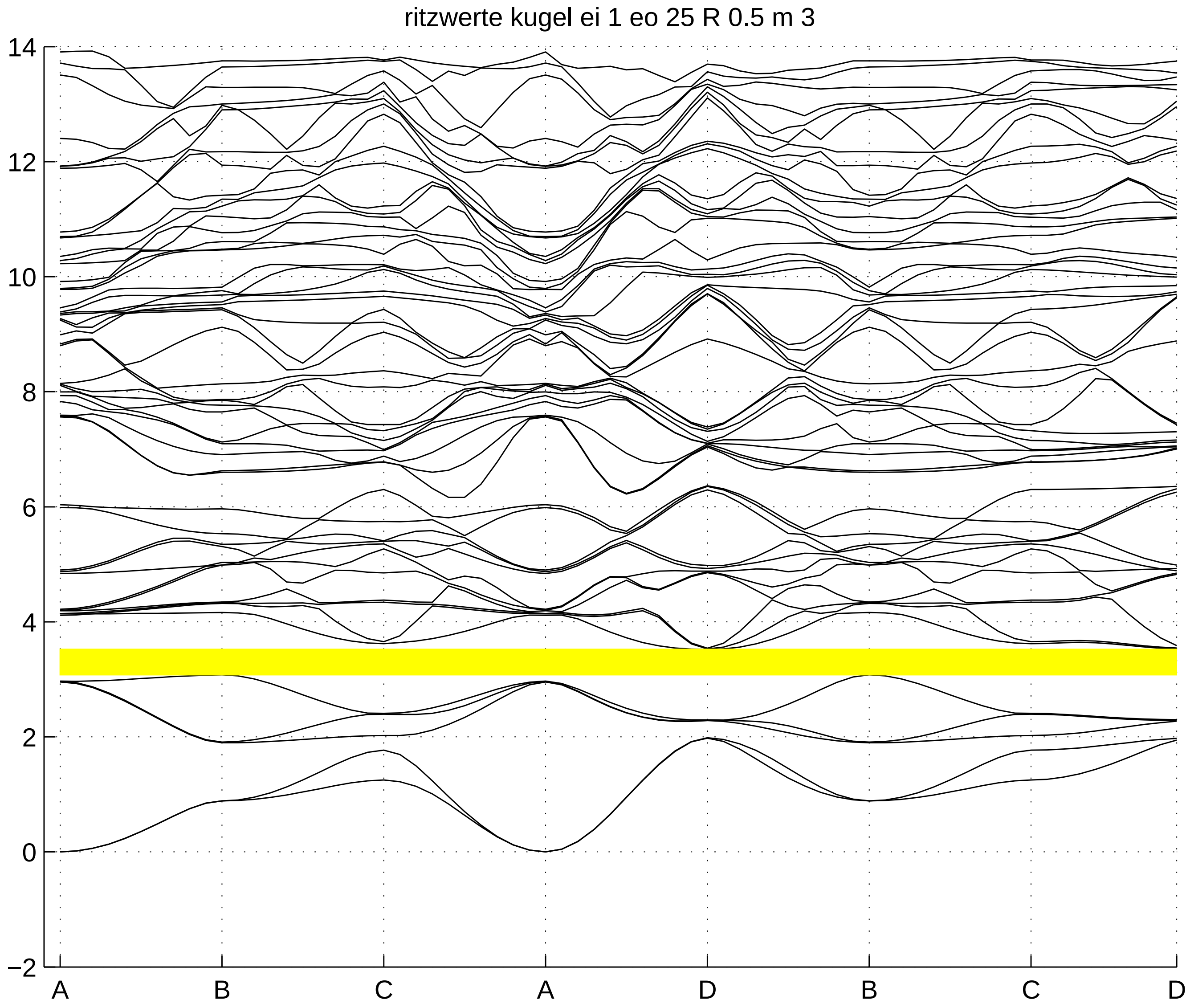
Basis functions: combination of

a) plane waves: $A_n^{(k)} e^{i(2\pi n + k)\cdot x}, n \in \mathbb{Z}^3,\ A_n^{(k)} \in \mathbb{C}^3,\ A_n^{(k)} \cdot (2\pi n + k) = 0$

b) certain functions which are non-zero only on the ball $\left|x - \left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)\right| < \frac{1}{2}$, constructed via polynomials in r and spherical harmonics in φ, θ.

