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# PDE Eigenvalue Iterations with Applications in Two-dimensional Photonic Crystals*

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Abstract. The first part of this paper is devoted to the approximative solution of linear and Hermitian eigenvalue problems where the differential operator satisfies a Gårding inequality. For this, known iterative schemes for the matrix case such as the inverse power or Arnoldi method are extended to the infinite-dimensional case. This formally allows one to apply different spatial discretizations in each iteration step and thus, justifies the use of adaptive methods. The second part considers eigenvalue problems as they appear in two-dimensional models of photonic crystals for the computation of band-gaps. If the permittivity of the material is frequency-dependent, then this leads to a nonlinear eigenvalue problem. For this, we consider two strategies. First, a linearization combined with the application of the inverse power method and second, a direct application of Newton's iteration.

**Key words.** nonlinear eigenvalue problem, photonic crystals, inverse power method, Newton iteration

**AMS subject classifications. 65N25, 65J10, 65F15**

## 1. Introduction

Eigenvalue problems including partial differential equations (PDE) appear in several applications such as structural mechanics [BW73], fluid-solid structures [Vos03], or the simulation of Bose-Einstein condensates [PS03]. In general, such problems are considered in order to optimize certain properties or parameters of the underlying dynamical system [MV04]. In this paper, we focus on applications as they appear in the modeling of photonic crystals [Joh87, Kuc01]. These are special composite materials with a periodic structure that affect the propagation of electromagnetic waves and thus, can be used for trapping and guiding light. As these crystals can be designed and manufactured for industrial applications, the aim is to find so-called *photonic band-gaps*, which prevent light within a specified frequency range from propagating [JJWM08, Joh12]. Direct applications areas are optical fibers [GH14, Ch. 5], medical technologies with laser guides for cancer surgeries [Tsa12], and thin film solar cells [DJ12].

The corresponding mathematical model is given by a sequence of nonlinear PDE eigenvalue problems based on the Maxwell equations [SP05, DLP$^+$11]. An important role is played by the *electric permittivity* $\varepsilon$, which is periodic in space and characterizes certain properties of the crystal. If $\varepsilon$ is independent of the frequency, then we obtain a linear eigenvalue problem. In more realistic models, however, the permittivity is approximated by a rational function, which carries the nonlinearity to the eigenvalue problem.

Numerical methods for computing the spectrum of such materials have been studied intensively. This includes adaptive finite element methods [BKS$^+$06, GG12], Newton-type methods [Kre09, HLM16], and linearization techniques [SB11, EKE12]. In the latter

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case, a spatial discretization is assumed and yields then a linear but extended eigenvalue problem, for which well-known iteration schemes can be applied.

Corresponding iterative methods for the operator case have, so far, not received much attention in the literature. In the first part of this paper, we focus on linear and Hermitian PDE eigenvalue problems in the weak formulation. This corresponds to the case of a frequency-independent permittivity. Convergence of the (inverse) power method for compact operators mapping from a Hilbert space $\mathcal{H}$ to $\mathcal{H}$ was already shown in [ESL95]. In this setting, the proof basically follows the same lines as in the finite-dimensional case. General bounded operators were considered in [EE07] but only together with a power iteration based on the exact (und thus unknown) eigenvalue. Considering the weak formulation, which is more natural in view of spatial discretization methods, we are in a different setting. Nevertheless, the power method converges if an appropriate scaling is included. For the $p$-Laplacian eigenvalue problem, this was shown in [Boz16].

The second part of the paper focuses on the nonlinear case as it appears in two-dimensional photonic crystal modeling. Here we consider two different paths of either linearizing the problem or applying directly a Newton iteration. In the first case, we combine the techniques introduced in [SB11, EKE12] with a inverse power iteration applied to the resulting linear problem. The second strategy translates the local convergence of Newton's method from [Sch08] to the operator case. An analogous method for infinite-dimensional eigenvalue problems was developed in [AR68], and its local convergence was proven for Fredholm operators with index 0 mapping from a Hilbert space $\mathcal{H}$ to $\mathcal{H}$. The method converges in a similar way when the operators arise from the weak formulation considered here.

The paper is structured as follows. In Section 2 we introduce the problem setting, i.e., the linear PDE eigenvalue problem in its weak and operator formulation. Here we gather all the assumptions on the spaces and included operators. In particular, we assume an underlying Gelfand triple with a compact embedding. Section 3 then considers several iteration schemes including the inverse power method, the Arnoldi method, and Newton's method. Two-dimensional photonic crystals with frequency-dependent permittivity are then topic of Sections 4 and 5. First, we consider a special Hermitian case. For this, we apply a linearization and the inverse power method. More realistic models are then discussed in Section 5, for which we prove the local convergence of Newton's method.

## 2. Preliminaries

As described in the introduction, we consider the weak formulation of a PDE eigenvalue problem, given by the sesquilinear forms $a\colon \mathcal{V}\times\mathcal{V}\to\mathbb{C}$ and $(\cdot\,,\cdot)\colon \mathcal{V}\times\mathcal{V}\to\mathbb{C}$. This means that we search for a pair $(u,\lambda)\in\mathcal{V}\times\mathbb{C}$ such that for all test functions $v\in\mathcal{V}$ it holds that

$$a(u,v) = \lambda\,(u,v). \tag{2.1}$$

More precisely, considering Hermitian eigenvalue problems, we are interested in the smallest eigenpair. In the following, we gather assumptions on the space $\mathcal{V}$ and the included sesquilinear forms. Afterwards we discuss well-known PDE eigenvalue problems, which fit into the given framework.

### 2.1. **General setting.** We start with general assumptions on the involved function spaces.

*Assumption* 2.1 (Function spaces). We assume $\mathcal{V}$ to be a complex, separable, and reflexive Banach space. Furthermore, we assume the existence of a complex and separable Hilbert space $\mathcal{H}$ (the pivot space) such that $\mathcal{V}$, $\mathcal{H}$, $\mathcal{V}^*$ form a *Gelfand triple*, cf. [Zei90, Ch. 23.4] and [Bre10, Ch. 11.4]. This means, in particular, that the embedding $i_{\mathcal{V}\hookrightarrow\mathcal{H}}\colon \mathcal{V}\hookrightarrow\mathcal{H}$ is continuous and dense [Wlo87, Ch. 17.1]. The continuity constant is denoted by $C_{\mathcal{V}\hookrightarrow\mathcal{H}}$.

*Assumption* 2.2 (Compactness). The embedding $\mathcal{V}\hookrightarrow\mathcal{H}$ is compact.

With the pivot space $\mathcal{H}$ in hand, we assume that the sesquilinear $(\cdot\,,\cdot)$ in (2.1) is also defined for functions in $\mathcal{H}$. We even assume that this defines the inner product in the Hilbert space $\mathcal{H}$ and set $\|\cdot\| := \|\cdot\|_{\mathcal{H}} = (\cdot\,,\cdot)^{1/2}$. Further, $j_{\mathcal{H}}\colon \mathcal{H}\to\mathcal{H}^*$ denotes the Riesz isomorphism. The norm in the space $\mathcal{V}$ is denoted by $\|\cdot\|_{\mathcal{V}}$. For the sesquilinear form $a$ we consider the following assumptions.

*Assumption* 2.3 (Sesquilinear form). The sesquilinear form $a\colon \mathcal{V}\times\mathcal{V}\to\mathbb{C}$ is assumed to be continuous and Hermitian such that $a(u,u)\in\mathbb{R}$ for all $u\in\mathcal{V}$. Furthermore, $a$ satisfies a Gårding inequality, i.e.,

$$a(u,u)\geq \alpha\,\|u\|_{\mathcal{V}}^2 - \beta\,\|u\|^2$$

for real constants $\alpha>0$, $\beta\geq 0$ and all $u,v\in\mathcal{V}$.

*Remark* 2.4. The previous Assumption 2.3 implies that $a_\beta(u,v) := a(u,v)+\beta\,(u,v)$ is $\mathcal{V}$-coercive and thus, defines an inner product in $\mathcal{V}$. As a result, $\mathcal{V}$ is actually a Hilbert space and the corresponding norm

$$\|u\|_\beta := a_\beta(u,u)^{1/2}\geq\sqrt{\alpha}\,\|u\|_{\mathcal{V}}$$

is equivalent to $\|\cdot\|_{\mathcal{V}}$. Further, all eigenvalues are real and satisfy $\lambda>-\beta$.

In order to be well-posed, an eigenvalue problem of the form (2.1) requires boundary conditions. Throughout this paper, we assume that these conditions are included in the space $\mathcal{V}$, cf. the examples in the following subsection. We close this preliminary part with the proof of Young's inequality in the specific case of complex vectors.

