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Bandgap Calculations For Photonic Crystals*

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Abstract

We study the propagation of light in a three-dimensional periodic photonic crystal, of which the electric permittivity is a complex nonlinear function of both space and frequency. We introduce the correct functional space $V_{\boldsymbol{k}}^{(\varepsilon)}$ needed to ensure that the operator corresponding to the weak formulation has a discrete spectrum, i.e., at most countably many isolated eigenvalues of finite multiplicity. Moreover, for two-dimensional photonic crystals, we present an a posteriori error estimator that can be used for the development of adaptive finite element methods.

Keywords: photonic crystals, eigenvalue problem, adaptive finite element method, a posteriori error estimator

1 Introduction

Photonic crystals are periodic materials that affect the propagation of electromagnetic waves. We say that a crystal is one-, two- or three-dimensional if its structure is periodic in one, two or three dimensions, respectively and constant in the other dimensions of $\mathbb{R}^3$. Such structures are sketched in Fig. 1.1. Photonic crystals can occur naturally (e.g. on

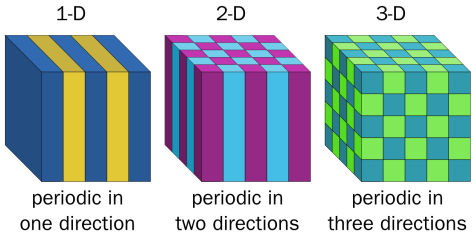

Fig. 1.1: From left to right: Sketchs of one-, two- and three-dimensional crystals.

butterfly wings or in opal stone) but they can also be designed and manufactured with the aim of modifying and controlling the propagation of electromagnetic waves in the *visible spectrum*, hence the name *photonic* crystals. The key property of such periodic structures is that, for certain material configurations, gaps between the bands of possibly propagating wavelengths can occur [Kuc01]. These gaps charaterize intervals of wavelengths that cannot

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propagate in the periodic structure. The occurrence of bandgaps in photonic crystals makes them interesting for wide range of applications in optical or electronic devices (e.g. wave guides or optical filters for solar cells).Therefore, finding materials and geometries with especially wide bandgaps is an ongoing research and engineering effort.

To analyze the interaction of electromagnetic waves with periodic dielectric materials, one can calculate the eigenfrequencies and the eigenfunctions representing the corresponding electric and magnetic fields resulting from the time-harmonic Maxwell equations. To calculate these eigenfrequencies one models an infinite periodic structure in space and formulates the time-harmonic Maxwell equations with no charge or current present.

The resulting Maxwell eigenvalue problems depend on various parameters and may be nonlinear in the eigenvalue. The parameters describing the material of the structure are typically nonlinear functions of the desired frequency. The configuration of the periodic geometry may also be modified and can be considered as a parameter. Finally, through the mathematical treatment of the PDE eigenvalue problem another parameter, the wavevector, is introduced in order to reduce the problem from an infinite domain to a family of problems, parametrized by the wavevector, on a finite domain.

In order to solve the problem of finding a material and geometric structure with an especially wide bandgap, one needs to solve many of those nonlinear eigenvalue problems during each step of the optimization process. Therefore, it is essential to have an efficient way of solving these eigenvalue problems. It is known [BO91] that an efficient way of discretizing PDE eigenvalue problems on geometrically complicated domains is an adaptive finite element method (AFEM). To investigate the performance of AFEM for the described problems, reliable and efficient error estimators for nonlinear parameter dependent eigenvalue problems are needed.

Solving the finite-dimensional nonlinear problem resulting from the AFEM discretization, in general, cannot be done directly, as the systems are usually large. Thus, an iterative solution process produces another error to be considered in the error analysis. It is therefore desirable to balance the errors and computational work between the discretization error of the AFEM and the error in the solution of the resulting finite dimensional nonlinear eigenvalue problems.

2 The model problem

The behavior of electromagnetic waves in media can be modeled mathematically by the macroscopic Maxwell equations. In this section we will derive the governing partial differential equations for the propagation of electromagnetic waves (e.g. light) in general and explain some assumptions that can be made to simplify the model in the case of considering periodic, dielectric materials with no charge or current present.

We follow the derivation of the model problem in [Kuc01], which was itself inspired by the works in [JJWM08] and [DLP$^+$11].

2.1 The Maxwell equations

The *macroscopic Maxwell equations* model any kind of behavior of electromagnetic waves in media. In absence of free charges and currents, they are given by

$$\begin{aligned} \nabla \times \mathbf{E} &= -\frac{\partial \mathbf{B}}{\partial t}, & \nabla \cdot \mathbf{B} &= 0, \\ \nabla \times \mathbf{H} &= \frac{\partial \mathbf{D}}{\partial t}, & \nabla \cdot \mathbf{D} &= 0, \qquad \text{in } \mathbb{R}^3 \end{aligned} \tag{2.1}$$

with $\mathbf{E}$ *the (macroscopic) electric field*, $\mathbf{H}$ *the (macroscopic) magnetic field*, $\mathbf{D}$ *the displacement field*, $\mathbf{B}$ *the magnetic induction field*, and c *the speed of light*. All quantities are expressed in SI units and are, in general, dependent on space and time.

Remark 2.1. *In this paper, bold letters are used to designate three-dimensional quantities only. Non-bold symbols are used to denote one-, two, and d-dimensional quantities, where d is a parameter in* $\mathbb{N}$*. Moreover, we use the standard notation* $\nabla\times$*,* $\nabla\cdot$*, and* ∇ *to denote the curl, the divergence and the gradient operators, respectively.*

To determine the relationship between $\mathbf{E}$ and $\mathbf{D}$, as well as between $\mathbf{H}$ and $\mathbf{B}$, several physical models exist. $\mathbf{D}$ is usually defined through $\mathbf{E}$ and a *polarization field* $\mathbf{P}$ as in [DLP+11, pp. 2]:

$$\mathbf{D} = \varepsilon_0 \mathbf{E} + \mathbf{P}, \tag{2.2}$$

The polarization $\mathbf{P}$ is determined by *the electric susceptibility* χ_ε of the material, a measure of how easily a dielectric material polarizes in response to an electric field. The simplest model for the polarization field is

$$\mathbf{P} = \varepsilon_0 \chi_\varepsilon \mathbf{E}, \tag{2.3}$$

where the polarization is proportionally related to the electric field through the electric susceptibility factor and the vacuum permittivity. This model describes an instantaneous polarization of the material on application of an electric field, which is physically not realistic. Therefore we introduce a time-lag into the model through a time dependency of χ_ε and a convolution operation. Eq. (2.3) is modified as follows:

$$\mathbf{P}(t) = \varepsilon_0 \int_{-\infty}^{t} \chi_\varepsilon(t-s)\mathbf{E}(s)\,\mathrm{d}s = \varepsilon_0 \left(\chi_\varepsilon \star \mathbf{E}\right)(t). \tag{2.4}$$

Considering the problem in the frequency domain instead of the time domain by applying a Fourier transformation [Wer11, Ch. V.2] to Eqs. (2.1) and (2.4) has multiple advantages. One of them is that it enables a spectral analysis of the electromagnetic field. Another one is that we regain a proportional relation between $\mathbf{P}$ and $\mathbf{E}$ after Fourier transformation of Eq. (2.4):

$$\mathbf{P}(\omega) = \varepsilon_0 \chi_\varepsilon(\omega)\mathbf{E}(\omega). \tag{2.5}$$

Note that we represent a function $f(t)$ and its Fourier transform $f(w)$ with the same symbol f. We have used the property that the Fourier transform of a convolution in the time domain is a multiplication in the frequency domain, i.e., $(f \star g)(\omega) = f(\omega)g(\omega)$. With this tool we have recovered a relationship similar to Eq. (2.3), but in frequency domain.

If we apply a Fourier transformation Eq. (2.2) and insert Eq. (2.5) into it, we get the linear relationship

$$\mathbf{D}(\omega) = \varepsilon_0 \mathbf{E}(\omega) + \varepsilon_0 \chi_\varepsilon(\omega)\mathbf{E}(\omega) = \varepsilon_0 \left(1 + \chi_\varepsilon(\omega)\right)\mathbf{E}(\omega) = \varepsilon(\omega)\mathbf{E}(\omega), \tag{2.6}$$

where $\varepsilon(\omega) = \varepsilon_0(1 + \chi_\varepsilon(\omega))$ is the Fourier transform of *the electric permittivity* $\varepsilon(t)$ of the material.

An analogous consideration yields

$$\mathbf{B}(\omega) = \mu(\omega)\mathbf{H}(\omega) \tag{2.7}$$

for μ the (Fourier transform of the) *magnetic permeability*. In general, the permeability may depend on the frequency ω. However, we consider here only nonmagnetic materials and therefore restrict ourselves to the case of a constant μ, which we scale to $\mu = 1$.

We proceed by applying a Fourier transformation to the entire system of Maxwell's equations

$$\begin{aligned} \nabla \times \mathbf{E}(\boldsymbol{x}, \omega) &= -i\omega \mathbf{B}(\boldsymbol{x}, \omega), & \nabla \cdot \mathbf{B} &= 0, \\ \nabla \times \mathbf{H}(\boldsymbol{x}, \omega) &= i\omega \mathbf{D}(\boldsymbol{x}, \omega), & \nabla \cdot \mathbf{D} &= 0, \qquad \text{in } \mathbb{R}^3. \end{aligned}$$

We have used the property that the Fourier transform of a time derivative in the time domain is a multiplication by $i\omega$ in the frequency domain, i.e., $\frac{\partial f}{\partial t}(\omega) = i\omega f(\omega)$. This yields time independent equations in which the displacement and induction fields can be replaced by use of the linear relations in Eq. (2.6) and Eq.(2.7) in frequency domain. This yields

$$\begin{aligned} \nabla \times \mathbf{E} &= -i\omega\mu\mathbf{H}, & \nabla \cdot (\mu\mathbf{H}) &= 0, \\ \nabla \times \mathbf{H} &= i\omega\varepsilon\mathbf{E}, & \nabla \cdot (\varepsilon\mathbf{E}) &= 0, \qquad \text{in } \mathbb{R}^3. \end{aligned}$$

In matrix form we get the eigenvalue problem

$$\begin{bmatrix} 0 & -\frac{i}{\varepsilon}\nabla\times \\ \frac{i}{\mu}\nabla\times & 0 \end{bmatrix} \begin{bmatrix} \mathbf{E} \\ \mathbf{H} \end{bmatrix} = \omega \begin{bmatrix} \mathbf{E} \\ \mathbf{H} \end{bmatrix}. \tag{2.8}$$

Note that the constraints

$$\nabla \cdot (\varepsilon\mathbf{E}) = 0, \quad \nabla \cdot (\mu\mathbf{H}) = 0$$

are naturally fulfilled in this formulation, since

$$i\omega\nabla \cdot (\varepsilon\mathbf{E}) = \nabla \cdot (\nabla \times \mathbf{H}) = 0$$

and

$$-i\omega\nabla \cdot (\mu\mathbf{H}) = \nabla \cdot (\nabla \times \mathbf{E}) = 0.$$

Indeed, the divergence of a curl-operator vanishes for all vector fields on $\mathbb{R}^3$.