By symmetry, only the following part of the Brillouin zone K needs to be considered: `Show[B, T]`

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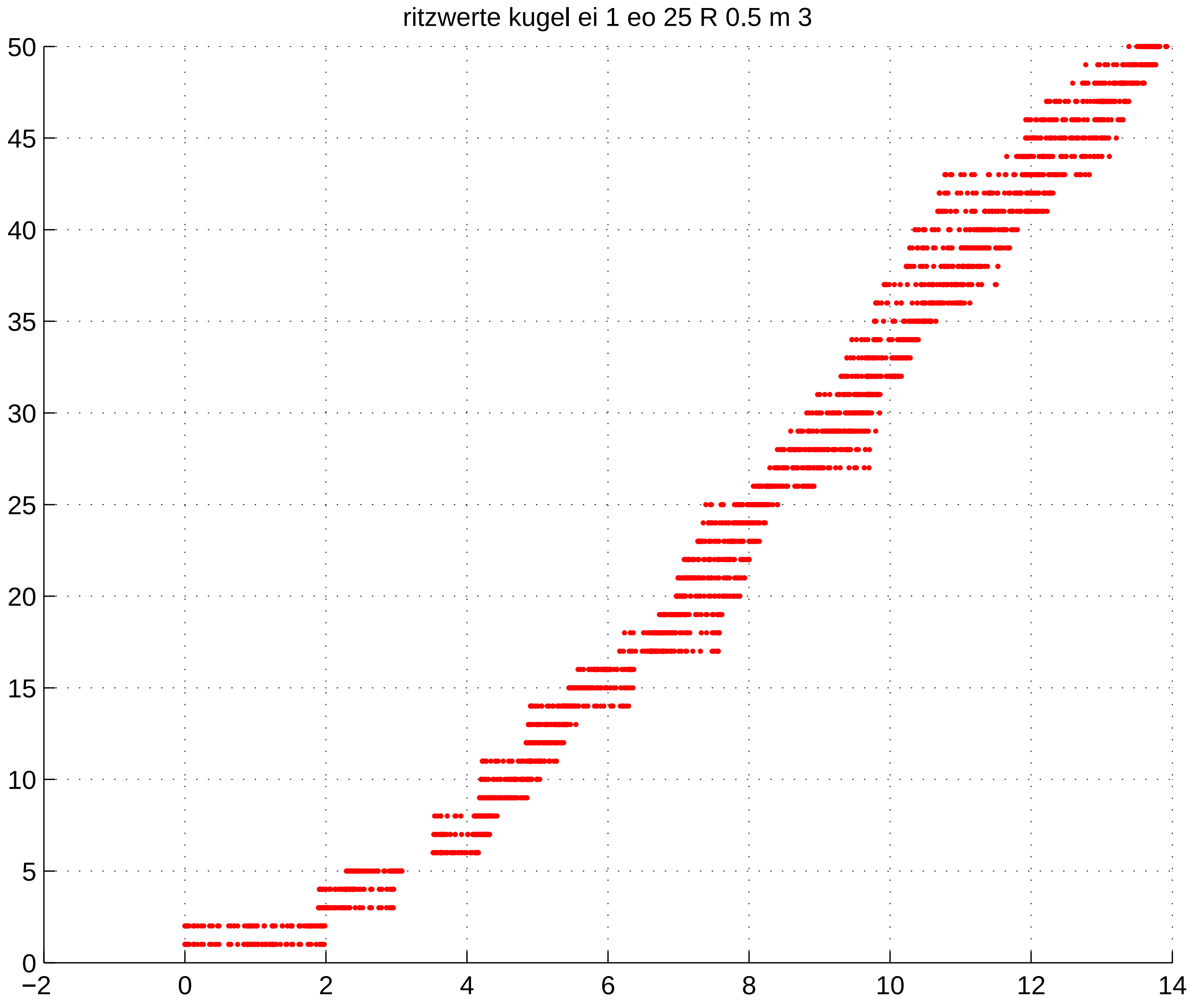