**Lemma 2.5** (Young's inequality). *Consider $\mathbf{a},\mathbf{b}\in\mathbb{C}^2$. Then, for every $\delta>0$ we have an estimate of the form*

$$|\mathbf{a}\cdot\overline{\mathbf{b}}+\overline{\mathbf{a}}\cdot\mathbf{b}|\leq\frac{1}{\delta}\,|\mathbf{a}|^2+\delta\,|\mathbf{b}|^2.$$

*Proof.* For any two vectors $\mathbf{c},\mathbf{d}\in\mathbb{C}^2$, the following estimates hold:

$$\begin{aligned}0&\leq|\mathbf{c}+\mathbf{d}|^2=(\mathbf{c}+\mathbf{d})\cdot\overline{(\mathbf{c}+\mathbf{d})}=|\mathbf{c}|^2+|\mathbf{d}|^2+\mathbf{c}\cdot\overline{\mathbf{d}}+\overline{\mathbf{c}}\cdot\mathbf{d},\\ 0&\leq|\mathbf{c}-\mathbf{d}|^2=(\mathbf{c}-\mathbf{d})\cdot\overline{(\mathbf{c}-\mathbf{d})}=|\mathbf{c}|^2+|\mathbf{d}|^2-\mathbf{c}\cdot\overline{\mathbf{d}}-\overline{\mathbf{c}}\cdot\mathbf{d}.\end{aligned}$$

As a result, we have $|\mathbf{c}\cdot\overline{\mathbf{d}}+\overline{\mathbf{c}}\cdot\mathbf{d}|\leq|\mathbf{c}|^2+|\mathbf{d}|^2$. The claim then follows by setting $\mathbf{c}=\mathbf{a}/\sqrt{\delta}$, and $\mathbf{d}=\mathbf{b}\sqrt{\delta}$. □

2.2. **Examples.** We present a couple of well-known examples, which fit into the given framework if formulated in the weak setting.

**Example 2.6** (Laplace eigenvalue problem)**.** Consider the eigenvalue problem $-\Delta u=\lambda u$ in a bounded domain $\Omega$ with homogeneous Dirichlet boundary conditions. For this, we set $\mathcal{V}:=H^1_0(\Omega)$ with $\|\cdot\|_{\mathcal{V}}:=\|\nabla\cdot\|_{L^2(\Omega)}$ and $\mathcal{H}:=L^2(\Omega)$ with the standard inner product. The corresponding sesquilinear form reads $a(u,v):=\int_\Omega\nabla u\cdot\overline{\nabla v}\,\mathrm{d}x$. Note that this implies $a(u,u)=\|u\|_{\mathcal{V}}^2$ and thus, $\alpha=1$ and $\beta=0$. The weak form of the Laplace eigenvalue problem then reads: find a pair $(u,\lambda)\in\mathcal{V}\times\mathbb{C}$ such that for all $v\in\mathcal{V}$ it holds that

$$a(u,v)=\lambda\,(u,v).$$

**Example 2.7** (Schrödinger eigenvalue problem)**.** The computation of the ground state of the linear Schrödinger operator leads to the sesquilinear form

$$a(u,v) := \int_\Omega \nabla u(x) \cdot \overline{\nabla v(x)} + W(x)\, u(x)\overline{v(x)}\, \mathrm{d}x$$

with a real-valued potential $W \in L^\infty(\Omega)$ defining $\beta := \max\{0, -\min_{x\in\Omega} W(x)\}$. For homogeneous Dirichlet boundary conditions this leads to the same spaces $\mathcal{V}$ and $\mathcal{H}$ as in Example 2.6. Further, $a$ satisfies the Gårding inequality with $\alpha = 1$ and $\beta$ as defined above. For periodic boundary conditions one has to replace the space $\mathcal{V}$ accordingly.

In this paper, we focus on applications with photonic crystals. The dynamics of the electromagnetic fields inside such a crystal can be modelled by the Maxwell equations in the whole domain $\mathbb{R}^d$, cf. [DLP$^+$11, Ch. 1]. These equations combine the magnitudes of the time-harmonic electric and magnetic fields $E$, $H$ and the frequency $\omega$, which takes the role of an eigenvalue.

A crucial parameter within the equations is the electric permittivity of the materials inside the crystal. We assume the permittivity $\varepsilon$ to be piecewise-constant and periodic in space as well as bounded in the sense that

$$0 < \varepsilon_0 \le \varepsilon(x,\omega) \le \varepsilon_\infty < \infty$$

for all $x \in \mathbb{R}^d$ and $\omega \in \mathbb{R}^+$. The positive constant $\varepsilon_0$ equals the electric permittivity of void. In the two-dimensional case, i.e., when $\varepsilon$ is periodic within a two-dimensional plane and constant along the direction orthogonal to this plane, the Maxwell eigenvalue problem decouples into so-called *transverse magnetic* (TM) and *transverse electric* (TE) modes. Thanks to the periodicity of $\varepsilon$, which implies a discrete translational symmetry in the system, a Floquet transformation can be applied to reduce the problem posed in $\mathbb{R}^2$ to a family of problems on a bounded domain $\Omega$ called the *Wigner-Seitz cell* of the crystal lattice, see e.g. [Kuc01, DLP$^+$11].

**Example 2.8** (TM mode)**.** In the two-dimensional setting we consider the TM mode with a real-valued frequency-independent function $\varepsilon(x)$. The resulting PDE eigenvalue problem describes the third component of the electric field $E_3$, with which one can directly compute the components $H_1$ and $H_2$. Let $\mathbf{k}$ be a fixed wave vector in the so-called *irreducible Brillouin zone* $\mathcal{K} \subset \mathbb{R}^2$, cf. [DLP$^+$11, Ch. 1], and $u_\mathbf{k}$ the *Floquet transform* of $E_3(x)$ at $\mathbf{k}$. Then, $u_\mathbf{k}$ satisfies the eigenvalue problem

$$-\nabla_\mathbf{k} \cdot \nabla_\mathbf{k}\, u_\mathbf{k}(x) = \omega^2 \mu_0\, \varepsilon(x) u_\mathbf{k}(x)$$

for all $x \in \Omega$ and $\nabla_\mathbf{k} := \nabla + i\mathbf{k}$ denoting the *shifted gradient*. For the corresponding weak form we define $\lambda := \omega^2\mu_0$. Including periodic boundary conditions, we set $\mathcal{V} = H^1_{\mathrm{per}}(\Omega)$ with the standard $H^1$-norm and $\mathcal{H} = L^2(\Omega)$. Note that $\mathcal{V}$ is densely embedded in $\mathcal{H}$ and thus, Assumption 2.1 is satisfied, cf. [Bre10, Ch. 4.4]. The sesquilinear form $a$ and the (weighted) inner product in $\mathcal{H}$ then read

$$a(u,v) := \int_\Omega \nabla_\mathbf{k} u(x) \cdot \overline{\nabla_\mathbf{k} v(x)}\, \mathrm{d}x, \tag{2.2}$$

and

$$(u,v) := \int_\Omega \varepsilon(x) u(x) \overline{v(x)}\, \mathrm{d}x.$$

The following lemma shows that $a$ indeed satisfies Assumption 2.3.

**Lemma 2.9.** *For a fixed wave vector $\mathbf{k} \in \mathbb{R}^2$ the sesquilinear form $a$ defined in* (2.2) *in Example 2.8 is Hermitian, continuous, and satisfies Gårding's inequality for any $\beta > 0$.*

*Proof.* Clearly, the sesquilinear form $a$ is Hermitian. For the continuity we apply Cauchy-Schwarz and obtain for all $u, v \in \mathcal{V}$,

$$a(u,v) \leq \int_\Omega |\nabla_{\mathbf{k}} u||\nabla_{\mathbf{k}} v| \,\mathrm{d}x \leq \Big(\int_\Omega |\nabla_{\mathbf{k}} u|^2 \,\mathrm{d}x\Big)^{1/2}\Big(\int_\Omega |\nabla_{\mathbf{k}} v|^2 \,\mathrm{d}x\Big)^{1/2}.$$