Remark 2.2. *These constraints, however, need to be kept in mind, especially during the discretization of the problem. Indeed, finite-dimensional subspaces do not necessarily inherit the property that* $\nabla \cdot (\nabla \times \mathbf{F}) = 0$ *for all* $\mathbf{F}$ *and the constraints need then to be enforced.*

The system now consist of two equations in two variables, which can be combined into a single second order differential equation. Substituting either $\mathbf{E}$ or $\mathbf{H}$ yields to one of the following equivalent eigenvalue problems, respectively

$$\nabla \times \left(\frac{1}{\varepsilon}\nabla \times \mathbf{H}\right) = \nabla \times (i\omega\ \mathbf{E}) = i\omega\,(-i\omega\mu\ \mathbf{H}) = \omega^2\mu\ \mathbf{H} \quad \text{in } \mathbb{R}^3$$

and

$$\nabla \times \left(\frac{1}{\mu}\nabla \times \mathbf{E}\right) - \omega^2\varepsilon\ \mathbf{E} = 0 \quad \text{in } \mathbb{R}^3. \tag{2.9}$$

We make the arbitrary choice to work with Eq. (2.9) in the remainder. In general, the dependence on time and space of $\mathbf{E}$ and $\mathbf{H}$ can be very complex. In order to simplify the system, we assume the time dependency to be harmonic, i.e., we take the ansatz $\mathbf{E}(x,\omega) = \mathbf{E}(x)e^{i\tau\omega}$. This ansatz is justified for a linear system like the Maxwell equations. Indeed, it is known from Fourier analysis that any general solution can be built on a linear combination of these harmonic modes.

In this way, we can eliminate the ω-dependence of the electromagnetic field from the eigenvalue problem

$$\nabla \times \left(\frac{1}{\mu}\nabla \times \mathbf{E}(\boldsymbol{x})\right) - \omega^2 \varepsilon(\boldsymbol{x},\omega)\mathbf{E}(\boldsymbol{x}) = 0 \quad \text{in } \mathbb{R}^3. \tag{2.10}$$

2.2 Simplification in the two-dimensional case

In the case of a two-dimensional crystal, i.e., a periodic medium which has material properties that are independent of at least one coordinates, the eigenvalue problem Eq. (2.10) can be substantially simplified. To see this, we consider that the electric permittivity $\varepsilon(x)$ is independent of x_3, i.e., $\varepsilon(\boldsymbol{x}) = \varepsilon(x_1, x_2)$. It follows by symmetry that the electromagnetic field $(\boldsymbol{E}, \boldsymbol{H})$ is independent of x_3 as well. In this case, Eq. (2.8) reduces to a matrix equation where the sets of variables (E_1, E_2, H_3) and (E_3, H_1, H_2) are decoupled [Kuc01]. The first set of variables characterizes the transverse electric polarized field $(\boldsymbol{E}_{TE}, \boldsymbol{H}_{TE}) := (E_1, E_2, 0, 0, 0, H_3)$, whereas the second set of variables characterizes the transverse magnetic polarized field $(\boldsymbol{E}_{TM}, \boldsymbol{H}_{TM}) := (0, 0, E_3, H_1, H_2, 0)$. With this decoupling the eigenvalue problem (2.8) can be reduced to a pair of two-dimensional scalar eigenvalue problems:

$$\begin{aligned} -\Delta E_3 &= \omega\varepsilon(x_1, x_2, \omega)E_3, \\ -\nabla \cdot \frac{1}{\varepsilon(x_1, x_2, \omega)}\nabla H_3 &= \omega H_3 \end{aligned} \tag{2.11}$$

The fact that Eq. (2.11) contains gradient and divergence operators instead of curl operators, as in Eq. (2.10), makes the spectral analysis of two-dimensional photonic crystals easier (see Section 7).

3 Periodic structures

The strong formulation of the model problem derived in Section 2.1 reads: Find $(\omega, \mathbf{E}) \in \mathbb{C} \times V$ such that

$$L(\varepsilon,\omega)\mathbf{E}(\boldsymbol{x}) := \nabla \times (\frac{1}{\mu}\nabla \times \mathbf{E}(\boldsymbol{x})) - \omega^2\, \varepsilon(\boldsymbol{x},\omega)\mathbf{E}(\boldsymbol{x}) = 0 \quad \text{in } \mathbb{R}^3, \tag{3.1}$$

where $\varepsilon(\boldsymbol{x},\omega)$ is periodic in $\boldsymbol{x}$ and V is a suitable function space to be introduced and discussed in Sec. 4 and Sec. 7.

This problem is defined in $\mathbb{R}^3$ and can be reduced to a pair of problems in $\mathbb{R}^2$ for two-dimensional crystals (see Sec. 2.2). In any case, it is not possible to solve the problem numerically in the unbounded domains $\mathbb{R}^3$ or $\mathbb{R}^2$. However, thanks to the *periodicity* of

the coefficient ε in space, the problem can be transformed into an equivalent family of parametric problems on a *bounded domain*.

In the remainder of this section we introduce the necessary notation and tools, as well as the conditions on problem (3.1) in order to transform it in the desired way. For the sake of clarity, the examples and drawings are mostly representing a two-dimensional periodic structure. The results are, however, valid for any dimension $d \in \mathbb{N}$.

3.1 Geometry

We introduce some notation to handle the periodicity of the geometry. More detailed introductions can be found in the physics book [Kit04], or in the mathematics books [JJWM08], [DLP+11], and [Kuc01, pp. 218]. Let

- G be a lattice in $\mathbb{R}^d$ (e.g. $G = \mathbb{Z}^2$ for $d = 2$),
- Ω denote the *Wigner-Seitz primitive cell of the lattice*, it is the fundamental periodicity zone of the lattice (e.g. $\Omega = [0, 1)^2$ for $G = \mathbb{Z}^2$),
- G^* is the *reciprocal lattice* , $G^* = \{\gamma \in \mathbb{R}^d \mid g \cdot \gamma \in 2\pi\mathbb{Z} \text{ for all } g \in G\}$ (e.g. $G^* = 2\pi\mathbb{Z}^2$ for $G = \mathbb{Z}^2$),
- $\mathcal{K}$ is called *Brillouin zone* and is the primitive cell of the reciprocal lattice G^* (e.g. $\mathcal{K} = [0, 2\pi)^2$ for $G^* = 2\pi\mathbb{Z}^2$),
- $\mathcal{B}$ is *the irreducible Brillouin zone*, the fundamental symmetry element of the Brillouin zone (e.g. for $\mathcal{K} = [0, 2\pi)^2$: $\mathcal{B}$ is the triangle spanned between the points $\Gamma = (\pi, \pi)$, $X = (2\pi, \pi)$, $M = (2\pi, 2\pi)$, see Fig. 3.2).

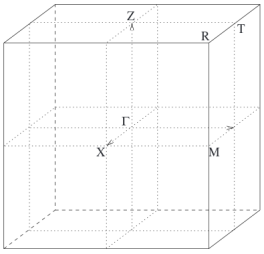


Fig. 3.1: Brillouin zone and symmetry points in cubic lattice [DLP+11, Ch. 2.2]

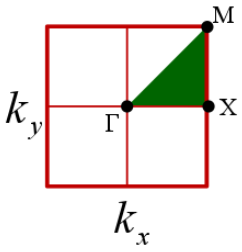


Fig. 3.2: Brillouin zone of a square lattice [Rum14, Lect. 7]

3.2 Floquet transformation

In order to reduce the model problem, which is posed on the entire space $\mathbb{R}^d$, to a more manageable size, we use a transformation of the system that is suitable for the periodic setting: *the Floquet transformation*. This exposition of the Floquet transformation follows [Eng10].

For a function u defined on $\mathbb{R}^d$ decaying sufficiently fast at infinity, a d-dimensional lattice G, and a vector $k \in \mathbb{R}^d$, define the Floquet transformation by

$$\mathcal{F}u(x, k) = \mathcal{F}\{u(\cdot)\}(x, k) := \sum_{n \in G} u(x - n)e^{-ik\cdot(x-n)}. \tag{3.2}$$

The condition that u has to decay sufficiently fast at infinity is similar to the assumptions for the Fourier transformation and can be assumed in the case of electromagnetic fields in infinite domains [Kuc93]. Floquet transformation, as opposed to Fourier transformation, introduces the additional variable k, the so-called *wavevector*. This, and of course the periodicity of ε, allows us to reduce problem (3.1) to a bounded domain, namely the Wigner-Seitz cell Ω, with appropriate, i.e., periodic, boundary conditions. However, with the additional variable k the problem becomes parameter-dependent. Let us proceed with some general properties of the Floquet transformation.

Lemma 3.1. *The Floquet transform of a function u is* periodic *with respect to x and* quasi-periodic *(or cyclic) with respect to k, i.e.,*

$$\begin{aligned} \mathcal{F}u(x+g,k) &= \mathcal{F}u(x,k) && \text{for all } g \in G, \\ \mathcal{F}u(x,k+\gamma) &= e^{-i\gamma\cdot x}\mathcal{F}u(x,k) && \text{for all } \gamma \in G^*. \end{aligned}$$

Proof. Observe that for all $g \in G$ we have

$$\mathcal{F}u(x+g,k) = \sum_{n\in G} u(x+g-n)e^{-ik\cdot(x+g-n)} = \sum_{m\in G} u(x-m)e^{-ik\cdot(x-m)} = \mathcal{F}u(x,k)$$

for $m = n - g$. Moreover, for all $\gamma \in G^*$ we have

$$\begin{aligned} \mathcal{F}u(x,k+\gamma) &= \sum_{n\in G^*} u(x-n)e^{-i(k+\gamma)\cdot(x-n)} = \sum_{n\in G^*} u(x-n)e^{-ik\cdot(x-n)}e^{-i\gamma\cdot(x-n)} \\ &= e^{-i\gamma\cdot x}\sum_{n\in G^*} u(x-n)e^{-ik\cdot(x-n)} = e^{-i\gamma\cdot x}\mathcal{F}u(x,k) \end{aligned}$$

as $\gamma \cdot n \in 2\pi\mathbb{Z}$ for all $\gamma \in G^*, n \in G$ and therefore $e^{i\gamma\cdot n} = 1$. □

Lemma 3.2. *For the* gradient *of the Floquet transform and* multiplication with a periodic function *we have*

$$\begin{aligned} \nabla\mathcal{F}u &= \mathcal{F}\big((\nabla - ik)u\big), \\ \mathcal{F}(\nabla u) &= (\nabla + ik)\,\mathcal{F}u, \\ \varepsilon\mathcal{F}u &= \mathcal{F}\varepsilon u, \end{aligned}$$

where ε is a G-periodic function, i.e., $\varepsilon(x+g) = \varepsilon(x)$ for all $g \in G$.