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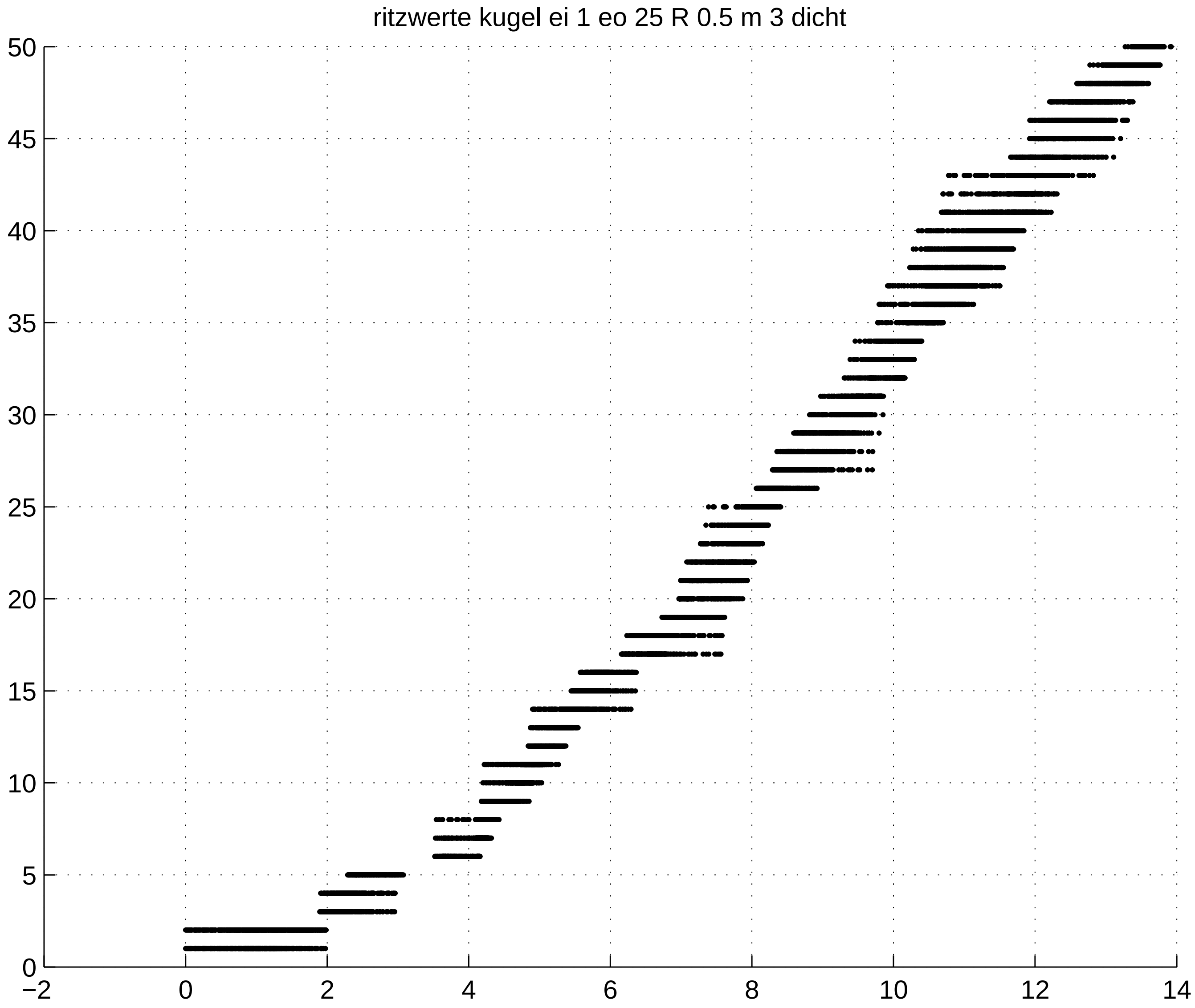
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jointly with V. Hoang, C. Wieners:

$2D$-situation: $\varepsilon = \varepsilon(x_1, x_2)$, *polarized* wave $E = (0, 0, u)$

$\Rightarrow 0 = \text{div}(\varepsilon E) = \frac{\partial}{\partial x_3}(\varepsilon u) = \varepsilon \frac{\partial u}{\partial x_3}$, i.e. $\frac{\partial u}{\partial x_3} = 0$, $u = u(x_1, x_2)$.