Young's inequality from Lemma 2.5 with $\delta = 1$ then yields

$$\begin{aligned}\int_\Omega |\nabla_{\mathbf{k}} u|^2 \,\mathrm{d}x &= \int_\Omega |\nabla u|^2 + |\mathbf{k}|^2|u|^2 + \nabla u \cdot \overline{(i\mathbf{k}u)} + (i\mathbf{k}u)\cdot \overline{\nabla u}\,\mathrm{d}x \\ &\leq \int_\Omega |\nabla u|^2 + |\mathbf{k}|^2|u|^2 + |\nabla u|^2 + |\mathbf{k}|^2|u|^2 \leq 2\max\{1, |\mathbf{k}|^2\}\|u\|_{\mathcal{V}}^2,\end{aligned}$$

which proves the continuity of $a$. To show the Gårding inequality, we first consider the case $\mathbf{k} = 0$. Then, for any $\tilde\beta \leq 1$,

$$a(u,u) = \int_\Omega |\nabla u|^2 \,\mathrm{d}x \geq (1-\tilde\beta)\|\nabla u\|^2_{L^2(\Omega)} + \tilde\beta\,\|u\|^2_{\mathcal{V}} - \frac{\tilde\beta}{\varepsilon_0}\int_\Omega \varepsilon(x) u\overline{u}\,\mathrm{d}x \geq \tilde\beta\|u\|^2_{\mathcal{V}} - \frac{\tilde\beta}{\varepsilon_0}\|u\|^2,$$

i.e., $\alpha = \tilde\beta$ and $\beta = \tilde\beta\varepsilon_0^{-1}$. Otherwise, for $\mathbf{k} \neq 0$, we apply once more Lemma 2.5 for some parameter $\delta > 0$ and get

$$\begin{aligned}a(u,u) = \int_\Omega |\nabla_{\mathbf{k}} u|^2 \,\mathrm{d}x &\geq \int_\Omega |\nabla u|^2 + |\mathbf{k}|^2|u|^2 - \big|\nabla u \cdot \overline{(i\mathbf{k}u)} + (i\mathbf{k}u)\cdot\overline{\nabla u}\big|\,\mathrm{d}x \\ &\geq \int_\Omega |\nabla u|^2 + |\mathbf{k}|^2|u|^2 - \frac{|\nabla u|^2}{\delta} - \delta|\mathbf{k}|^2|u|^2\,\mathrm{d}x.\end{aligned}$$

Now assume $\delta > 1$ such that $\alpha := (1-\delta^{-1})\min\{1, |\mathbf{k}|^2\} > 0$. Then, $a$ satisfies a Gårding inequality with $\beta := \varepsilon_0^{-1}(\delta - \delta^{-1})\,|\mathbf{k}|^2 > 0$. Note that $\beta$ can be chosen arbitrarily small with an appropriate choice of $\delta > 1$. □

**Example 2.10** (TE mode)**.** In the eigenvalue problem corresponding to the TE modes, the permittivity $\varepsilon$ appears on the other side of the eigenvalue problem. More precisely, for a fixed wave vector $\mathbf{k}$, we search for $u_{\mathbf{k}}$ such that

$$-\nabla_{\mathbf{k}} \cdot \frac{1}{\varepsilon(x)}\nabla_{\mathbf{k}}\, u_{\mathbf{k}}(x) = \lambda\, u_{\mathbf{k}}(x) \qquad \text{in } \Omega.$$

Considering again periodic boundary conditions, we set $\mathcal{V} = H^1_{\mathrm{per}}(\Omega)$ and $\mathcal{H} = L^2(\Omega)$ with the standard inner products. In this case, the sesquilinear form $a$ has the form

$$a(u,v) := \int_\Omega \frac{1}{\varepsilon(x)}\nabla_{\mathbf{k}} u \cdot \overline{\nabla_{\mathbf{k}} v}\,\mathrm{d}x.$$

The proof of the Gårding inequality follows similarly as in Lemma 2.9.

More general eigenvalue problems are discussed in Sections 4 and 5. There we consider a TM mode with an electric permittivity, which depends on the frequency $\omega$. This then leads to a nonlinear eigenvalue problem.

2.3. **Operator formulation.** The weak formulation of the eigenvalue problem (2.1) can be equivalently written as an operator equation in the dual space of $\mathcal{V}$. This also yields a convenient formulation for the introduction of iterative schemes. We introduce the operator $\mathcal{A}\colon \mathcal{V} \to \mathcal{V}^*$ by

$$\langle \mathcal{A}u, v\rangle := a(u,v).$$

Further, we define $\mathcal{I}\colon \mathcal{V} \to \mathcal{V}^*$ as the embedding of $\mathcal{V}$ in $\mathcal{V}^*$ induced by the Gelfand triple $\mathcal{V}, \mathcal{H}, \mathcal{V}^*$ from Assumption 2.1 with respect to the inner product in $\mathcal{H}$, cf. [Zei90, Ch. 23.4].

To be precise, this means that $\langle \mathcal{I}u, v\rangle := (u, v)$ for all $u, v \in \mathcal{V}$. The operator equation corresponding to (2.1) then reads

$$\mathcal{A}u = \lambda\, \mathcal{I}u \qquad \text{in } \mathcal{V}^*. \tag{2.3}$$

Note that this equation is stated in the dual space of $\mathcal{V}$, which means that we consider test functions in $\mathcal{V}$ as in (2.1). Hence, the two formulations (2.1) and (2.3) are equivalent.

Recall the definition of the shifted sesquilinear form $a_\beta$ from Remark 2.4. With this, we define the corresponding operator $\mathcal{A}_\beta\colon \mathcal{V} \to \mathcal{V}^*$, which is then positive and thus, invertible.

## 3. Iterative Methods on Operator Level

In this section, we analyze iterative methods to find the smallest eigenpair to the operator eigenvalue problem (2.3). We emphasize that we do not apply any spacial discretization but perform the eigenvalue iteration directly to the operator equation.

We first consider the inverse power method for which we prove the convergence in $\mathcal{V}$. Second, we discuss Arnoldi's method for the operator case, based on Krylov subspaces as in the matrix case. Finally, we consider a Newton iteration and its connection to the inverse power method.

3.1. **Inverse power method.** Power and inverse power methods come in various variants with different kinds of scaling, see e.g. [AK08, Ch. 10.3] or [Saa11, Ch. 4] for the matrix case. One may even consider the scaling with the exact eigenvalue $\lambda$ as done, e.g., in [EE07, AHP18]. Clearly, the latter is only of interest for theoretical observations rather than actual computations.

As every iteration scheme we need a starting function $u^0 \in \mathcal{V}$. In order to permit the iterates to converge to the wanted eigenfunction, one needs an additional assumption on $u^0$, e.g., having a non-vanishing component in the direction of this eigenfunction.

3.1.1. *Rayleigh quotient iteration.* A direct implementation of the inverse power method for the operator case would apply the operator $\mathcal{A}^{-1}\mathcal{I}$ over and over again with an appropriate normalization. We emphasize that $\mathcal{A}$ is invertible, since the corresponding sesquilinear form $a$ satisfies a Gårding inequality if Assumption 2.3 is satisfied. However, the *Rayleigh quotient* is not guaranteed to remain positive. Thus, we consider the shifted eigenvalue problem

$$\mathcal{A}_\beta u := (\mathcal{A} + \beta\mathcal{I})\, u = (\lambda + \beta)\, \mathcal{I}u =: \mu\, \mathcal{I}u \qquad \text{in } \mathcal{V}^*. \tag{3.1}$$

This then leads to the following algorithm: Given an initial function $u^0 \in \mathcal{V}$, which we assume not to be orthogonal to the first eigenfunction, with normalization $\|u^0\| = 1$ we solve for $j = 1, 2, \dots$ the variational problem

$$\mathcal{A}_\beta u^j = \mu^{j-1}\, \mathcal{I}\tilde{u}^{j-1} \qquad \text{in } \mathcal{V}^*. \tag{3.2}$$

Therein, $\tilde{u}^j := u^j/\|u^j\|$ includes the normalization and $\mu^j$ the Rayleigh quotient, i.e.,

$$\mu^j := \frac{\langle \mathcal{A}_\beta u^j, u^j\rangle}{\langle \mathcal{I}u^j, u^j\rangle} = \frac{a_\beta(u^j, u^j)}{(u^j, u^j)} = \frac{\|u^j\|_\beta^2}{\|u^j\|^2}.$$

Note that the power iteration (3.2) includes a normalization although the iterates $u^j$ themselves are not normalized. The approximation of the smallest eigenvalue $\lambda$ is then given by $\lambda^j := \mu^j - \beta$. It remains to discuss the convergence of the suggested iteration.

**Theorem 3.1.** *Given Assumptions 2.1-2.3, the power iteration* (3.2) *converges to an eigenpair* $(u^*, \lambda^*)$ *of* (2.3) *in the sense that the sequences* $u^j$ *and* $\lambda^j := \mu^j - \beta$ *satisfy* $u^j \to u^*$ *in* $\mathcal{V}$ *and* $\lambda^j \to \lambda^*$ *with* $\mathcal{A}u^* = \lambda^*\mathcal{I}u^*$ *in* $\mathcal{V}^*$.