Proof. See that

$$\begin{aligned} \nabla\mathcal{F}u &= \nabla\left(\sum_{n\in G} u(x-n)e^{-ik\cdot(x-n)}\right) \\ &= \sum_{n\in G}\Big(\nabla u(x-n)e^{-ik\cdot(x-n)} + u(x-n)(-ik)e^{-ik\cdot(x-n)}\Big) \\ &= \sum_{n\in G}(\nabla - ik)\,u(x-n)e^{-ik\cdot(x-n)} \\ &= \mathcal{F}(\nabla - ik)u \end{aligned}$$

and

$$\begin{aligned} \varepsilon\mathcal{F}u &= \varepsilon(x)\sum_{n\in G} u(x-n)e^{-ik\cdot(x-n)} = \sum_{n\in G}\varepsilon(x)u(x-n)e^{-ik\cdot(x-n)} \\ &= \sum_{n\in G}\varepsilon(x-n)u(x-n)e^{-ik\cdot(x-n)} = \mathcal{F}(\varepsilon u). \end{aligned}$$

□

Theorem 3.3 ([Eng10, p. 1323], [Kuc01, Ch. 7.3]). *The Floquet transformation, considered as a mapping*

$$\begin{aligned}\mathcal{F} : L^2(\mathbb{R}^d) &\to L^2(\mathcal{K}, L^2(\mathbb{T}^d)) \\ u \quad &\mapsto (k \mapsto \mathcal{F}u(k, \cdot)),\end{aligned}$$

where $\mathbb{T}^d$ is the d-dimensional Torus, i.e., the unit cell with periodic boundary conditions, is isometric *and its inverse is given by*

$$(\mathcal{F}^{-1}v)(x) = \frac{1}{|\mathcal{K}|}\int_{\mathcal{K}} v(x,k)e^{ik\cdot x}\,\mathrm{d}k$$

where $v \in L^2(\mathcal{K}, L^2(\mathbb{T}^d))$.

Proof. See that

$$\begin{aligned}\mathcal{F}^{-1}(\mathcal{F}u)(x) &= \frac{1}{|\mathcal{K}|}\int_{\mathcal{K}} \mathcal{F}u(x,k)e^{ik\cdot x}\,\mathrm{d}k \\ &= \frac{1}{|\mathcal{K}|}\int_{\mathcal{K}} \left(\sum_{n\in G} u(x-n)e^{-ik\cdot(x-n)}\right) e^{ik\cdot x}\,\mathrm{d}k \\ &= \frac{1}{|\mathcal{K}|}\int_{\mathcal{K}} \left(\sum_{n\in G} u(x-n)e^{ik\cdot n}\right)\mathrm{d}k \\ &= \frac{1}{|\mathcal{K}|}\sum_{n\in G}\left(u(x-n)\int_{\mathcal{K}} e^{ik\cdot n}\,\mathrm{d}k\right) \\ &= \frac{1}{|\mathcal{K}|}\sum_{n\in G} u(x-n)|\mathcal{K}|\delta(n) \\ &= u(x).\end{aligned}$$

More detailed proofs in terms of Fourier series are available in [DLP+11, Kuc01]. □

Transformation of the model problem

In order to reduce the size of the domain on which our model problem is posed, we apply a Floquet transformation to Eq. (3.1). We obtain a family of problems, parametrized in $\boldsymbol{k} \in \mathcal{K}$, on the bounded Wigner-Seitz cell Ω:

$$L(\varepsilon,\omega,\boldsymbol{k})\mathcal{F}\mathbf{u}(\boldsymbol{x},\boldsymbol{k}) = (\nabla + i\boldsymbol{k}) \times \frac{1}{\mu}(\nabla + i\boldsymbol{k}) \times \mathcal{F}\mathbf{u}(\boldsymbol{x},\boldsymbol{k}) - \omega^2\,\varepsilon(\boldsymbol{x},\omega)\mathcal{F}\mathbf{u}(\boldsymbol{x},\boldsymbol{k}) = 0 \quad \text{in } \Omega.$$

To make the notation more concise we introduce, for fixed $\boldsymbol{k} \in \mathcal{K}$, $\nabla_{\boldsymbol{k}} := \nabla + i\boldsymbol{k}$ and $\mathbf{u}_{\boldsymbol{k}}(\boldsymbol{x}) := \mathcal{F}\mathbf{u}(\boldsymbol{x},\boldsymbol{k})$. The model problem becomes: Find $(\omega, \mathbf{E}) \in \mathbb{C} \times V$ such that

$$L(\varepsilon,\omega,\boldsymbol{k})\mathbf{u}_{\boldsymbol{k}}(\boldsymbol{x}) := \nabla_{\boldsymbol{k}} \times \left(\frac{1}{\mu}\nabla_{\boldsymbol{k}} \times \mathbf{u}_{\boldsymbol{k}}(\boldsymbol{x})\right) - \omega^2\,\varepsilon(\boldsymbol{x},\omega)\mathbf{u}_{\boldsymbol{k}}(\boldsymbol{x}) = 0 \quad \text{in } \Omega. \tag{3.3}$$

This is the eigenvalue problem which we will consider in the following.

3.3 Band diagrams

The transformed eigenvalue problem (3.3) is typically solved for fixed $k \in \mathcal{K}$ and the resulting eigenvalues, or eigen*frequencies*, $\omega_j(k), k \in \mathcal{K}, j = 1, 2, \ldots$, can be visualized for varying k. We shall see in the following sections dedicated to the spectral theory of the operators involved in Eq. (3.3) that it is possible to enumerate the resulting eigenvalues in this way as they turn out to be discrete and of finite multiplicity. Actually, it is even known [KS14, Prop. 2.1] that the relation $\omega_j(k)$ is analytic in k.

In dimension $d \geq 1$, it is difficult to visualize in a clear way the relations $\omega_j(k)$ for all $k \in \mathcal{K} \subset \mathbb{R}^d$. Therefore, these relations $\omega_j(k)$ are typically only plotted for a parametrization of some areas of the Brillouin zone $\mathcal{K}$. Usually a parametrization of the boundary of the irreducible Brillouin zone $\mathcal{B}$ is used.

See Fig. 3.3 for an illustration of such a parametrization for the square lattice, $\mathcal{K}$ centered around $\Gamma = (0, 0)$ and its irreducible Brillouin zone $\mathcal{B}$. See Fig. 3.4 for a band diagram on the cube from Fig. 3.1. This indeed illustrates where the notion *band* diagram and *band*gap comes from.

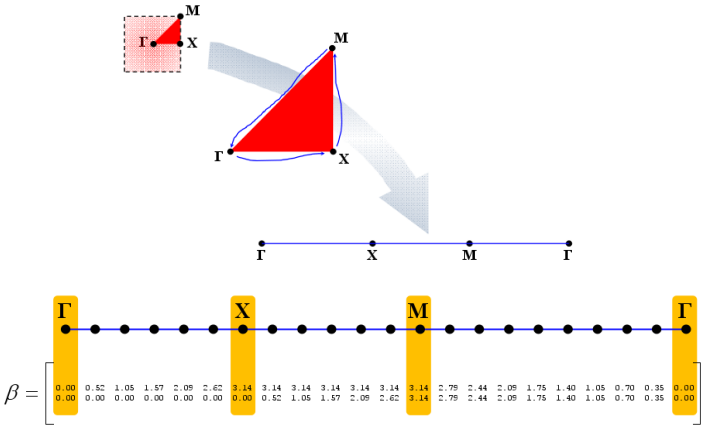


Fig. 3.3: Parametrization of the boundary of $\mathcal{B}$ [Rum14, Lec. 8]

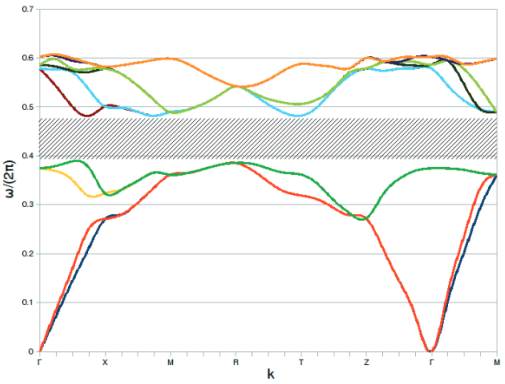


Fig. 3.4: Band diagram for eigenvalues of Eq. (3.3) on a three-dimensional cubic lattice [DLP+11, Ch. 2.2]

4 Function spaces

In the previous section we have transformed the model problem (3.1) defined on the entire space $\mathbb{R}^3$ into an equivalent family of eigenvalue problems (3.3) defined on a bounded domain Ω. In our case, Ω corresponds to the Wigner-Seitz cell of the periodic crystal.

The next step towards the spectral analysis of the operators in Eq. (3.3) is to define the appropriate function space V which should be searched for eigenfunctions $\boldsymbol{u_k}$.

4.1 Sobolev Spaces

In the case of two-dimensional photonic crystals, it has been seen that the Maxwell equations can be reduced to Eq. (2.11). In this case, the spectral analysis is based on the theory of standard Sobolev spaces

$$H^m(\Omega) \coloneqq W^{m,2}(\Omega) = \left\{ v \in L^2(\Omega) \;\middle|\; D^\alpha v \in L^2(\Omega), |\alpha| \leq m \right\},$$

for $m \in \geqslant$, with the associated norm

$$\|v\|^2_{H^m(\Omega)} \coloneqq \sum_{0 \leq |\alpha| \leq m} \|D^\alpha v\|^2_{L^2(\Omega)}.$$

In particular,

$$H^1(\Omega) = W^{1,2}(\Omega) = \left\{ v \in L^2(\Omega) \mid \nabla v \in L^2(\Omega) \right\}.$$

We have used here the standard notation from [AF03]. The spaces $H^m_0(\Omega)$ are defined as the closure of $C^\infty_0(\Omega)$ [AF03, Sect. 3.2] with respect to the norm $\|\cdot\|_{H^m(\Omega)}$. Through trace operators they provide a notion of Dirichlet boundary conditions on boundaries of measure zero. These trace operators are introduced in more details in Sec. 4.2.

4.1.1 Sobolev spaces for vector fields

The theory of standard Sobolev spaces is sufficient to analyze two-dimensional crystals. However, the Maxwell equations are posed in general in a three-dimensional space. Therefore, it is necessary to introduce another set of somewhat intermediate Sobolev spaces that account for the behavior of the differential operators occurring in the Maxwell equations: the curl and the divergence operators.

Let us consider a bounded domain $\Omega \in \mathbb{R}^3$ the Euclidean norm $\|\boldsymbol{f}\|^2_{(L^2(\Omega))^3} = \int_\Omega \boldsymbol{f} \cdot \bar{\boldsymbol{f}} \, \mathrm{d}\boldsymbol{x}$ for functions $\boldsymbol{f} \in \left(L^2(\Omega)\right)^3$. We define the following Sobolev spaces with the weak curl and divergence operators

$$H(\mathrm{curl}, \Omega) = \left\{ \boldsymbol{v} \in \left(L^2(\Omega)\right)^3 \;\middle|\; \nabla \times \boldsymbol{v} \in \left(L^2(\Omega)\right)^3 \right\},$$

with the norm

$$\|\boldsymbol{v}\|^2_{\mathrm{curl}} \coloneqq \|\boldsymbol{v}\|^2_{(L^2(\Omega))^3} + \|\nabla \times \boldsymbol{v}\|^2_{(L^2(\Omega))^3}$$

and

$$H(\mathrm{div}, \Omega) = \left\{ \boldsymbol{v} \in \left(L^2(\Omega)\right)^3 \;\middle|\; \nabla \cdot \boldsymbol{v} \in L^2(\Omega) \right\},$$

with the norm

$$\|\boldsymbol{v}\|^2_{\mathrm{div}} \coloneqq \|\boldsymbol{v}\|^2_{(L^2(\Omega))^3} + \|\nabla \cdot \boldsymbol{v}\|^2_{L^2(\Omega)}.$$

4.1.2 Periodic function spaces

As we are interested in periodic materials, we need spaces of periodic functions, or functions fulfilling periodic boundary conditions. If $G \subset \mathbb{R}^3$ is a lattice, we can define an equivalence relation $\boldsymbol{x} \sim \boldsymbol{y} \Leftrightarrow \boldsymbol{x} - \boldsymbol{y} \in G$. The corresponding residue class $\mathbb{R}^3/G$ is a compact manifold which can be identified with the Wigner-Seitz cell Ω of the lattice [DLP+11, Ch. 1.2.6].