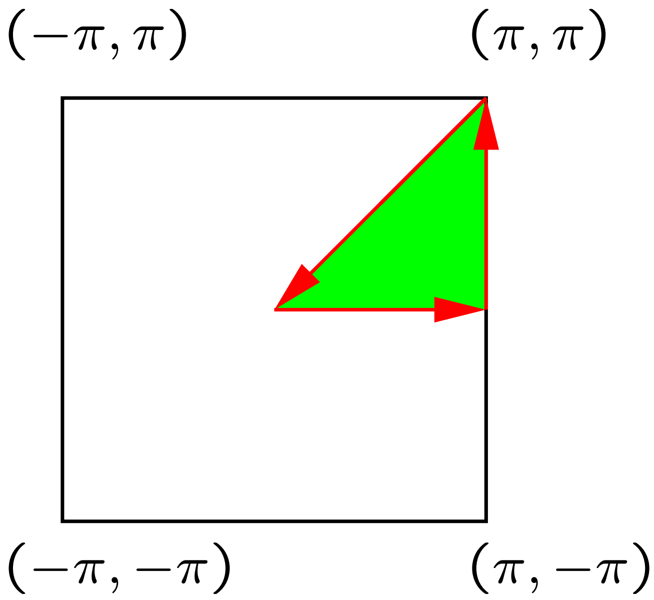
$$\Rightarrow \text{curl curl } E = \begin{pmatrix} 0 \\ 0 \\ -\Delta u \end{pmatrix}$$

Maxwell's equation gives, with $\lambda = \omega^2$, $\Delta = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2}$

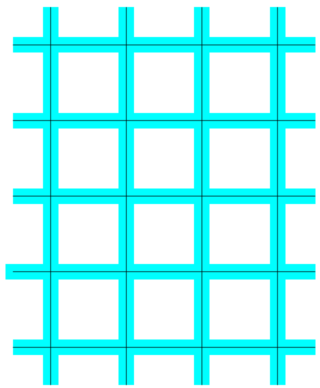
$$(\,*\,) \qquad \boxed{-\Delta u = \lambda \varepsilon u} \qquad \text{equation on whole of } \mathbb{R}^2$$

A Candidate

Let $\Lambda = \mathbb{Z}^2$, $\Omega = (0,1)^2$ and $K = [-\pi, \pi]^2$. We set $\varepsilon(x) = 1$ 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)