*Proof.* We follow the proof in [Boz16] showing the convergence of the inverse power method for the $p$-Laplacian. The first step is to show the monotonic decrease of the sequence $\mu^j$. For this, we consider (3.2) with test functions $u^j$ and $\tilde{u}^{j-1}$ leading to

$$\|u^j\|_\beta^2 \le \mu^{j-1}\|u^j\|, \qquad \mu^{j-1} = \mu^{j-1}\|\tilde{u}^{j-1}\|^2 \le \sqrt{\mu^{j-1}}\|u^j\|_\beta.$$

A combination of these two estimates yields $\|u^j\|_\beta \le \sqrt{\mu^{j-1}}\|u^j\|$ and thus,

$$\sqrt{\mu^j} = \frac{\|u^j\|_\beta}{\|u^j\|} \le \sqrt{\mu^{k-1}}. \tag{3.3}$$

The monotonicity and $\mu^j \ge 0$, which follows from the positivity of $\mathcal{A}_\beta$, imply that there exists the limit $\mu^* := \lim_{j\to\infty} \mu^j \ge 0$.

As a second step, we conclude from estimate (3.3) that $\|\tilde{u}^j\|_\beta = \sqrt{\mu^j} \le \sqrt{\mu^0}$. Since the norms $\|\cdot\|_\beta$ and $\|\cdot\|_\mathcal{V}$ are equivalent, we obtain that $\tilde{u}^j$ is uniformly bounded in $\mathcal{V}$. Thus, there exists a convergent subsequence and an element $\tilde{u}^* \in \mathcal{V}$, which satisfy (without relabeling)

$$\tilde{u}^j \rightharpoonup \tilde{u}^* \quad \text{in } \mathcal{V}, \qquad \tilde{u}^j \to \tilde{u}^* \quad \text{in } \mathcal{H}.$$

Note that we have used here the compact embedding $\mathcal{V} \hookrightarrow \mathcal{H}$ from Assumption 2.2. Obviously, we have $\|\tilde{u}^*\| = \lim_{j\to\infty} \|\tilde{u}^j\| = 1$. Further, we know from previous calculations that

$$\|u^j\|_\beta^2 \le \mu^{j-1}\|u^j\| \le \mu^0\|u^j\| \le C_{\mathcal{V}\hookrightarrow\mathcal{H}}\mu^0\|u^j\|_\mathcal{V} \lesssim \|u^j\|_\beta.$$

This means that also the sequence $u^j$ is uniformly bounded in $\mathcal{V}$. Thus, there exists a limit $u^* \in \mathcal{V}$ such that (again without relabeling)

$$u^j \rightharpoonup u^* \quad \text{in } \mathcal{V}, \qquad u^j \to u^* \quad \text{in } \mathcal{H}.$$

In the following we compare the two limits $u^*$ and $\tilde{u}^*$. For this, we consider

$$\mu^j = \frac{a_\beta(u^j, u^j)}{\|u^j\|^2} = \mu^{j-1}\frac{(\tilde{u}^{j-1}, u^j)}{\|u^j\|^2} = \frac{\mu^{j-1}}{\|u^j\|}(\tilde{u}^{j-1}, \tilde{u}^j)$$

Taking the limit $j \to \infty$ on both sides, we conclude that

$$\mu^* = \frac{\mu^*}{\|u^*\|}\|\tilde{u}^*\|^2 = \frac{\mu^*}{\|u^*\|},$$

i.e., $\|u^*\| = 1$. As a result, the sequence $(\tilde{u}^j)$ converges to $u^*/\|u^*\| = u^*$. The uniqueness of the limit then yields $u^* = \tilde{u}^*$.

To show that the pair $(u^*, \lambda^*)$ with $\lambda^* := \mu^* - \beta$ is indeed an eigenpair of (2.3), we apply the limit to equation (3.2) and seek

$$a_\beta(u^*, v) = \mu^*(u^*, v) \qquad \text{for all } v \in \mathcal{V}.$$

Thus, we have $a(u^*, v) = \lambda^*(u^*, v)$ for all $v \in \mathcal{V}$ or, in operator form, $\mathcal{A}u^* = \lambda^*\mathcal{I}u^*$. The weak convergence $\tilde{u}^j \rightharpoonup \tilde{u}^* = u^*$ in $\mathcal{V}$ additionally implies

$$\sqrt{\mu^*} = \|u^*\|_\beta \le \liminf_{j\to\infty} \|\tilde{u}^j\|_\beta = \liminf_{j\to\infty} \sqrt{\mu^j} = \sqrt{\mu^*}.$$

Note that the inequality is strict, if and only if the convergence is not strong. This implies $\tilde{u}^j, u^j \to u^*$ in $\mathcal{V}$. The unique solvability (up to scaling) then implies that every convergent subsequence has the same limit. □

*Remark* 3.2. In order to show that $(u^*, \lambda^*)$ is the smallest eigenpair, one needs an additional assumption on $u^0$, see e.g. [Boz16] using the maximum principle and $u^0 \ge 0$.

*Remark* 3.3. A second strategy to prove Theorem 3.1 is to reformulate the eigenvalue problem in terms of the resolvent. Assumption 2.2 shows that the resolvent is a compact operator such that the results in [ESL95] can be applied.

3.1.2. *An alternative power method.* In Theorem 3.1 we have shown that the inverse power method (3.2) provides in the limit an eigenvalue (the limit of the Rayleigh quotient) and an eigenfunction. However, one may also omit the Rayleigh quotient, which leads to the iteration

$$\mathcal{A}_\beta v^j = \mathcal{I}\tilde{v}^{j-1} \qquad \text{in } \mathcal{V}^* \tag{3.4}$$

and the following convergence result.

**Lemma 3.4.** *Assume* $u^0 = v^0 \in \mathcal{V}$ *with* $\|u^0\| = 1$. *Let* $u^j$ *and* $v^j$ *be the sequences obtained from the iteration procedures* (3.2) *and* (3.4), *respectively. Then, we have the relation* $u^j = \mu^{j-1} v^j$ *for all* $j \geq 1$ *with the Rayleigh quotient* $\mu^j = \|u^j\|_\beta^2 / \|u^j\|^2$.

*Proof.* We prove this result by mathematical induction and observe first that

$$u^1 = \mu^0 \mathcal{A}_\beta^{-1}\mathcal{I}u^0 = \mu^0 \mathcal{A}_\beta^{-1}\mathcal{I}v^0 = \mu^0 v^1.$$

Now, assuming $u^j = \mu^{j-1}v^j$ is true for a fixed but arbitrary index $j$, we obtain

$$u^{j+1} = \mu^j \mathcal{A}_\beta^{-1}\mathcal{I}\frac{u^j}{\|u^j\|} = \mu^j \mathcal{A}_\beta^{-1}\mathcal{I}\frac{\mu^{j-1}v^j}{\mu^{j-1}\|v^j\|} = \mu^j \mathcal{A}_\beta^{-1}\mathcal{I}\frac{v^j}{\|v^j\|} = \mu^j v^{j+1}.$$

Note that we have used the fact that $\mu^j > 0$ and thus $|\mu^j| = \mu^j$. □

Lemma 3.4 directly implies the convergence of the iteration (3.4). In particular, we have $v^j = u^j/\mu^{j-1} \to u^*/\mu^* =: v^*$ in $\mathcal{V}$. Thus, the limit is not normalized but rather satisfies

$$\|v^*\| = \frac{\|u^*\|}{|\mu^*|} = \frac{1}{\mu^*}.$$

3.1.3. *Commutativity.* The convergence of the power method in the operator case directly leads to the question whether the application of the power method and the spatial discretization commute. If we discretize the shifted eigenvalue problem (3.1) by finite elements, then we obtain a system of the form

$$Kq = \mu\, Mq.$$

Therein, $q \in \mathbb{C}^n$ encodes a finite-dimensional approximation of the eigenfunction $u \in \mathcal{V}$, e.g., the coefficients w.r.t. a finite element basis. Since we have included the boundary conditions in the space $\mathcal{V}$, we assume that the mass matrix $M \in \mathbb{C}^{n,n}$ and the stiffness matrix $K \in \mathbb{C}^{n,n}$ are Hermitian and positive definite. With $A := M^{-1}K$ the discrete system is equivalent to the eigenvalue problem $Aq = \mu q$. Seeking for the smallest eigenvalue, we apply the *inverse power method* with normalization, i.e.,

$$q^j = A^{-1}\tilde{q}^{j-1} = A^{-1}\frac{q^{j-1}}{\|q^{j-1}\|_Z} = K^{-1}M\frac{q^{j-1}}{\|q^{j-1}\|_Z}. \tag{3.5}$$

As approximation for the eigenvalue we consider $\mu^j := 1/\|q^j\|_Z$ with $\|\cdot\|_Z$ being any norm in $\mathbb{C}^n$. The starting vector, which may be a given approximation of $u^0$, is denoted by $q^0$. We emphasize that the iteration converges despite of the choice of the norm as long as $q^0$ contains a non-zero component in direction of the first eigenvector.