Thus we can define the periodic Sobolev spaces

$$H^m_{\mathrm{per}}(\Omega) \coloneqq \left\{ v|_\Omega \mid v \in H^m(\mathbb{R}^3/G) \right\} \tag{4.1}$$

$$H_{\mathrm{per}}(\mathrm{curl}, \Omega) \coloneqq \left\{ \boldsymbol{v}|_\Omega \mid \boldsymbol{v} \in H(\mathrm{curl}, \mathbb{R}^3/G) \right\}, \tag{4.2}$$

$$H_{\mathrm{per}}(\mathrm{div}, \Omega) \coloneqq \left\{ \boldsymbol{v}|_\Omega \mid \boldsymbol{v} \in H(\mathrm{div}, \mathbb{R}^3/G) \right\}. \tag{4.3}$$

4.2 Trace operators

For the correct interpretation of boundary conditions and the construction of weak formulations in the spaces $H(\mathrm{curl}, \Omega)$ and $H(\mathrm{div}, \Omega)$ we need to introduce adequate trace operators.

From now on we assume that Ω is a bounded Lipschitz domain. In most application examples Ω will even have a polygonal boundary in order to make sense of the periodicity. We define the trace operators

$$\gamma(v) = v|_{\partial\Omega} \text{ for all } v \in C^\infty(\overline{\Omega}), \qquad \gamma_t(\boldsymbol{v}) = \mathbf{n} \times \boldsymbol{v}|_{\partial\Omega} \text{ for all } \boldsymbol{v} \in C^\infty(\overline{\Omega})^3,$$
$$\gamma_n(\boldsymbol{v}) = \mathbf{n} \cdot \boldsymbol{v}|_{\partial\Omega} \text{ for all } \boldsymbol{v} \in C^\infty(\overline{\Omega})^3, \quad \gamma_T(\boldsymbol{v}) = (\mathbf{n} \times \boldsymbol{v}|_{\partial\Omega}) \times \mathbf{n} \text{ for all } \boldsymbol{v} \in C^\infty(\overline{\Omega})^3,$$

where $\mathbf{n}$ is the unit outward normal to Ω. The operators γ_t, γ_T have continuous extensions $H(\mathrm{curl}, \Omega) \to H^{-\frac{1}{2}}(\partial\Omega)^3$ [DLP+11]. In the remainder we denote these extensions with the same symbols γ_t, γ_T. Similarly, we keep the same symbols for denoting the continuous extensions of the operators $\gamma : H^1(\Omega) \to H^{\frac{1}{2}}(\partial\Omega)$ and $\gamma_n : H(\mathrm{div}, \Omega) \to H^{-\frac{1}{2}}(\partial\Omega)$.

Equivalently, $\gamma_T(\boldsymbol{v})$ can be written as

$$\gamma_T(\boldsymbol{v}) = (\mathbf{n} \times \boldsymbol{v}|_{\partial\Omega}) \times \mathbf{n} = \boldsymbol{v}|_{\partial\Omega} - (\boldsymbol{v}|_{\partial\Omega} \cdot \mathbf{n})\mathbf{n}.$$

Note that $\gamma_t, \gamma_T : H(\mathrm{curl}, \Omega) \to H^{-\frac{1}{2}}(\partial\Omega)^3$ are non-surjective operators. In order to obtain the integration by parts formula of $\boldsymbol{u}, \boldsymbol{v} \in H(\mathrm{curl}, \Omega)$, it is necessary to restrain the codomain of γ_t and γ_T to the so-called *trace spaces* $Y_t = \mathrm{range}(\gamma_t)$ and $Y_T = \mathrm{range}(\gamma_T)$ respectively, where $Y_t, Y_T \subset H^{-\frac{1}{2}}(\partial\Omega)^3$ can be characterized completely [BCS02].

It follows that for $\boldsymbol{u}, \boldsymbol{v} \in H(\mathrm{curl}, \Omega)$:

$$\int_\Omega (\nabla \times \boldsymbol{u} \cdot \boldsymbol{v} - \boldsymbol{u} \cdot \nabla \times \boldsymbol{v}) \, \mathrm{d}\boldsymbol{x} = \langle \gamma_T(\boldsymbol{v}), \gamma_t(\boldsymbol{u}) \rangle_{Y_T \times Y_t}. \tag{4.4}$$

Remark 4.1. *We use here the notation from [DLP+11] and [Mon03, Ch. 3.5].*

4.3 Helmoltz decomposition

Before deriving the weak formulation for the eigenvalue problem in Eq. (3.3), we need to address an inherent problem concerning any equation involving the curl operator. Contrarily to the kernel of the gradient operator which consists of the constant functions and is therefore finite-dimensional, the kernel of the curl operator is infinite-dimensional. Indeed the gradient of any function $f \in H^1(\Omega)$ satisfies $\nabla \times \nabla f = 0$.

This is why the kernel of the curl operator cannot be eliminated simply by fixing boundary conditions as for the gradient operator. Instead we shall decompose the space $H_{\mathrm{per}}(\mathrm{curl}, \Omega)$ into subspaces of curl-free and divergence-free functions, respectively.

We recall that Ω denotes the Wigner-Seitz cell of G.

Lemma 4.2. *For $\boldsymbol{k} \in \mathcal{K}$, the map $\langle \cdot, \cdot \rangle_{\boldsymbol{k}} : H_{per}(curl, \Omega) \times H_{per}(curl, \Omega) \to \mathbb{C}$,*

$$\langle \boldsymbol{u}, \boldsymbol{v} \rangle_{\boldsymbol{k}} \coloneqq \int_\Omega \boldsymbol{u} \cdot \overline{\boldsymbol{v}} \; + (\nabla_{\boldsymbol{k}} \times \boldsymbol{u}) \cdot \overline{(\nabla_{\boldsymbol{k}} \times \boldsymbol{v})} \, \mathrm{d}\boldsymbol{x} \,,$$

is an inner product in $H_{per}(curl, \Omega)$.

Proof. For all $\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w} \in H_{\mathrm{per}}(\mathrm{curl}, \Omega)$ and $\lambda \in \mathbb{C}$:

1. $\overline{\langle \boldsymbol{v}, \boldsymbol{u} \rangle}_{\boldsymbol{k}} = \langle \boldsymbol{u}, \boldsymbol{v} \rangle_{\boldsymbol{k}}$
2. $\langle \lambda(\boldsymbol{u} + \boldsymbol{w}), \boldsymbol{v} \rangle = \lambda \Big(\langle \boldsymbol{u}, \boldsymbol{v} \rangle_{\boldsymbol{k}} + \langle \boldsymbol{w}, \boldsymbol{v} \rangle_{\boldsymbol{k}} \Big)$
3. $\langle \boldsymbol{u}, \boldsymbol{u} \rangle_{\boldsymbol{k}} = \|\boldsymbol{u}\|^2_{(L^2(\Omega))^3} + \|\nabla_{\boldsymbol{k}} \times \boldsymbol{u}\|^2_{L^2(\Omega)} \geq 0$ and $\langle \boldsymbol{u}, \boldsymbol{u} \rangle_{\boldsymbol{k}} = 0 \Leftrightarrow \boldsymbol{u} = 0$. □

With Lem. 4.2, we can define the norm associated to $\langle \cdot, \cdot \rangle_{\boldsymbol{k}}$ by

$$\|\boldsymbol{u}\|_{\boldsymbol{k}} \coloneqq \sqrt{\langle \boldsymbol{u}, \boldsymbol{u} \rangle_{\boldsymbol{k}}} = \sqrt{\|\boldsymbol{u}\|^2_{(L^2(\Omega))^3} + \|\nabla_{\boldsymbol{k}} \times \boldsymbol{u}\|_{(L^2(\Omega))^3}} .$$

Lemma 4.3 ([DP01,])**.** *The sequence*

$$0 \longrightarrow H^1_p(\Omega) \xrightarrow{\nabla_{\boldsymbol{k}}} H_{per}(curl, \Omega) \xrightarrow{\nabla_{\boldsymbol{k}} \times} H_{per}(div, \Omega) \xrightarrow{\nabla_{\boldsymbol{k}} \cdot} L^2(\Omega) \longrightarrow 0$$

is exact.

It follows from Lem. 4.3 that $\nabla_{\boldsymbol{k}} H^1_{\mathrm{per}}(\Omega) = \ker(\nabla_{\boldsymbol{k}} \times)$ and thus, $\nabla_{\boldsymbol{k}} H^1_{\mathrm{per}}(\Omega)$ is a closed subspace of $H_{\mathrm{per}}(\mathrm{curl}, \Omega)$. Therefore we can decompose

$$H_{\mathrm{per}}(\mathrm{curl}, \Omega) = \nabla_{\boldsymbol{k}} H^1_{\mathrm{per}}(\Omega) \oplus \Big(\nabla_{\boldsymbol{k}} H^1_{\mathrm{per}}(\Omega) \Big)^{\perp}$$

with orthogonality in the $\langle \cdot, \cdot \rangle_{\boldsymbol{k}}$ inner product.

Theorem 4.4 (Shifted Helmholtz decomposition)**.** *Let G be a lattice in $\mathbb{R}^3$, $\Omega = \mathbb{R}^3/G$ the Wigner-Seitz primitive cell of G, $\mathcal{K}$ the corresponding Brillouin zone, and $\boldsymbol{k} \in \mathcal{K}$. Then,*

$$H_{per}(curl, \Omega) = \nabla_{\boldsymbol{k}} H^1_{per}(\Omega) \oplus V^{(1)}_{\boldsymbol{k}} \tag{4.5}$$

where $V^{(1)}_{\boldsymbol{k}} \coloneqq \Big\{ \boldsymbol{u} \in H_{per}(curl, \Omega) \;\Big|\; \int_\Omega \boldsymbol{u} \cdot \overline{\nabla_{\boldsymbol{k}} \xi} \, \mathrm{d}\boldsymbol{x} = 0 \text{ for all } \xi \in H^1_{per}(\Omega) \Big\}$.