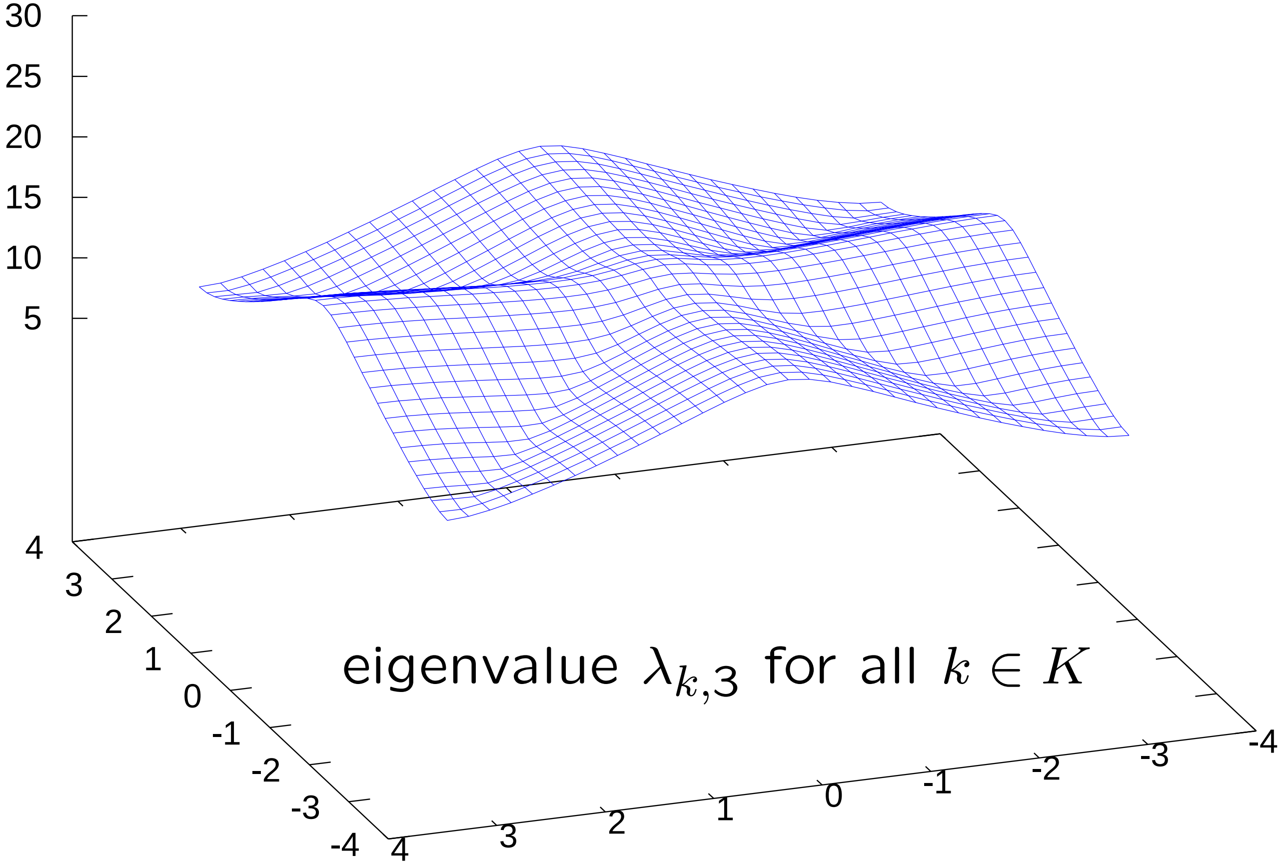


Brillouin zone K



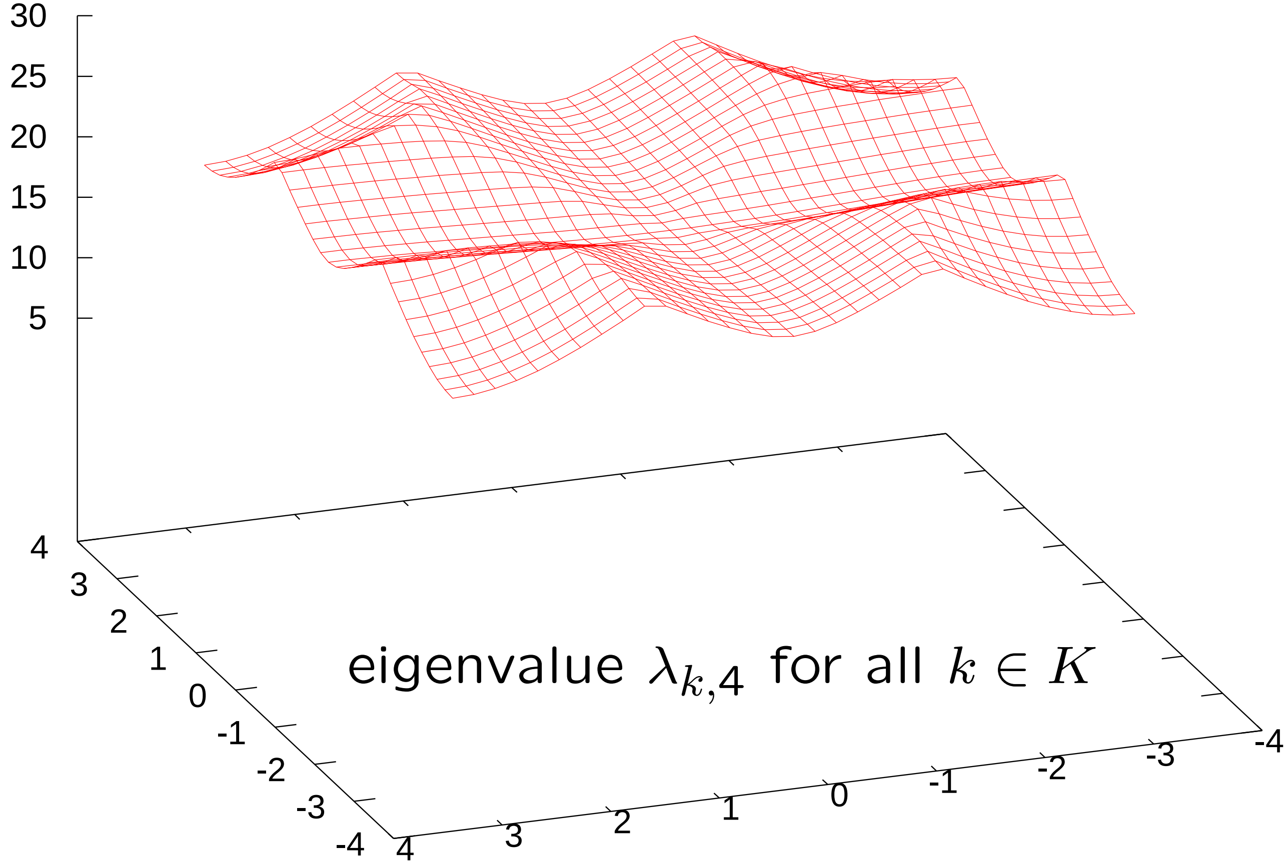
periodic material distribution ε

A Candidate



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