We now consider the spatial discretization of (3.4), i.e., we first apply the inverse power method to the PDE eigenvalue problem (3.1) and then discretize. We emphasize that this allows a different discretization scheme in each iteration step and thus, adaptivity.

However, we assume here an invariant mesh used for the spatial discretization and thus, the same matrices $M$ and $K$ appear as before.

$$Kq^j = M\tilde{q}^{j-1} = M\frac{q^{j-1}}{\|q^{j-1}\|_M}.$$

Note that the applied normalization is here w.r.t the $M$-norm, since this corresponds to the $L^2$-inner product in the infinite-dimensional case. Thus, the iteration equals (3.5) if we choose the normalization matrix

*Remark* 3.5. If we discretize the iteration scheme introduced in (3.2), then also this is equivalent to the inverse power iteration (3.5). To see this, the normalization matrix $Z$ has to be chosen accordingly.

3.2. **A Krylov subspace method.** The natural extension of the inverse power method in order to approximate several eigenvalues is a subspace iteration, cf. [Saa11, Ch. 5]. This includes several starting functions, for which a power iteration is applied, and an additional orthogonalization step. The computation of several eigenvalues is also of interest in the calculation of band-gaps of a photonic crystal. Here, we consider the Arnoldi method in the operator setting. For this, we need an extension of the Krylov subspaces used in numerical linear algebra.

3.2.1. *Krylov spaces.* Krylov subspaces play in crucial role for iterative eigenvalue computations, see, e.g., [Saa11, Ch. 6.1]. In order to generalize these methods to the PDE setting, we need Krylov subspaces for general Hilbert spaces [GHS14].

Let $u^0$ be a function in $\mathcal{V}$, e.g., an initial guess for the power method in Section 3.1, and $\mu^0 := \|u^0\|_\beta^2$. With this, we define the *Krylov subspace*

$$\mathfrak{K}_\beta^m(u^0) := \operatorname{span}\big\{u^0,\ \mathcal{A}_\beta^{-1}\mathcal{I}u^0,\ \dots,\ (\mathcal{A}_\beta^{-1}\mathcal{I})^{m-1}u^0\big\} \subseteq \mathcal{V}. \tag{3.6}$$

Obviously, this defines a closed subspace of $\mathcal{V}$. We emphasize that $\mathfrak{K}_\beta^m(u^0)$ is spanned - as in the finite-dimensional case - by the iterates of the power method. To see this note that $(\mathcal{A}_\beta^{-1}\mathcal{I})^j u^0$ equals the corresponding iterate of the power method up to a constant. Thus, if we denote the sequence resulting from the modified inverse power method (3.4) by $u^j_{\text{pow}}$, then we have

$$\mathfrak{K}_\beta^m(u^0) = \operatorname{span}\big\{u^0,\ u^1_{\text{pow}},\ \dots,\ u^{m-1}_{\text{pow}}\big\}.$$

3.2.2. *Arnoldi's method.* We translate the Arnoldi algorithm from the matrix setting [Saa11, Ch. 6.2] to the present operator case. Let $\{v_1, \dots, v_m\}$ denote a basis of $\mathfrak{K}_\beta^m(u^0)$, e.g., obtained by a Gram-Schmidt orthogonalization process. Then, the new iterate of the Arnoldi method is then given by $u^m := \sum_{i=1}^m \alpha_i v_i \in \mathfrak{K}_\beta^m(u^0)$, whose coefficients $\alpha := [\alpha_1, \dots, \alpha_m]^T$ and corresponding $\mu^m \in \mathbb{R}$ are derived by the Galerkin projection

$$\sum_{i=1}^m \alpha_i\, a_\beta(v_i, v_j) = \mu^m \sum_{i=1}^m \alpha_i\, (v_i, v_j) \qquad \text{for } j = 1, \dots, m.$$

This is equivalent to the $m$-dimensional eigenvalue problem $\tilde{K}\alpha = \mu^m \tilde{M}\alpha$, for which we search for the smallest eigenpair. Here, $\tilde{K}$ and $\tilde{M}$ are stiffness and mass matrices restricted to the Krylov basis, i.e.,

$$\tilde{K}_{ij} := a_\beta(v_i, v_j), \qquad \tilde{M}_{ij} := (v_i, v_j).$$

Thus, the extra costs going form the power method to the Arnoldi method are identical as in the finite-dimensional setting, namely the solution of a small (but dense) eigenvalue problem. Note that the resulting approximation of the eigenvalue, namely $\mu^m$, is again the Rayleigh quotient of the iterate $u^m$. The obtained pair of the Arnoldi method provides the best-approximation within the Krylov subspace $\mathfrak{K}_\beta^m(u^0)$ in the sense that

$$\langle \operatorname{Res}(u^m, \mu^m), v\rangle = 0$$

for all $v \in \mathfrak{K}_\beta^m(u^0)$ and with the residual defined by $\operatorname{Res}(u, \mu) := \mathcal{A}_\beta u - \mu \mathcal{I} u \in \mathcal{V}^*$ for any pair $(u, \mu) \in \mathcal{V} \times \mathbb{C}$. Obviously, this implies that the Arnoldi method is superior to the inverse power method. The norm of the residual may also be used as a error estimator as it equals the backward error.

The gain of the Arnoldi method can also be characterized in terms of the Courant *min-max principle* in Hilbert spaces, cf. [Cou20] or [WS72, Ch. 1]. This means that the $j$-th eigenvalue is defined by minimizing over all $j$-dimensional subspaces of $\mathcal{V}$, i.e.,

$$\lambda_j + \beta = \mu_j = \min_{\substack{\mathcal{V}^{(j)} \subset \mathcal{V},\\ \dim \mathcal{V}^{(j)} = j}} \ \max_{v \in \mathcal{V}^{(j)}} \frac{a_\beta(v, v)}{(v, v)}.$$

With this, one shows that computed approximations of the eigenvalues are larger than the exact ones. With the same arguments one can show that the Arnoldi iteration provides better approximations than the inverse power method and thus, converges as well. Recall that the Arnoldi method computes $\mu^m_{\mathrm{Arnoldi}}$ satisfying

$$\mu_1 \le \mu^m_{\mathrm{Arnoldi}} = \min_{\substack{\mathcal{V}^{(1)} \subset \mathfrak{K}_\beta^m(u^0),\\ \dim \mathcal{V}^{(1)} = 1}} \ \max_{v \in \mathcal{V}^{(1)}} \frac{a_\beta(v, v)}{(v, v)} \le \max_{v \in \operatorname{span}\{u^{m-1}_{\mathrm{pow}}\}} \frac{a_\beta(v, v)}{(v, v)} = \mu^{m-1}_{\mathrm{pow}}.$$

Note that the inequality holds, since $u^{m-1}_{\mathrm{pow}}$ is an element of the Krylov subspace $\mathfrak{K}_\beta^m(u^0)$ and thus, $\operatorname{span}\{u^{m-1}_{\mathrm{pow}}\}$ is one particular one-dimensional subspace.

3.3. **Newton iteration.** Yet another approach to solve the eigenvalue problem (2.3) is to apply Newton's method [MV04, Sch08]. For this, we rewrite the problem as

$$\mathcal{F}(\lambda) := \begin{bmatrix} (\mathcal{A} - \lambda \mathcal{I})u \\ (y, u) - 1 \end{bmatrix} = 0$$

with a fixed function $y \in \mathcal{V}$ serving as normalization. Further, the second equation balances the number of equations and variables. The resulting iteration reads

$$\begin{bmatrix} \mathcal{A} - \lambda^{j-1}\mathcal{I} & -\mathcal{I}u^{j-1} \\ (y, \cdot) & 0 \end{bmatrix} \begin{bmatrix} u^j - u^{j-1} \\ \lambda^j - \lambda^{j-1} \end{bmatrix} = - \begin{bmatrix} \mathcal{A}u^{j-1} - \lambda^j \mathcal{I} u^{j-1} \\ (y, u^{j-1}) - 1 \end{bmatrix}. \tag{3.7}$$

This means that all iterates are normalized to $(y, u^j) = 1$ and $u^j$ satisfies

$$(\mathcal{A} - \lambda^{j-1}\mathcal{I})u^j = (\lambda^j - \lambda^{j-1})\,\mathcal{I}u^{j-1}.$$

The similarities to the power method are obvious. More precisely, Newton's method leads to a *shifted inverse iteration* with the shift given by the previous eigenvalue approximation. The precise algorithm is given in [MV04, Alg. I]. This then leads to a third-order convergence of the eigenvalue in the matrix case, which was proven in [Osb64].