Proof. For all $\boldsymbol{u} \in H_{\mathrm{per}}(\mathrm{curl}, \Omega),\ \xi \in \nabla H^1_{\mathrm{per}}(\Omega)$,

$$\langle \boldsymbol{u}, \nabla_{\boldsymbol{k}} \xi \rangle_{\boldsymbol{k}} = \int_\Omega \boldsymbol{u} \cdot \overline{\nabla \xi} \ + (\nabla_{\boldsymbol{k}} \times \boldsymbol{u}) \cdot \overline{(\nabla_{\boldsymbol{k}} \times \nabla_{\boldsymbol{k}} \xi)} \, \mathrm{d}\boldsymbol{x} = \int_\Omega \boldsymbol{u} \cdot \overline{\nabla_{\boldsymbol{k}} \xi} \, \mathrm{d}\boldsymbol{x} \,,$$

since $\nabla_{\boldsymbol{k}} \times \nabla_{\boldsymbol{k}} \xi = \underbrace{\nabla \times \nabla \xi}_{0} + \underbrace{\nabla \times (i\boldsymbol{k}\xi) + i\boldsymbol{k} \times \nabla \xi}_{0} + \underbrace{i\boldsymbol{k} \times i\boldsymbol{k}\xi}_{0} = 0.$

Therefore,

$$\left(\nabla_{\boldsymbol{k}} H^1_{\mathrm{per}}(\Omega)\right)^\perp = \left\{ \boldsymbol{u} \in H_{\mathrm{per}}(\mathrm{curl}, \Omega) \;\middle|\; \langle \boldsymbol{u}, \nabla_{\boldsymbol{k}} \xi \rangle_{\boldsymbol{k}} = 0 \text{ for all } \xi \in H^1_{\mathrm{per}}(\Omega) \right\} = V^{(1)}_{\boldsymbol{k}}. \quad (4.6)$$

The result follows from Lem. 4.3. □

In addition to Thm. 4.4, we will need a slightly different decomposition in order to perform the spectral analysis of the eigenvalue problem in Eq. (3.3).

Theorem 4.5. *Let $\boldsymbol{k}$ and Ω as in Thm. 4.4, $D \subset \mathbb{C}$ an open connected set and $\varepsilon : \Omega \times D \to \mathbb{C}$ satisfy the following conditions:*

- *$\varepsilon(\cdot, \omega)$ is analytic in D*
- *$|\varepsilon| \leq C_1 < \infty$ almost everywhere in Ω*
- *$\mathrm{Re}(\varepsilon) > C_0 > 0$ almost everywhere in Ω.*

Then

$$H_{per}(curl, \Omega) = \nabla_{\boldsymbol{k}} H^1_{per}(\Omega) \oplus V^{(\varepsilon)}_{\boldsymbol{k}} \quad (4.7)$$

where $V^{(\varepsilon)}_{\boldsymbol{k}} := \left\{ \boldsymbol{u} \in H_{per}(curl, \Omega) \;\middle|\; \int_\Omega \varepsilon \boldsymbol{u} \cdot \overline{\nabla_{\boldsymbol{k}} \xi} \, \mathrm{d}\boldsymbol{x} = 0 \text{ for all } \xi \in H^1_{per}(\Omega) \right\}$.

Before proving this theorem, we show that the bilinear form $\langle \varepsilon \cdot, \cdot \rangle_{(L^2(\Omega))^3}$ is coercive and bounded. In the remainder we simplify the notation by omitting the indices $L^2(\Omega)$ and $(L^2(\Omega))^3$ when referring to the inner product and norm of these spaces. Whether the omitted index is $L^2(\Omega)$ or $(L^2(\Omega))^3$ will be clear from the context.

With

$$|\langle \varepsilon \boldsymbol{u}, \boldsymbol{v} \rangle| = \left| \int_\Omega \varepsilon \boldsymbol{u} \cdot \boldsymbol{v} \, \mathrm{d}\boldsymbol{x} \right| \leq \|\varepsilon \boldsymbol{u}\| \|\boldsymbol{v}\| \leq C_1 \|\boldsymbol{u}\| \|\boldsymbol{v}\| \quad (4.8)$$

we show the boundedness and with

$$|\langle \varepsilon \boldsymbol{u}, \boldsymbol{u} \rangle| = \left| \int_\Omega \varepsilon |\boldsymbol{u}|^2 \, \mathrm{d}\boldsymbol{x} \right| \geq \int_\Omega \mathrm{Re}(\varepsilon) |\boldsymbol{u}|^2 \, \mathrm{d}\boldsymbol{x} \geq C_0 \|\boldsymbol{u}\|^2$$

we show the coercivity. We can now prove Thm. 4.5.

Proof. We define $\langle \cdot, \cdot \rangle_{\varepsilon, \boldsymbol{k}} : H_{\mathrm{per}}(\mathrm{curl}, \Omega) \times H_{\mathrm{per}}(\mathrm{curl}, \Omega) \to \mathbb{C}$,

$$\langle \boldsymbol{u}, \boldsymbol{v} \rangle_{\varepsilon, \boldsymbol{k}} = \int_\Omega (\nabla_{\boldsymbol{k}} \times \boldsymbol{u}) \cdot \overline{(\nabla_{\boldsymbol{k}} \times \boldsymbol{v})} \ + \varepsilon \boldsymbol{u} \cdot \overline{\boldsymbol{v}} \, \mathrm{d}\boldsymbol{x} \,.$$

It follows that

$$\langle \boldsymbol{u}, \boldsymbol{u} \rangle_{\varepsilon, \boldsymbol{k}} = \int_\Omega |\nabla_{\boldsymbol{k}} \times \boldsymbol{u}|^2 + \langle \varepsilon \boldsymbol{u}, \boldsymbol{u} \rangle \, \mathrm{d}\boldsymbol{x} \ \geq \min(1, C_1) \|\boldsymbol{u}\|^2_{\boldsymbol{k}}$$

and

$$|\langle \boldsymbol{u}, \boldsymbol{v} \rangle_{\varepsilon,\boldsymbol{k}}| \leq | \int_\Omega (\nabla_{\boldsymbol{k}} \times \boldsymbol{u}) \cdot (\nabla_{\boldsymbol{k}} \times \boldsymbol{v}) \, \mathrm{d}\boldsymbol{x} \ | + |\langle \varepsilon \boldsymbol{u}, \boldsymbol{v} \rangle|$$
$$\leq \max(1, C_0)(\|\nabla_k \times \boldsymbol{u}\| \|\nabla_k \times \boldsymbol{v}\| + \|\boldsymbol{u}\| \|\boldsymbol{v}\|) \leq \frac{1}{2} \max(1, C_0) \|\boldsymbol{u}\|_{\boldsymbol{k}} \|\boldsymbol{v}\|_{\boldsymbol{k}}$$

where we have used Young's inequality:

$$(a_1 b_1 + a_2 b_2) \leq \sqrt{a_1^2 + a_2^2} \sqrt{b_1^2 + b_2^2}.$$

Therefore, $\langle \cdot, \cdot \rangle_{\varepsilon,\boldsymbol{k}}$ is sesquilinear, bounded, and coercive. We can thus use the same argument as in the proof of Lem. 4.5 in [Mon03] to show the decomposition in Eq. (4.7). □

Remark 4.6. *Functions* $\boldsymbol{u}^{(1)} \in V_{\boldsymbol{k}}^{(1)}$ *and* $\boldsymbol{u}^{(\varepsilon)} \in V_{\boldsymbol{k}}^{(\varepsilon)}$ *satisfy*

$$\nabla_{\boldsymbol{k}} \cdot \boldsymbol{u}^{(1)} = 0 \qquad \textit{and} \qquad \nabla_{\boldsymbol{k}} \cdot \boldsymbol{u}^{(\varepsilon)} = 0,$$

respectively, in the weak sense.

4.4 Embedding theorems

It is well-known that the space $H^1_{\mathrm{per}}(\Omega)$ is compactly embedded in $L^2(\Omega)$ [Ces96]. Contrarily, the embeddings of $H_{\mathrm{per}}(\mathrm{curl}, \Omega)$ and $H_{\mathrm{per}}(\mathrm{div}, \Omega)$ into $\left(L^2(\Omega)\right)^3$ are not compact. Indeed, these spaces contain the subspace

$$\ker(\nabla\times) \cap \ker(\nabla\cdot) = \{\boldsymbol{u} \in H_{\mathrm{per}}(\mathrm{curl}, \Omega) \cap H_{\mathrm{per}}(\mathrm{div}, \Omega) \mid \nabla \times \boldsymbol{u} = 0, \nabla \cdot \boldsymbol{u} = 0\},$$

which is a closed subspace of $\left(L^2(\Omega)\right)^3$ of infinite dimension [Ces96].

Lemma 4.7. *[BCG06] The space* $V_{\boldsymbol{k}}^{(1)}$ *is compactly embedded in* $\left(L^2(\Omega)\right)^3$.

Lemma 4.8. *The space* $V_{\boldsymbol{k}}^{(\varepsilon)}$ *is compactly embedded in* $\left(L^2(\Omega)\right)^3$.

Proof. We follow the proof of Thm. 4.7 in [Mon03]. Let $\{\boldsymbol{v}_n\}_{n\in\mathbb{N}}$ be a bounded sequence in $V_{\boldsymbol{k}}^{(\varepsilon)}$. Since $V_{\boldsymbol{k}}^{(\varepsilon)} \subset H_{\mathrm{per}}(\mathrm{curl}, \Omega)$, we can use the decomposition in Eq. (4.5) for all $n = 1, 2, ...$, namely

$$\boldsymbol{v}_n = \nabla_{\boldsymbol{k}} \xi_n + \boldsymbol{w}_n \text{ with } \xi_n \in H^1_{\mathrm{per}}(\Omega), \ \boldsymbol{w}_n \in V_{\boldsymbol{k}}^{(1)}$$

Since $V_{\boldsymbol{k}}^{(1)}$ is compactly embedded into $\left(L^2(\Omega)\right)^3$, there exists a subsequence $\{\boldsymbol{w}_{n_m}\}_{m\in\mathbb{N}}$ of $\{\boldsymbol{w}_n\}$ that is strongly convergent in $\left(L^2(\Omega)\right)^3$ to a limit $\boldsymbol{w} \in V_{\boldsymbol{k}}^{(1)}$. Since $V_{\boldsymbol{k}}^{(1)} \subset H_{\mathrm{per}}(\mathrm{curl}, \Omega)$, we can use the decomposition in Eq. (4.7):

$$\boldsymbol{w} = -\nabla_{\boldsymbol{k}} \xi + \boldsymbol{v} \text{ with } \xi \in H^1_{\mathrm{per}}(\Omega), \boldsymbol{v} \in V_{\boldsymbol{k}}^{(\varepsilon)}$$

Therefore, using the boundedness and coercivity of $\langle \varepsilon \cdot, \cdot \rangle$, we show that $\boldsymbol{v}$ is the limit of $\{\boldsymbol{v}_{n_m}\}$:

$$\begin{aligned} C_1 \|\boldsymbol{v} - \boldsymbol{v}_{n_m}\|^2 &\leq \langle \varepsilon(\boldsymbol{v} - \boldsymbol{v}_{n_m}), (\boldsymbol{v} - \boldsymbol{v}_{n_m}) \rangle \\ &= \langle \varepsilon(\boldsymbol{v} - \boldsymbol{v}_{n_m}), (\boldsymbol{v} - \nabla_{\boldsymbol{k}} \xi) - (\boldsymbol{v}_{n_m} - \nabla_{\boldsymbol{k}} \xi_{n_m}) \rangle \\ &= \langle \varepsilon(\boldsymbol{v} - \boldsymbol{v}_{n_m}), (\boldsymbol{w} - \boldsymbol{w}_{n_m}) \rangle \\ &\leq C_0 \|\boldsymbol{v} - \boldsymbol{v}_{n_m}\| \|\boldsymbol{w} - \boldsymbol{w}_{n_m}\|. \end{aligned}$$

Thus,

$$\|\boldsymbol{v} - \boldsymbol{v}_{n_m}\| \leq \frac{C_1}{C_0} \cdot \|\boldsymbol{w} - \boldsymbol{w}_{n_m}\| \xrightarrow{m\to\infty} 0$$

and it follows that $V_{\boldsymbol{k}}^{(\varepsilon)}$ is compactly embedded in $\left(L^2(\Omega)\right)^3$. □

5 Spectral theory

After introducing the notation for eigenvalue problems of operator equations, we can finally come to the results from spectral theory which we will be using for our photonic crystal bandgap calculations. We need some general notation to formulate the classical results.