A Candidate



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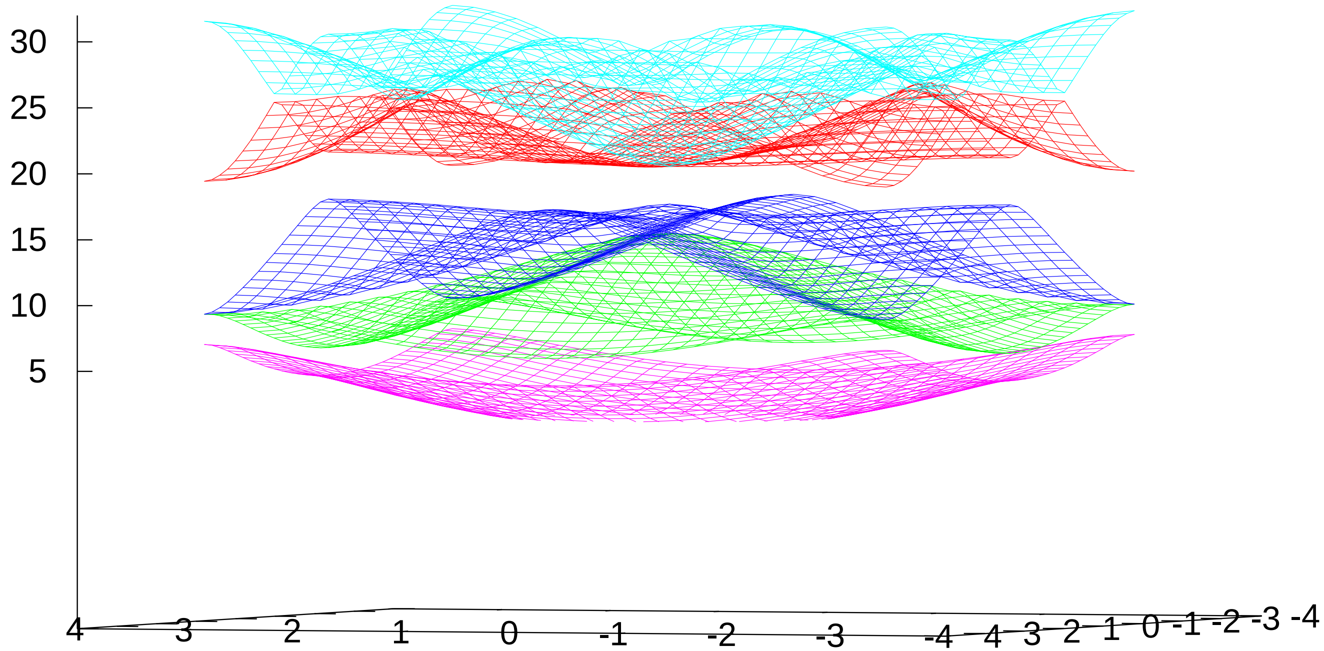
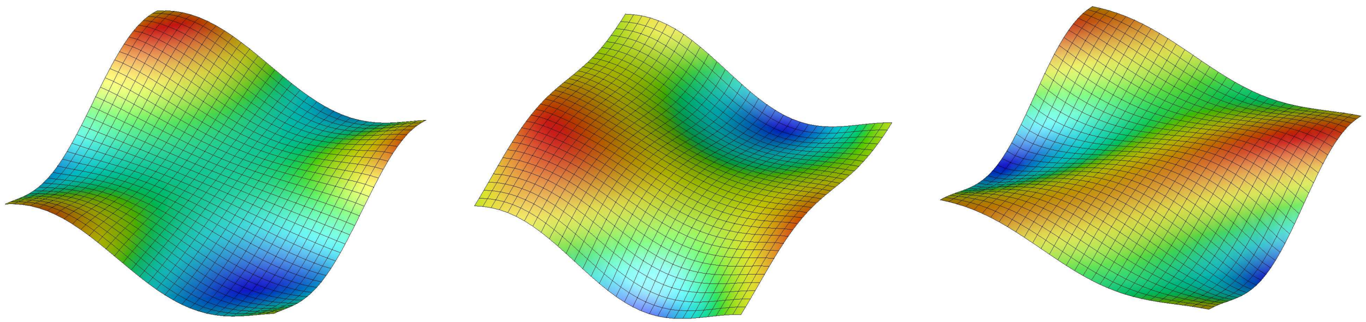
eigenvalue $\lambda_{k,4}$ for all $k \in K$