A simplified Newton algorithm would not update the shift in every step. If we even consider a constant shift and set this to zero, then – up to scaling – we end up with the power iteration given in (3.2). We will apply Newton's method in Section 5 for a nonlinear eigenvalue problem arising from two-dimensional photonic crystals.

# 4. A Nonlinear Model Problem for Photonic Crystals

In this section, we consider an extension of the TM mode from Example 2.8, in which the electric permittivity $\varepsilon$ depends on the frequency and thus, the eigenvalue. This then leads to a nonlinear eigenvalue problem. Assuming that $\varepsilon$ is a rational function in the frequency, we are able to reformulate the eigenvalue problem to a linear one satisfying Assumptions 2.1 and 2.3. The lack of compactness and convergence properties of the inverse power method are discussed.

4.1. **A simplified Drude-Lorentz model.** We consider a photonic crystal made up of two different materials. For this, we decompose the computational domain $\Omega$ into two subdomains $\Omega = \Omega_1 \cup \Omega_2$, each representing one material. We define the corresponding indicator functions on $\Omega_j$ by $\chi_j\colon \Omega \to \{1, 0\}$, $j = 1, 2$. On both subdomains we assume the electric permittivity to be constant in space and thus,

$$\varepsilon(x,\omega) = \varepsilon_1(\omega)\chi_1(x) + \varepsilon_2(\omega)\chi_2(x). \tag{4.1}$$

To skimp the length of this section, the material contained in $\Omega_1$ is assumed to be linear, i.e., we set the electric permittivity in this subdomain to a constant $\varepsilon_1(\omega) \equiv \alpha_1 > 0$. For the frequency dependence in the second material we consider a simplified version of the Drude-Lorentz model, see e.g. [LL10] or [Jac99, Ch. 7.5]. More precisely, we assume the electric permittivity to be of the form

$$\varepsilon_2(\omega) = \alpha_2 + \sum_{\ell=1}^{L} \frac{\xi_\ell^2}{\eta_\ell^2 - \omega^2} \tag{4.2}$$

with a positive constant $\alpha_2 > 0$ and real parameters $\eta_\ell, \xi_\ell$ such that $\eta_\ell^2, \xi_\ell^2 \geq 0$. Since $\omega$ only appears squared, we introduce $\lambda := \omega^2$ and obtain

$$\lambda\, \varepsilon_2(\lambda) = \lambda\, \alpha_2 + \sum_{\ell=1}^{L} \frac{\lambda\, \xi_\ell^2}{\eta_\ell^2 - \omega^2} = \lambda\, \alpha_2 - \Xi + \sum_{\ell=1}^{L} \frac{\xi_\ell^2 \eta_\ell^2}{\eta_\ell^2 - \lambda}$$

with

$$\Xi := \sum_{\ell=1}^{L} \xi_\ell^2 > 0.$$

Due to the inclusion of $\Xi$, the fractional terms are in a strictly proper form, i.e., the degree of the polynomial in terms of $\lambda$ in the numerator is strictly smaller than the degree of the polynomial in the denominator. All in all, this leads to the nonlinear eigenvalue problem

$$\begin{aligned} -\frac{1}{\mu_0} \nabla_{\mathbf{k}} \cdot \nabla_{\mathbf{k}} u_{\mathbf{k}}(x) &+ \Xi\, \chi_2(x) u_{\mathbf{k}}(x) \\ &= \lambda \big(\alpha_1 \chi_1(x) + \alpha_2 \chi_2(x)\big) u_{\mathbf{k}}(x) + \sum_{\ell=1}^{L} \frac{\xi_\ell^2 \eta_\ell^2}{\eta_\ell^2 - \lambda} \chi_2(x) u_{\mathbf{k}}(x) \end{aligned} \tag{4.3}$$

with $\nabla_{\mathbf{k}}$ denoting again the shifted gradient introduced in Example 2.8. Our aim is to turn this into a linear eigenvalue problem in order to apply the iterative methods from the previous sections. For this, we follow the ideas presented in [SB11, EKE12, Eff13], which consider the corresponding finite-dimensional case. The main clue is to rewrite the sum, which may be regarded as a transfer function, by means of a realization, i.e.,

$$\sum_{\ell=1}^{L} \frac{\xi_\ell^2 \eta_\ell^2}{\eta_\ell^2 - \lambda} = \mathbf{b}^* \big(\mathbf{A} - \lambda \mathbf{I}\big)^{-1} \mathbf{b}. \tag{4.4}$$

Due to the simple structure of the permittivity, we can directly read of the vector $\mathbf{b} = [\xi_1\eta_1, \dots, \xi_L\eta_L]^T \in \mathbb{R}^L$ and $\mathbf{A} \in \mathbb{R}^{L\times L}$ as the diagonal (and thus Hermitian) matrix with $\mathbf{A}_{j,j} = \eta_j^2$ for $j = 1, \dots, L$. By $\mathbf{I} \in \mathbb{R}^{L\times L}$ we denote the identity matrix.

*Remark* 4.1. For other models of the permittivity, the choice (and even the dimension) of $\mathbf{A}$ and $\mathbf{b}$ may not be as straightforward. Further, the identity matrix $\mathbf{I}$ may be replaced by another positive Hermitian matrix. Proper realizations for such cases may be found using the techniques in [SUBG18].

4.2. **Spaces and embeddings.** For the weak formulation and linearization of the eigenvalue problem we need to introduce several function spaces. First, we introduce

$$H := L^2(\Omega), \qquad V := H^1_{\mathrm{per}}(\Omega), \qquad X := \{v \in H \mid v \text{ vanishes on } \Omega_1\}.$$

These spaces form Hilbert spaces with the standard inner products

$$(u, v) := (u, v)_H := \int_\Omega u\overline{v}\,\mathrm{d}x, \quad (u, v)_V := (u, v) + (\nabla u, \nabla v), \quad (u, v)_X := \int_{\Omega_2} u\overline{v}\,\mathrm{d}x$$

for $u$ and $v$ in the respective spaces $H$, $V$, or $X$. Second, we define the product spaces

$$\mathcal{V} := V \otimes X^L, \qquad \mathcal{H} := H \otimes X^L.$$

Also these product spaces are Hilbert spaces. In $\mathcal{H}$ we consider the inner product

$$(\boldsymbol{z}_1, \boldsymbol{z}_2)_{\mathcal{H}} := (u, v)_H + \sum_{\ell=1}^{L} (x_\ell, y_\ell)_X$$

for $\boldsymbol{z}_1 = [u; \boldsymbol{x}]$, $\boldsymbol{z}_2 = [v; \boldsymbol{y}] \in \mathcal{H}$ consisting of $u, v \in H$ and $\boldsymbol{x}, \boldsymbol{y} \in X^L$. Note that we use here the notation $[u; \boldsymbol{x}] := [u, \boldsymbol{x}^T]^T$. Analogously, we define an inner product in $\mathcal{V}$ by replacing $(u, v)_H$ by $(u, v)_V$. This also defines the norms $\|\boldsymbol{z}\|^2_{\mathcal{H}} := (\boldsymbol{z}, \boldsymbol{z})_{\mathcal{H}}$ and $\|\boldsymbol{z}\|^2_{\mathcal{V}} := (\boldsymbol{z}, \boldsymbol{z})_{\mathcal{V}}$.

*Remark* 4.2. Although the embedding $V \hookrightarrow H$ is compact, the embedding $\mathcal{V} \hookrightarrow \mathcal{H}$ is not. This is due to the fact that the identity operator is not compact in infinite dimensions.