Let $L(V)$ be the space of all linear bounded operators on a Banach space V, equipped with the operator norm.

Definition 5.1 ([Wer11], Ch. VI.1)**.** The *resolvent set* of an operator T is defined as

$$\rho(T) \coloneqq \left\{\lambda \in \mathbb{C} \mid (\lambda I - T)^{-1} \text{ exists in } L(V)\right\}. \tag{5.1}$$

The *spectrum* of an operator is defined as the complement of the resolvent set, $\sigma(T) \coloneqq \mathbb{C} \setminus \rho(T)$. Those $\lambda \in \sigma(T)$ for which $\lambda I - T$ is not injective are called *eigenvalues* of T.

The main results in classical spectral theory have been obtained for *compact self-adjoint* operators [Wer11, Ch. VI.3], *self-adjoint* operators [Wer11, Cor. VII.1.2] and *Fredholm* operators. We will only recapture the theory for compact self-adjoint operators and Fredholm operators here, as the theory for self-adjoint operators requires a more involved notation and will not be used for the operators occurring in our model problem.

5.1 Compact self-adjoint operators

The main result on the spectrum of compact self-adjoint operators can be found in [Wer11, Th. VI.3.2 and Cor. VI.3.3]. It describes a spectral decomposition of the Hilbert space on which the operator is defined.

Theorem 5.2 ([Wer11], Thm. VI.3.2)**.** *Let T be a compact, normal (or self-adjoint) operator on a Hilbert space H. Then there exists an orthonormal system $e_1, e_2, \dots$ and a null-sequence $(\lambda_1, \lambda_2, \dots) \in \mathbb{C} \setminus \{0\}$ (or $\mathbb{R} \setminus \{0\}$) such that*

$$H = \ker T \oplus \overline{lin}\{e_1, e_2, \dots\}$$

and

$$Tx = \sum_i \lambda_i (x, e_i) e_i \quad \text{for all } x \in H.$$

Corollary 5.3 ([Wer11], Cor. VI.3.3)**.** *T can also be described through orthogonal projections as*

$$T = \sum_{j=1}^{\infty} \mu_i E_i$$

where μ_i are the eigenvalues not counted by their multiplicity and E_i the orthogonal projections on the eigenspaces corresponding to μ_i.

5.2 Min-max principles

Since the spectrum of *compact* self-adjoint operators is discrete, we can investigate properties of the eigenvalues. Courant's maximum principle gives a concrete analytic description for all eigenvalues.

Theorem 5.4 ([Wer11], Ch. VI.7)**.** *Let T be a compact, self-adjoint operator on a Hilbert space H. Then*

$$\lambda_i = \sup_{\substack{U \subset H \\ dim(U)=i}} \min_{x \in U \setminus \{0\}} \frac{(Tx,x)}{(x,x)} = \min_{\substack{V \subset H \\ dim(V)=i-1}} \max_{x \in V^\perp \setminus \{0\}} \frac{(Tx,x)}{(x,x)} \tag{5.2}$$

Remark 5.5. *Unfortunately, the minimum and maximum in Eq. (5.2) are usually impossible to compute. However, these results can be a good starting point for estimates of numerically calculated eigenvalues.*

5.3 Nonlinear operator valued functions

The spectral theory mentioned so far only applies to the classical spectral problem for an operator A and the resolvent and spectrum defined for $T = A - \lambda I$, where I is the identity operator. The spectral problems we will be studying, however, will contain additional terms in λ and therefore we will need a generalized notion of the *spectrum* of such operators.

We will study the spectra of operator valued functions $T : D \to L(H)$ defined on open subsets $D \subset \mathbb{C}$.

Definition 5.6 ([Eng10])**.** The resolvent set of a function $T : D \to L(H)$ is defined as

Note that each $T(\lambda)$ is a linear bounded operator on H and therefore has a resolvent set defined by Eq. (5.1)

$$\rho(T(\lambda)) = \{\mu \in \mathbb{C} \mid (T(\lambda) - \mu I)^{-1} \text{ exists in } L(H)\}.$$

Therefore if $\lambda \in \rho(T)$, the equation $T(\lambda)\mathbf{v} = 0$ has no nonzero solution $\mathbf{v}$. As in the linear case, the spectrum of T is then defined as the complement of the resolvent set.

Definition 5.7 ([Eng10])**.** The *spectrum* of an operator valued function $T : D \to L(H)$ is defined as

$$\sigma(T) = \mathbb{C} \setminus \rho(T).$$

This contains the continuous and the discrete spectrum (the eigenvalues) as in the classical linear operator case.

Definition 5.8 ([Eng10])**.** A $\lambda_0 \in D$ is called an *eigenvalue* of T if $T(\lambda_0)u = 0$ has a nonzero solution $u \in H$.

Remark 5.9. *This description of the spectrum of a nonlinear operator-valued function is from [Eng10]. Another description, by a min-max principle, of the spectrum of a nonlinear operator can be found in [Vos09].*

5.4 Fredholm operators

Definition 5.10 ([Wer11], Ch. VI.2)**.** A bounded operator T between two Banach spaces is called a *Fredholm operator* if its kernel and cokernel are finite dimensional and its range is closed. The *index of a Fredholm operator* is the number

$$\mathrm{ind}(T) = \dim(\ker T) + \dim(\mathrm{im}\ T)^{\perp}.$$

For a nonlinear operator-valued function $T(\lambda)$ this definition can be taken for each fixed $\lambda \in D$. Then, the $\lambda \in \sigma(T)$ for which $T(\lambda)$ is a Fredholm operator are exactly the eigenvalues. They have finite multiplicity as $\dim(\ker T(\lambda)) < \infty$.

Theorem 5.11 ([McL00], Thm. 2.22)**.** *Let B_λ be a compact operator on a Banach space. Then $T_\lambda := I - B_\lambda$ is Fredholm and ind$(T_\lambda) = 0$.*

Theorem 5.12 ([McL00], Thm. 2.27)**.** *Let $T_\lambda : X \to Y$ be a Fredholm operator between two Banach spaces with ind$(T_\lambda) = 0$. There are two, mutually exclusive possibilities:*

- *The homogeneous equation $T_\lambda u = 0$ has only the trivial solution $u = 0$. In this case, for each $f \in Y$, the inhomogeneous equation $T_\lambda u = f$ has a unique solution $u \in X$;*
- *The homogeneous equation $T_\lambda u = 0$ has exactly p linearly independent solutions $u_1, ..., u_p$ for some finite $p > 1$.*

Theorem 5.13. *The analytic Fredholm theorem. [[GK69], Ch. 1, Thm. 5.1] Let $B : D \to L(H)$ an operator-valued function that is analytic on D and such that $B(\lambda)$ is a compact operator for each $\lambda \in D$. Then for all $\lambda \in D$, with the possible exception of certain isolated points, the number $\alpha(\lambda)$ of linearly independent solutions of*

$$(I - B(\lambda))\, u = 0$$

is constant: $\alpha(\lambda) = n$. At the isolated points mentioned, $\alpha(n) \geq n$.

Remark 5.14. *In order to use this theorem for our model problem (3.3), we must show that our operators $T(\lambda)$ can be written as $T(\lambda) = I - B(\lambda)$ for compact operators $B(\lambda)$. $T(\lambda)$ are then Fredholm operators and the analytic Fredholm theorem can be applied, as I is the identity and $B(\lambda)$ are compact operators.*

6 The nonlinear eigenvalue problem

For the calculation of bandgaps of a three-dimensional photonic crystal we have so far introduced the model problem (3.3)

$$L(\varepsilon, \omega, \boldsymbol{k})\boldsymbol{u_k}(\boldsymbol{x}) = \nabla_{\boldsymbol{k}} \times \left(\frac{1}{\mu}\nabla_{\boldsymbol{k}} \times \boldsymbol{u_k}(\boldsymbol{x})\right) - \omega^2\, \varepsilon(\boldsymbol{x}, \omega)\boldsymbol{u_k}(\boldsymbol{x}) = 0 \quad \text{in } \Omega, \tag{6.1}$$

where $\Omega \subset \mathbb{R}^3$ is the *fundamental periodicty cell* of the crystal lattice and k is the *wavevector*, a parameter from the *Brillouin zone* $\mathcal{K}$.

If the crystal is only periodic in two dimensions and constant in the third one, the model problem reduces to the two-dimensional scalar problem [Kuc01].

$$L(\varepsilon, \omega, k)u_k(x) = (\nabla + ik) \cdot \frac{1}{\mu}(\nabla + ik)u_k(x) - \omega^2\, \varepsilon(x, \omega)u_k(x) = 0 \quad \text{in } \Omega \subset \mathbb{R}^2. \tag{6.2}$$

If we examine Eqs. (6.1) and (6.2) closer we see that, determined by the dependencies of ε on x and ω, different types of eigenvalue problems need to be solved. The case where ε does not depend on the frequency ω has been investigated numerically in various papers (e.g. [DLP$^+$11], [Gia12], citeBofCG06). In that case, Eq. (6.1) reduces to a generalized linear eigenvalue problem for $\lambda = \omega^2$, namely:

Find $(\lambda, \boldsymbol{u_k}) \in \mathbb{C} \times V$ with $\|\boldsymbol{u_k}\|_V = 1$ such that

$$\begin{aligned} & \nabla_{\boldsymbol{k}} \times \left(\frac{1}{\mu} \nabla_{\boldsymbol{k}} \times \boldsymbol{u_k}(\boldsymbol{x}) \right) = \lambda \, \varepsilon(\boldsymbol{x}) \boldsymbol{u_k}(\boldsymbol{x}) \quad \text{in } \Omega \\ \Leftrightarrow \quad & A_k \boldsymbol{u_k} = \lambda M \boldsymbol{u_k} \\ \Leftrightarrow \quad & T_{\boldsymbol{k}}(\lambda) \boldsymbol{u_k} \coloneqq (A_{\boldsymbol{k}} - \lambda M) \boldsymbol{u_k} = 0. \end{aligned}$$

Remark 6.1. *For the solution of this generalized linear eigenvalue problem many numerical algorithms have been proposed and studied, such as discretization by a finite element method and iterative solution of the resulting algebraic eigenvalue problem by the* Arnoldi method *or the* Lanczos method *for symmetric problems [BDD$^+$00].*

Let us now consider the case where ε does depend on the frequency ω in a not specified manner which includes any nonlinear dependence. To that end, assume that the domain Ω is divided into s subdomains Ω_j in which the permittivity does not depend on space anymore, only on the frequency. Let $\mathcal{I}_j$ be the indicator functions on these subdomains with

$$\mathcal{I}_i(x) = \begin{cases} 1 & \text{if } x \in \Omega_i, \\ 0 & \text{otherwise.} \end{cases}$$

Then the permittivity can be written as $\varepsilon(\omega, x) = \sum_{j=1}^{s} \varepsilon_j(\omega) \mathcal{I}_j(x)$.