A Candidate

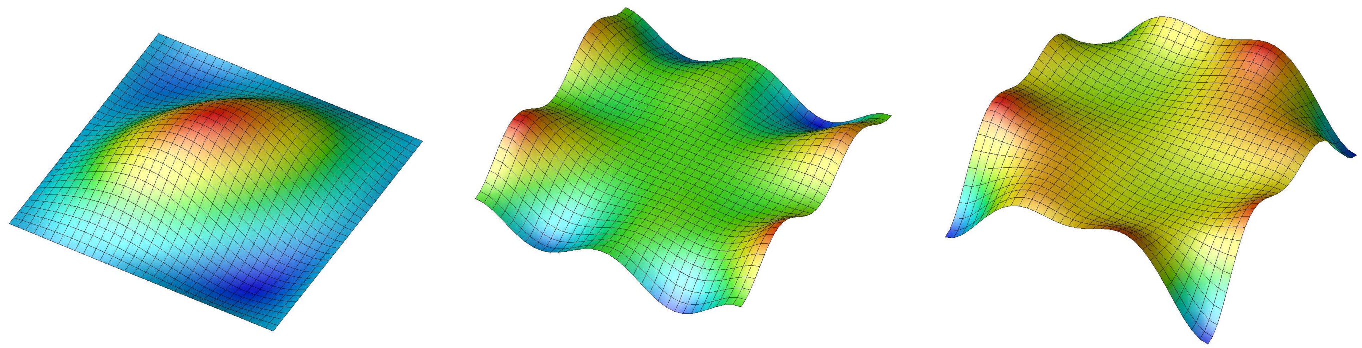


eigenvalues $\lambda_{k,1}, ..., \lambda_{k,5}$ for all $k \in K$

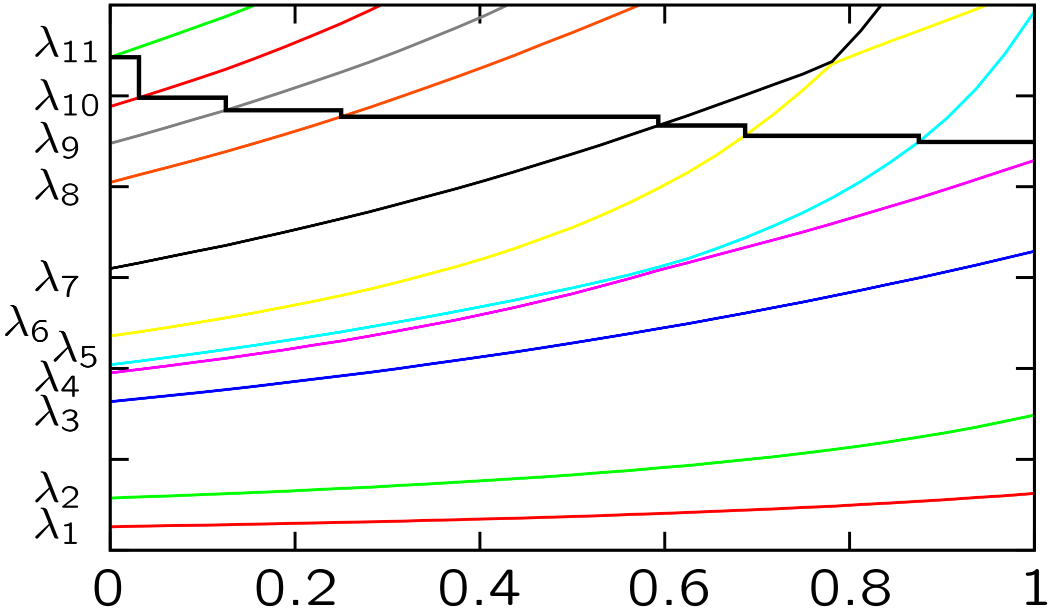
A Candidate



eigenfunctions $u_{k,1}, ..., u_{k,6}$ for $k = (\pi, \pi)$



Spectral Homotopy for $k = (2.5130, 0.4046)$



$\lambda_{10}^{(s)} \geq 27.13$ for $s \geq 1/32$ $\quad\lambda_7^{(s)} \geq 23.37$ for $s \geq 19/32$