For the weak formulation of the nonlinear eigenvalue problem (4.3) we need several embeddings. First, $\mathcal{I}\colon V \to V^*$ denotes the continuous inclusion map defined by the Gelfand triple $V$, $H$, $V^*$, cf. Section 2.3. Second, we define the extension of the mapping $u \mapsto (u, \cdot\,)_X$ as $\mathcal{I}_2\colon V \to V^*$, i.e.,

$$u \mapsto \langle \mathcal{I}_2 u, \cdot\,\rangle_{V^*,V} := (\chi_2 u,\, \chi_2\,\cdot\,)_X = \int_{\Omega_2} u\,\overline{\cdot}\,\mathrm{d}x.$$

In the same manner, based on the indicator function $\chi_1$, we define $\mathcal{I}_1\colon V \to V^*$. The weighted combination of these two embeddings yields $\mathcal{I}_\alpha\colon V \to V^*$, given by

$$\mathcal{I}_\alpha := \alpha_1\mathcal{I}_1 + \alpha_2\mathcal{I}_2.$$

Finally, we introduce the embedding $\overline{\mathcal{I}}_2\colon X \to V^*$. For $u \in X$ this is defined by

$$u \mapsto \langle \overline{\mathcal{I}}_2 u, \cdot\,\rangle_{V^*,V} := (u,\, \chi_2\,\cdot\,)_X = \int_{\Omega_2} u\,\overline{\cdot}\,\mathrm{d}x.$$

The corresponding dual operator $\overline{\mathcal{I}}_2^*\colon V \to X^*$ satisfies for $v \in V$ and $u \in X$ that

$$\langle \overline{\mathcal{I}}_2^* v, u\rangle_{X^*,X} = \langle v, \overline{\mathcal{I}}_2 u\rangle_{V,V^*} = (\chi_2 v, u)_X.$$

**Lemma 4.3.** *With the Riesz isomorphism $j_X\colon X \to X^*$, the introduced embeddings satisfy that $\overline{\mathcal{I}}_2\, j_X^{-1}\, \overline{\mathcal{I}}_2^* = \mathcal{I}_2\colon V \to V^*$.*

*Proof.* Consider $u, v \in V$. Then, the claimed identity can be seen by

$$\langle \overline{\mathcal{I}}_2\, j_X^{-1}\, \overline{\mathcal{I}}_2^* u, v\rangle_{V^*,V} = \langle \overline{\mathcal{I}}_2^* u, \chi_2 v\rangle_{X^*,X} = (\chi_2 u, \chi_2 v)_X = \langle \mathcal{I}_2 u, v\rangle_{V^*,V}. \qquad \square$$

*Remark* 4.4. In the remainder of this paper, we often omit to write the Riesz isomorphisms $j_H\colon H \to H^*$ or $j_X\colon X \to X^*$ if their presence is clear from the context. Thus, we may write $\overline{\mathcal{I}}_2 \overline{\mathcal{I}}_2^* = \mathcal{I}_2$.

4.3. **Weak formulation and linearization.** The goal of this subsection is to transform the nonlinear eigenvalue problem into a linear one by introducing new variables. Thus, we aim to write (4.3) into

$$\mathbb{A}\boldsymbol{z} = \lambda\, \mathbb{I}\boldsymbol{z}.$$

Based on the proper form of the permittivity given in (4.4), we obtain the following weak form of the eigenvalue problem. For a given (and fixed) wave vector $\mathbf{k} \in \mathcal{K}$, find a pair $(u_{\mathbf{k}}, \lambda) \in V \times \mathbb{R}$ such that

$$\tfrac{1}{\mu_0}\mathcal{A}_{\mathbf{k}} u_{\mathbf{k}} + \Xi\, \mathcal{I}_2 u_{\mathbf{k}} = \lambda\, \mathcal{I}_\alpha u_{\mathbf{k}} + \mathbf{b}^*\big(\mathbf{A} - \lambda \mathbf{I}\big)^{-1} \mathbf{b}\, \mathcal{I}_2 u_{\mathbf{k}}. \tag{4.5}$$

We emphasize that this equation is stated in $V^*$. The operator $\mathcal{A}_{\mathbf{k}}$ denotes the weak form of the shifted Laplacian, cf. Example 2.8. For the linearization of (4.5) we introduce a new variable

$$\boldsymbol{x} := (\mathbf{A} - \lambda\mathbf{I})^{-1}\mathbf{b}\, \overline{\mathcal{I}}_2^* u_{\mathbf{k}} \in X^L. \tag{4.6}$$

Note that this includes a hidden application of $j_X$. With Lemma 4.3 this leads to a linear eigenvalue problem where we search for a pair $(\boldsymbol{z}, \lambda)$ with $\boldsymbol{z} := [u_{\mathbf{k}}; \boldsymbol{x}] \in \mathcal{V}$ such that

$$\begin{bmatrix} \frac{1}{\mu_0}\mathcal{A}_{\mathbf{k}} + \Xi\, \mathcal{I}_2 & -\overline{\mathcal{I}}_2 \mathbf{b}^* \\ -\mathbf{b}\, \overline{\mathcal{I}}_2^* & \mathbf{A}\, j_X \end{bmatrix} \boldsymbol{z} = \lambda \begin{bmatrix} \mathcal{I}_\alpha & \\ & \mathbf{I}\, j_X \end{bmatrix} \boldsymbol{z}. \tag{4.7}$$

This formulation consists of two equations stated in the dual spaces of $V$ and $X^L$, respectively. Note that $j_X$ should be understood here as the componentwise application of the Riesz isomorphism.

*Remark* 4.5. The linearized eigenvalue problem (4.7) contains an operator on the left-hand side with a generalized saddle point structure.

**Lemma 4.6.** *The eigenvalue problems* (4.5) *and* (4.7) *are equivalent. This means that an eigenpair* $(u_{\mathbf{k}}, \lambda)$ *of* (4.5) *defines a solution of* (4.7) *by* $([u_{\mathbf{k}}; \boldsymbol{x}], \lambda)$ *with* $\boldsymbol{x}$ *as defined in* (4.6) *and vice versa.*

*Proof.* The second block row of (4.7) is given by $(\mathbf{A} - \lambda\mathbf{I}) j_X\, \boldsymbol{x} = \mathbf{b}\, \overline{\mathcal{I}}_2^* u_{\mathbf{k}}$, which implies (4.6). Substituting this formula for $\boldsymbol{x}$ into the first block row yields together with $\overline{\mathcal{I}}_2 \overline{\mathcal{I}}_2^* = \mathcal{I}_2$ from Lemma 4.3 that (4.7) is indeed equivalent to the nonlinear eigenvalue problem (4.5). $\square$

Defining $\mathbb{A}, \mathbb{I}\colon \mathcal{V} \to \mathcal{V}^*$ in an obvious manner, we can write (4.7) in the form $\mathbb{A}\boldsymbol{z} = \lambda\, \mathbb{I}\boldsymbol{z}$. Although the to $\mathbb{I}$ corresponding sesquilinear form reads $\mathfrak{i}\colon \mathcal{V} \times \mathcal{V} \to \mathbb{C}$,

$$\mathfrak{i}(\boldsymbol{z}_1, \boldsymbol{z}_2) := \big\langle \mathcal{I}_\alpha u, v\big\rangle_{V^*,V} + \big(\boldsymbol{x}_1, \boldsymbol{x}_2\big)_{X^L}$$

for $\boldsymbol{z}_1 = [u; \boldsymbol{x}_1]$, $\boldsymbol{z}_2 = [v; \boldsymbol{x}_2] \in \mathcal{V}$, we may also consider $\mathfrak{i}$ as a sesquilinear form mapping from $\mathcal{H} \times \mathcal{H}$ to $\mathbb{C}$. We now show that this defines an inner product in $\mathcal{H}$.

**Lemma 4.7.** *The sesquilinear form* $\mathfrak{i}$ *considered as mapping* $\mathcal{H} \times \mathcal{H} \to \mathbb{C}$*, defines an inner product in* $\mathcal{H}$*.*

*Proof.* Obviously, $\mathfrak{i}$ is Hermitian and sesquilinear. Further, for any $\boldsymbol{z} = [u; \boldsymbol{x}] \in \mathcal{H}$ and $\underline{\alpha} := \min\{\alpha_1, \alpha_2\} > 0$, it holds that

$$\mathfrak{i}(\boldsymbol{z}, \boldsymbol{z}) \geq \underline{\alpha}\, \|u\|^2 + \big(\boldsymbol{x}, \boldsymbol{x}\big)_{X^L} \geq \min(\underline{\alpha}, 1)\, \|\boldsymbol{z}\|^2_{\mathcal{H}},$$

which proves the positivity. □

4.4. **Shifted eigenvalue problem.** In the previous subsection, the nonlinear eigenvalue problem was brought into the form $\mathbb{A}\boldsymbol{z} = \lambda\, \mathbb{I}\boldsymbol{z}$. In order to use the framework presented in Section 2, we need to apply a shift to gain positivity of the differential operator. Recall from the discussion of the linear case that the operator $\mathcal{A}_{\mathbf{k}}$ is not elliptic. From Lemma 2.9 we know, however, that $\mathcal{A}_{\mathbf{k},\beta} := \mathcal{A}_{\mathbf{k}} + \beta\mathcal{I}$ is elliptic for every $\beta > 0$. For fixed $\beta > 0$ and $\underline{\alpha} := \min\{\alpha_1, \alpha_2\}$ we introduce $\tilde{\beta} := \beta/(\underline{\alpha}\, \mu_0)$ and shift the linearized eigenvalue problem by $\tilde{\beta}\, \mathbb{I}\boldsymbol{z}$. This then provides the appearance of $\mathcal{A}_{\mathbf{k},\beta}$. More precisely, we obtain the shifted operator

$$\mathbb{A}_\beta := \mathbb{A} + \tilde{\beta}\, \mathbb{I} = \begin{bmatrix} \frac{1}{\mu_0}\mathcal{A}_{\mathbf{k}} + \Xi\, \mathcal{I}_2 + \tilde{\beta}\, \mathcal{I}_\alpha & -\overline{\mathcal{I}}_2 \mathbf{b}^* \\ -\mathbf{b}\, \overline{\mathcal{I}}_2^* & \mathbf{A} + \tilde{\beta}\, \mathbf{I} \end{bmatrix}. \tag{4.8}$$