For $\mu = 1$ we consider Eq. (6.1) in the weak formulation, i.e. ,we multiply by test functions from V, integrate over Ω and apply the integration by parts formula given in Eq. (4.4). We obtain the following eigenvalue problem:

Find $(\omega, \boldsymbol{u_k}) \in \mathbb{C} \times V$ with $\|\boldsymbol{u_k}\|_V = 1$ such that for all $\boldsymbol{v} \in V$

$$\int_\Omega (\nabla_{\boldsymbol{k}} \times \boldsymbol{u_k}) \cdot (\nabla_{\boldsymbol{k}} \times \boldsymbol{v}) = \omega^2 \sum_{j=1}^{s} \varepsilon_j(\omega) \int_{\Omega_j} \boldsymbol{u_k} \cdot \boldsymbol{v} \, \mathrm{d}\boldsymbol{x} \tag{6.3}$$

$$\Leftrightarrow \quad a_{\boldsymbol{k}}(\boldsymbol{u_k}, \boldsymbol{v}) = \omega^2 \sum_{j=1}^{s} \varepsilon_j(\omega) \, m_j(\boldsymbol{u_k}, \boldsymbol{v}) \tag{6.4}$$

In operator form, the problem is:

Find $(\omega, \boldsymbol{u_k}) \in \mathbb{C} \times V$ with $\|\boldsymbol{u_k}\|_V = 1$ such that for all $\boldsymbol{v} \in V$

$$T_k(\omega) \boldsymbol{u_k} \coloneqq (A_{\boldsymbol{k}} - \omega^2 \sum_{j=1}^{s} \varepsilon_j(\omega) M_j) \boldsymbol{u_k} = 0 \tag{6.5}$$

which is a nonlinear eigenvalue problem for the operator valued function $T_{\boldsymbol{k}}(\omega)$ with the nonlinearities depending on the form of the ε_j.

Remark 6.2. *There are typically two possible approaches to solve a nonlinear eigenvalue problem. The first one consists in turning the system into a linear eigenvalue problem by means of an appropriate linearization technique [MMMM06, BDD$^+$00, EKE12, EK12]. This approach is often used for eigenvalue problems which are polynomial in the eigenvalue. The second approach consists in applying* Newton's method *or* inverse iteration *such as [HLM16, SP04] directly to the nonlinear eigenvalue problem.*

7 Spectral analysis

In order to solve problem (6.5), we must first analytically determine what sort of solutions, i.e. , eigenvalues and eigenfunctions, can be expected. Fortunately, the spectrum of $T_k(\omega)$ was rigorously analyzed in [Eng10] for the two-dimensional case. In this paper we consider the three-dimensional problem in a similar way.

In the remainder we assume that $\varepsilon(\boldsymbol{x}, \omega)$ satisfies the conditions of Thm. 4.5.

7.1 Two-dimensional case

Let us briefly recapture the results from [Eng10] for the two-dimensional case. The operator $T_k(\omega)$ in the two-dimensional case is given by

$$(T_k(\omega)u_k, v) = \int_\Omega \nabla_k u_k \cdot \overline{\nabla_k v} - \omega^2 \int_\Omega \varepsilon(\omega, x)\ u_k \bar{v}\, \mathrm{d}x\,. \tag{7.1}$$

The can be decomposed into

$$T_k(\omega) = I - B_k(\omega)$$

with

$$(Iu, v) = \int_\Omega \nabla_k u_k \cdot \overline{\nabla_k v} + u_k \bar{v}\, \mathrm{d}x\,.$$

and

$$(B_k(\omega)u, v) = \int_\Omega \left(\omega^2 \varepsilon(\omega, x) + 1\right)\ u_k \bar{v}\, \mathrm{d}x\,.$$

After showing that $B_k(\omega)$ is *bounded* and *compact* for fixed ω, Thms. 5.11, 5.12, and 5.13 can be applied to show that the spectrum of $T_k(\omega)$ consists of at most *countably many isolated eigenvalues* with finite geometrical multiplicity [Eng10, Th. 4.1].

7.2 Three-dimensional case

For the three-dimensional case described by Eq. (6.3) we consider a similar approach as in [Eng10].

Let us first consider the biggest search space V that is possible, i.e. , we search solutions $\boldsymbol{u}$ of Eq. (6.3) in the whole space $H_{\mathrm{per}}(\mathrm{curl}, \Omega)$. We see that any of theses solutions $\boldsymbol{u}$ has to satisfy

$$t_{\omega,\boldsymbol{k}}(\boldsymbol{u}, \boldsymbol{v}) \coloneqq \int_\Omega \nabla_{\boldsymbol{k}} \times \boldsymbol{u} \cdot \overline{\nabla_{\boldsymbol{k}} \times \boldsymbol{v}} - \omega^2 \int_\Omega \varepsilon(\boldsymbol{x}, \omega)\boldsymbol{u} \cdot \bar{\boldsymbol{v}}\, \mathrm{d}\boldsymbol{x} = 0 \tag{7.2}$$

for all $\boldsymbol{v} \in H_{\mathrm{per}}(\mathrm{curl}, \Omega)$. In particular, for $\boldsymbol{v} = \nabla_{\boldsymbol{k}}\xi,\ \xi \in H^1_{\mathrm{per}}(\Omega)$, any solution $\boldsymbol{u}$ has to satisfy

$$\omega^2 \int_\Omega \varepsilon(\boldsymbol{x}, \omega)\boldsymbol{u} \cdot \overline{\nabla_{\boldsymbol{k}}\xi}\, \mathrm{d}\boldsymbol{x} = 0.$$

Therefore, we restrain the search space to $V \coloneqq V_{\boldsymbol{k}}^{(\varepsilon)}$.

The sesquilinear form in Eq. (7.3) can be written in the form

$$t_{\omega,\boldsymbol{k}}(\boldsymbol{u}, \boldsymbol{v}) = \langle \boldsymbol{u}, \boldsymbol{v} \rangle_{\boldsymbol{k}} - b_{\omega,\boldsymbol{k}}(\boldsymbol{u}, \boldsymbol{v})$$

with

$$b_{\omega,\boldsymbol{k}}(\boldsymbol{u}, \boldsymbol{v}) \coloneqq \int_\Omega \left(\omega^2 \varepsilon(\boldsymbol{x}, \omega) + 1\right) \boldsymbol{u} \cdot \bar{\boldsymbol{v}}\, \mathrm{d}\boldsymbol{x}\,. \tag{7.3}$$

Lemma 7.1. *The sesquilinear form in Eq. (7.3) is bounded in* $V_{\boldsymbol{k}}^{(\varepsilon)}$.

Proof. It follows straightforwardly from Eq. (4.8). □

In operator form, the spectral problem (6.5) can be rewritten in the form

$$0 = \langle \boldsymbol{u}, \boldsymbol{v} \rangle - \langle B(\omega)\boldsymbol{u}, \boldsymbol{v} \rangle$$

where $B(\omega)$ is the operator-valued function corresponding to $b_{\omega,\boldsymbol{k}}$.

Lemma 7.2. *The operator* $B(\omega)$ *is compact for all* $\omega \in D$.

Proof. Let $\{\boldsymbol{u}_n\}_{n\in\mathbb{N}} \in V_{\boldsymbol{k}}^{(\varepsilon)}$ be a given bounded sequence. Then, by Lem. 4.8, $\{\boldsymbol{u}_n\}$ has a convergent subsequence $\{\boldsymbol{u}_{n_m}\}_{m\in\mathbb{N}}$ in $\left(L^2(\Omega)\right)^3$. Let $\boldsymbol{u}_{n_m}$ and $\boldsymbol{u}_{n_{m'}}$ denote two elements in the subsequence $\{u_{n_m}\}$. Then

$$\begin{aligned}
&\|B(\omega)\boldsymbol{u}_{n_m} - B(\omega)\boldsymbol{u}_{n_{m'}}\|_{\boldsymbol{k}}^2 \\
&\qquad = \left| b_{\omega,\boldsymbol{k}}(\boldsymbol{u}_{n_m} - \boldsymbol{u}_{n_{m'}}, B(\omega)\boldsymbol{u}_{n_m} - B(\omega)\boldsymbol{u}_{n_{m'}}) \right| \\
&\qquad \leq C \left\| B(\omega)\boldsymbol{u}_{n_m} - B(\omega)\boldsymbol{u}_{n_{m'}} \right\|_{\boldsymbol{k}} \left\| \boldsymbol{u}_{n_m} - \boldsymbol{u}_{n_{m'}} \right\|_{(L^2(\Omega))^3}
\end{aligned}$$

where C is the bounding constant of Lem. 7.1. Therefore, $\{B(\omega)\boldsymbol{u}_{n_m}\}_{m\in\mathbb{N}}$ converges since $\{\boldsymbol{u}_{n_m}\}$ converges. □

Thanks to Thm. 5.11, we know that

$$T(\omega) \coloneqq I - B(\omega)$$

is a Fredholm operator-valued function with $\operatorname{ind}(T(\omega)) = 0$ for all $\omega \in D$. It follows from Thm. 5.12 that all eigenvalues have finite geometric multiplicities.

Note that in the spectral problem described by Eq. (7.2) with the chosen search space $V = V_{\boldsymbol{k}}^{(\varepsilon)}$, $\omega = 0$ implies $\nabla_{\boldsymbol{k}} \times \boldsymbol{u} = 0$. By Lem. 4.3, it follows that $\boldsymbol{u} = 0$ is the only solution corresponding to $\omega = 0$, for all $\boldsymbol{k} \in \mathcal{K}$. Thus, the resolvent set of $T(\omega)$ is not empty since it contains $\omega = 0$.

With Thm. 5.13, we arrive thus to the following result:

Theorem 7.3. *The spectrum of the operator-valued function* $T(\omega)$ *consists of at most countably many isolated eigenvalues of finite geometrical multiplicities.*

8 Discretization

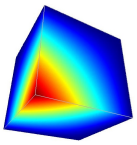
The operator $T_k(\omega)$ in Eq. (6.5) is defined on the Hilbert space $H_{\text{per}}(\text{curl}, \Omega)$, see Eq. (4.1), or for two dimensions as in Eq. (7.1) on $H^1_{\text{per}}(\Omega)$, see Eq. (4.1). In both cases we consider a conforming finite element discretization of the operator eigenvalue problem.