$\lambda_9^{(s)} \geq 24.90$ for $s \geq 4/32$ $\quad\lambda_6^{(s)} \geq 22.81$ for $s \geq 22/32$

$\lambda_8^{(s)} \geq 23.85$ for $s \geq 8/32$ $\quad\lambda_5^{(s)} \geq 22.47$ for $s \geq 28/32$

Spectral Homotopy for $k = (2.5130, 0.4046)$

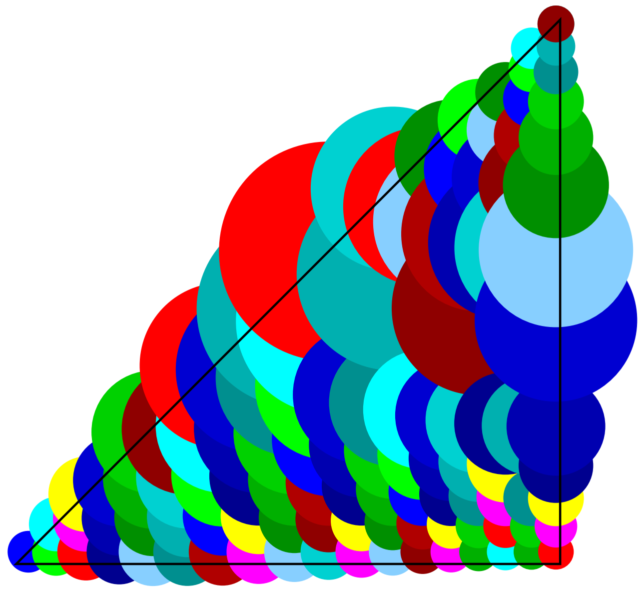
s	0	4/32	8/32	19/32
λ_1	(1.295, 1.296)	(1.402, 1.403)	(1.528, 1.529)	(2.017, 2.018)
λ_2	(2.875, 2.876)	(3.114, 3.115)	(3.396, 3.397)	(4.526, 4.527)
λ_3	(8.174, 8.175)	(8.840, 8.841)	(9.594, 9.595)	(12.189,12.190)
λ_4	(9.754, 9.755)	(10.563,10.564)	(11.523,11.524)	(15.397,15.398)
λ_5	(10.208,10.209)	(11.048,11.049)	(12.019,12.020)	(15.575,15.577)
λ_6	(11.788,11.789)	(12.783,12.784)	(14.019,14.020)	(19.920,19.921)
λ_7	(15.507,15.508)	(16.778,16.779)	(18.236,18.237)	(23.339,23.373)
λ_8	(20.246,20.247)	(21.907,21.913)	(23.786,23.832)	
λ_9	(22.386,22.387)	(24.210,24.213)		
λ_{10}	(24.419,24.420)			

s	19/32	22/32	28/32	1
λ_1	(2.017, 2.018)	(2.204, 2.205)	(2.690, 2.691)	(3.127, 3.128)
λ_2	(4.526, 4.527)	(4.979, 4.980)	(6.220, 6.221)	(7.433, 7.434)
λ_3	(12.189,12.190)	(13.046,13.048)	(14.981,14.985)	(16.445,16.452)
λ_4	(15.397,15.398)	(16.653,16.655)	(19.383,19.389)	(21.422,21.450)
λ_5	(15.575,15.577)	(17.188,17.190)	(22.451,22.465)	
λ_6	(19.920,19.921)	(22.809,22.813)		
λ_7	(23.339,23.373)			

A Verified Band Gap

This figure illustrates the covering

$$K \subset \bigcup_{k \in \text{grid}} \text{Ball}(k, r_k)$$



Eigenvalue bounds (in grid) and perturbation arguments give $\lambda_{k,3} \leq 18.2$, $\lambda_{k,4} \geq 18.25$ for all $k \in K$.

This proves the existence of a band gap

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

for the spectral problem $-\Delta u = \lambda \varepsilon u$ in $\mathbb{R}^2$.

The proof requires the close approximation of more than 5 000 eigenvalues and eigenfunctions (for 100 vectors $k \in$ grid with up to 7 homotopy steps each) and takes about 90 h computing time.