This means, we define a regular triangulation $\mathcal{T}_h$ of Ω where the boundaries of the different subdomains Ω_j coincide with edges of the triangulation. We follow the notation of [Ver13]. Let $\mathcal{N}_h$ be the set of nodes and $\mathcal{E}_h$ the set of edges or faces of the triangulation. For an element $K \in \mathcal{T}_h$ let $\mathcal{N}_K$ be the set of nodes and $\mathcal{E}_K$ the set of edges or faces of that element.

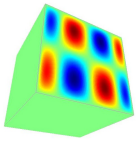
For an edge or face $E \in \mathcal{E}_h$ let $\mathcal{N}_E$ be the set of nodes on that edge or face. A *nodal shape function* $\lambda_z, z \in \mathcal{N}_h$, is defined as a piecewise linear function with

$$\lambda_z(z) = 1, \quad \lambda_z(x) = 0 \text{ for all } x \in \mathcal{N}_h \setminus \{z\}.$$

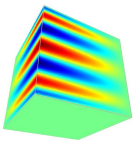
As discrete solution spaces we consider the finite element spaces $V_h = P_p(\mathcal{T}_h) \subset V = H^1_{\text{per}}(\Omega)$ of polynomial nodal elements of degree p, or *Lagrange elements* of order p, for $\Omega \subset \mathbb{R}^2$ and $V_h = N_p(\mathcal{T}_h) \subset V = H_{\text{per}}(\text{curl}, \Omega)$ the space of polynomial edge elements of degree p, or *Nédélec elements* [Néd80] of order p, for $\Omega \subset \mathbb{R}^3$. These are both conforming finite element spaces as they are contained in the respective solution spaces of the continuous problem. See Fig. 8.1A and Fig. 8.1C for examples of a higher order edge function and a second order nodal function on a three-dimensional quadrilateral element. For more illustrations and detailed descriptions of the finite element spaces see e.g. [AL14].



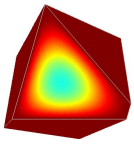
(A) A vertex function [Sol08].



(B) A face function [Sol08].



(C) An edge function [Sol08].



(D) A bubble function [Sol08].

Fig. 8.1: Examples of shape functions on a three-dimensional quadrilateral element.

Next, we consider the discretization of the operator $T_k(\omega)$ defined in Eqs. (6.3) and (7.1) respectively. Since in both cases the differential operator involved is linear and we chose conforming finite element spaces V_h, we can define the discrete operators $T_{k,h}(\omega_h)$ simply as restrictions of $T_k(\omega)$ to the finite dimensional spaces V_h, i.e.

$$(T_{k,h}(\omega_h)\boldsymbol{u}_{k,h}, \boldsymbol{v}_h) = (T_k(\omega_h)\boldsymbol{u}_{k,h}, \boldsymbol{v}_h) \qquad \text{for all } \boldsymbol{v}_h \in V_h. \tag{8.1}$$

Therefore, we immediately get the Galerkin orthogonality of the residual

$$(T_k(\omega - \omega_h)(\boldsymbol{u}_k - \boldsymbol{u}_{k,h}), \boldsymbol{v}_h) = 0 \qquad \text{for all } \boldsymbol{v}_h \in V_h \tag{8.2}$$

by choosing the above mentioned spaces V_h, if $(\omega, \boldsymbol{u}_k)$ is an eigenpair of the operator defined in Eq. (6.3) and $(\omega_h, \boldsymbol{u}_{k,h})$ is an eigenpair of (8.1).

In order to approximate the discretization error $e_h = (\omega, \boldsymbol{u}_k) - (\omega_h, \boldsymbol{u}_{k,h}) = (\omega - \omega_h, \boldsymbol{u}_k - \boldsymbol{u}_{k,h})$, which in general is unknown as $(\omega, \boldsymbol{u}_k)$ is unknown, we define some additional intermediate spaces of *bubble functions*, which are higher order polynomials inside the elements of $\mathcal{T}_h$ and vanish on the boundaries. See Fig. 8.1D for an example of a face bubble function on a three-dimensional element.

Definition 8.1. Let $K \in \mathcal{T}_h, E \in \mathcal{E}_h$ be an element and an edge or face of a given triangulation $\mathcal{T}_h$. The locally defined weighted products of the nodal shape functions

$$\psi_K = \beta_K \prod_{z \in \mathcal{N}_K} \lambda_z, \quad \psi_E = \beta_E \prod_{z \in \mathcal{N}_E} \lambda_z, \tag{8.3}$$

are called *bubble functions*, or *local cut-off functions* [Ver13], with

$$\beta_K = \begin{cases} (d+1)^{d+1} & \text{if } K \text{ is a simplex,} \\ (2d)^{2d} & \text{if } K \text{ is a parallelepiped,} \end{cases}$$

$$\beta_E = \begin{cases} 2^2 & \text{if } E \text{ is an edge,} \\ d^d & \text{if } E \text{ is a } (d-1)\text{-dimensional simplex,} \\ (2^{d-1})^{2^{d-1}} & \text{if } E \text{ is a } (d-1)\text{-dimensional parallelepiped.} \end{cases}$$

Remark 8.2. *The bubble functions fulfill certain inverse estimates for polynomials in local elementwise norms [Ver13, Ch. 3.6] which are used to derive lower bounds for error estimation in the next section.*

9 Error estimation

We will now consider the two-dimensional problem for the operator in Eq. (7.1). In order to derive a first residual based a posteriori error estimator for the nonlinear problem given by Eq. (7.1) we apply results for general nonlinear problems from [Ver13] modified to our setting of an eigenvalue problem.

To that end, we reformulate the eigenvalue problem for the operator in Eq. (7.1) as a general nonlinear problem. Find $(\omega, u) \in \mathbb{C} \times V$ such that

$$F(\omega, u) = 0 \tag{9.1}$$

with F defined by the weak formulation

$$\begin{aligned} \langle F(\omega,u),(\mu,v)\rangle_V = &\int_\Omega (\nabla + ik)u \cdot (\nabla + ik)v - \omega^2 \varepsilon(x,\omega) uv \; dx \\ &+ \mu \left(\int_\Omega u^2 \; dx - 1 \right) \qquad \text{for all } v \in V. \end{aligned}$$

The problem for the discretized operator in Eq. (8.1) takes the form: Find $(\omega_h, u_h) \in \mathbb{C} \times V_h$ such that

$$F_h(\omega_h, u_h) = 0 \tag{9.2}$$

with F_h the restriction of F to $\mathbb{C} \times V_h$, just as in Eq. (8.1).

In the discrete solution space V_h we will need an operator to describe the possible jumps of gradients of the piecewise continuous functions across edges of the triangulation $\mathcal{T}_h$.

Definition 9.1. The operator $[\![\cdot]\!]_E$ describes the *jump in normal direction* of a piecewise polynomial vector valued function across an edge E defined by

$$[\![\nabla v]\!]_E = (\nabla v|_{K_1} + \nabla v|_{K_2}) \cdot \mathbf{n}_E$$

for $E = K_1 \cap K_2 \in \mathcal{E}_h$ and $\mathbf{n}_E$ the normal vector on E.

Then we define the residual based error estimator

$$\eta_K^2 = \; h_K^2 \; \|(\nabla + ik) \cdot (\nabla + ik) u_h - \omega_h^2 \varepsilon(\omega_h) u_h\|_K^2 + \frac{1}{2} \sum_{E \in \mathcal{E}_K} h_E \; [\![(\nabla + ik) u_h]\!]_E^2 \tag{9.3}$$

elementwise for $K \in \mathcal{T}_h$.

Proposition 9.2. *Let (ω, u) be a regular solution of Eq. (9.1), i.e.,let ω be a simple eigenvalue of the operator defined in Eq. (7.1) and ε analytic in a neighbourhood of ω. If (ω_h, u_h) is a solution of the discretized problem (9.2) sufficiently close to (ω, u), then*

$$|\omega - \omega_h| + \|\nabla(u - u_h)\| \leq c_1 \Big(\sum_{K \in \mathcal{T}_h} \eta_K^2 \Big)^{\frac{1}{2}} =: c_1 \eta_h \tag{9.4}$$

and

$$\eta_h = \Big(\sum_{K \in \mathcal{T}_h} \eta_K^2 \Big)^{\frac{1}{2}} \leq c_2 \left(|\omega - \omega_h| + \|\nabla(u - u_h)\| \right) \tag{9.5}$$

for constants c_1, c_2 depending only on the polynomial degree of u_h and the regularity of the triangulation $\mathcal{T}_h$.

Proof. Proposition 5.1 in [Ver13] yields a direct equivalence between the discretization error $\|(\omega, u) - (\omega_h, u_h)\|_{\mathbb{C} \times V}$ and the residual $F(\omega_h, u_h)$ around points (ω, u) with simple eigenvalues ω. This equivalence, however, holds for the dual norm of the residual $\|F(\omega_h, u_h)\|_{V^\star}$ which is in general as hard to calculate as the solution itself. Thm. 5.5 [Ver13] then establishes upper and lower bounds for the dual norm of the residual through error estimators. Similar to Thm. 5.23 [Ver13], integration by parts of Eq. (9.1) yields the L^2-representation of the residual

$$\langle F(\omega_h, u_h), (\mu, v) \rangle_H = \sum_{K \in \mathcal{T}_h} \int_K \Big((\nabla + ik) \cdot (\nabla + ik) u_h + \omega_h^2 \varepsilon(\omega_h) u_h \Big) v + \sum_{E \in \mathcal{E}_h} \int_E [\![(\nabla + ik) u_h]\!] v.$$

The term $\int_\Omega u_h^2 - 1$ disappears as u_h is assumed to be a solution of (9.2). This L^2-representation then implies the upper bound in (9.4) for the error estimator η_K defined above.

For the lower bound in Eq. (9.5) we consider an intermediate space Y_h, $V_h \subset Y_h \subset V$, for which we know the lower bound

$$\eta_h \leq c_2 \|F(\omega_h, u_h)\|_{Y_h^\star}$$

with c_2 only depending on the shape regularity of the triangulation and the polynomial degree of V_h. Choosing Y_h as the space of element and edge bubble functions (8.3) introduced in the last section, we can use the inverse estimates in Proposition 3.37 [Ver13] and the resulting lower bounds in Thm. 3.59 [Ver13] and then apply the second part of Thm. 5.5 [Ver13] to get the lower bound in (9.5). □

Remark 9.3. *The condition that the discrete solution has to be* sufficiently close *to the exact solution and that ε has to be analytic in a neighbourhood of the actual eigenvalue are quite restrictive and might not apply in some situations which are important for applications. However, the error estimator η_h is a first step towards adaptive grid refinement for nonlinear photonic crystal bandgap calculations.*

Remark 9.4. *Compared with standard error estimators for linear eigenvalue problems (e.g. [Ver13, Ch. 4.7], [GG12]), the fully nonlinear approach in Proposition 9.2 does not include higher order terms. This is due to the direct equivalence of the error and the residual in the general nonlinear approach, where the eigenvalue is not interpreted as a parameter, but a variable. On the other hand, the lower bound in Proposition 9.2 is not local but global, due to the global term $\int_\Omega u^2 - 1$ in the nonlinear formulation of the problem.*

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