Due to $\mathcal{I} = \mathcal{I}_1 + \mathcal{I}_2$ we have

$$\begin{aligned} \tfrac{1}{\mu_0}\mathcal{A}_{\mathbf{k}} + \Xi\, \mathcal{I}_2 + \tilde{\beta}\, \mathcal{I}_\alpha &= \tfrac{1}{\mu_0}\mathcal{A}_{\mathbf{k}} + \Xi\, \mathcal{I}_2 + \tfrac{\beta}{\mu_0}\tfrac{\alpha_1}{\underline{\alpha}}\mathcal{I}_1 + \tfrac{\beta}{\mu_0}\tfrac{\alpha_2}{\underline{\alpha}}\mathcal{I}_2 \\ &= \tfrac{1}{\mu_0}\mathcal{A}_{\mathbf{k},\beta} + \Xi\, \mathcal{I}_2 + \tfrac{\beta}{\mu_0}\big(\underline{\alpha}^{-1}\mathcal{I}_\alpha - \mathcal{I}\big) \end{aligned}$$

with $\big(\underline{\alpha}^{-1}\mathcal{I}_\alpha - \mathcal{I}\big) \geq 0$. The shifted eigenvalue problem has the form $\mathbb{A}_\beta \boldsymbol{z} = (\lambda + \tilde{\beta})\, \mathbb{I}\boldsymbol{z}$. Corresponding to the operator $\mathbb{A}_\beta$, we define $\mathfrak{a}_\beta \colon \mathcal{V} \times \mathcal{V} \to \mathbb{C}$ by

$$\mathfrak{a}_\beta(\boldsymbol{z}_1, \boldsymbol{z}_2) := \big\langle \mathbb{A}_\beta \boldsymbol{z}_1, \boldsymbol{z}_2 \big\rangle = \mathfrak{a}(\boldsymbol{z}_1, \boldsymbol{z}_2) + \tilde{\beta}\, \mathfrak{i}(\boldsymbol{z}_1, \boldsymbol{z}_2)$$

for $\boldsymbol{z}_1 = [u; \boldsymbol{x}_1]$, $\boldsymbol{z}_2 = [v; \boldsymbol{x}_2] \in \mathcal{V}$.

**Lemma 4.8.** *The sesquilinear form $\mathfrak{a} \colon \mathcal{V} \times \mathcal{V} \to \mathbb{C}$ satisfies Assumption 2.3.*

*Proof.* Due to the given structure of $\mathbb{A}$ and the fact that $\mathbf{A}$ is Hermitian, it is easy to see that $\mathfrak{a}$ is continuous and Hermitian. It remains to show that $\mathfrak{a}_\beta$ is positive for some $\beta > 0$. For this, we consider $\boldsymbol{z} = [u; \boldsymbol{x}] \in \mathcal{V}$ and note that

$$\mathfrak{a}_\beta(\boldsymbol{z}, \boldsymbol{z}) \geq \big\langle \tfrac{1}{\mu_0}\mathcal{A}_{\mathbf{k},\beta} u + \Xi\, \mathcal{I}_2 u, u \big\rangle - 2\, \langle \overline{\mathcal{I}}_2 \mathbf{b}^* \boldsymbol{x}, u \rangle + \big((\mathbf{A} + \tilde{\beta}\, \mathbf{I})\boldsymbol{x}, \boldsymbol{x}\big)_X.$$

The definition of $\mathbf{b} = [\xi_1\eta_1, \dots, \xi_L\eta_L]^T$ yields the estimate

$$2\, \langle \overline{\mathcal{I}}_2 \mathbf{b}^* \boldsymbol{x}, u \rangle = 2\sum_{\ell=1}^{L} (\xi_\ell \eta_\ell x_\ell, u)_X \leq 2\sum_{\ell=1}^{L} \|\eta_\ell x_\ell\|_X \|\xi_\ell u\|_X \leq \max \eta_\ell^2\, \|\boldsymbol{x}\|_X^2 + \max \xi_\ell^2\, \|u\|_X^2$$

and thus, with $c_{\text{ell}}$ denoting the ellipticity constant of $\mathcal{A}_{\mathbf{k},\beta}$,

$$\mathfrak{a}_\beta(\boldsymbol{z}, \boldsymbol{z}) \geq \tfrac{1}{\mu_0} c_{\text{ell}}\, \|u\|_V^2 + (\Xi - \max \xi_\ell^2)\, \|u\|_X^2 + (\min \eta_\ell^2 - \max \eta_\ell^2 + \tilde{\beta})\, \|\boldsymbol{x}\|_X^2.$$

Assuming $\tilde{\beta} > \max \eta_\ell^2 - \min \eta_\ell^2$, we conclude $\mathfrak{a}_\beta(\boldsymbol{z}, \boldsymbol{z}) \gtrsim \|\boldsymbol{z}\|_{\mathcal{V}}^2$ and thus, positivity of $\mathfrak{a}_\beta$. □

4.5. **Convergence of the inverse power method.** We apply the inverse power method from Section 3.1 to the shifted eigenvalue problem (4.8). For an initial function $\boldsymbol{z}^0 = [u^0; \boldsymbol{x}^0] \in \mathcal{V}$ we thus consider the iteration

$$\mathbb{A}_\beta \boldsymbol{z}^j = \mu^{j-1}\, \mathbb{I}\, \tilde{\boldsymbol{z}}^{j-1} \qquad \text{in } \mathcal{V}^* \tag{4.9}$$

with the Rayleigh quotient

$$\mu^j := \frac{\mathfrak{a}_\beta(\boldsymbol{z}^j, \boldsymbol{z}^j)}{\mathfrak{i}(\boldsymbol{z}^j, \boldsymbol{z}^j)} = \frac{\|\boldsymbol{z}^j\|_\beta^2}{\|\boldsymbol{z}^j\|^2} \geq 0.$$

Note that we use here the norms $\|\boldsymbol{z}\|_\beta^2 = \mathfrak{a}_\beta(\boldsymbol{z}, \boldsymbol{z})$ and $\|\boldsymbol{z}\|^2 = \mathfrak{i}(\boldsymbol{z}, \boldsymbol{z})$, similar to Section 2.1. Further, $\tilde{\boldsymbol{z}}^{j-1}$ denotes the normalization in the $\mathfrak{i}$-norm, i.e., we define $\tilde{\boldsymbol{z}}^{j-1} := \boldsymbol{z}^{j-1}/\|\boldsymbol{z}^{j-1}\|$. Note, however, that in the present setting the embedding $\mathcal{V} \hookrightarrow \mathcal{H}$ is not compact and thus, Assumption 2.2 is not satisfied. Hence, Theorem 3.1 is not applicable but we are able to show the following result.

**Theorem 4.9.** *Consider the nonlinear eigenvalue problem* (4.5) *for a fixed wave vector* $\mathbf{k}$ *and a starting function* $u^0 \in V$*. Set* $\boldsymbol{z}^0 := [u^0; \boldsymbol{x}^0] \in \mathcal{V}$ *with* $\boldsymbol{x}^0 \in X^L$ *defined as in* (4.6)*. Then, the power iteration* (4.9) *converges in the sense that there exists a subsequence of* $u^j$*, which satisfies* $u^j \to u^*$ *in* $H$ *with* $u^*$ *being an eigenfunction of* (4.5)*. The corresponding eigenvalue is given by*

$$\lambda^* := \frac{\|\boldsymbol{z}^*\|_\beta^2}{\|\boldsymbol{z}^*\|^2} - \tilde{\beta},$$

*where* $\boldsymbol{z}^*$ *denotes the weak limit of* $\boldsymbol{z}^j$ *in* $\mathcal{V}$*.*

*Proof.* We proceed as in the proof of Theorem 3.1 and test (4.9) with $\boldsymbol{z}^j$ and $\tilde{\boldsymbol{z}}^{j-1}$, respectively. This then yields the estimates

$$\|\boldsymbol{z}^j\|_\beta^2 \leq \mu^{j-1}\|\boldsymbol{z}^j\|, \qquad \sqrt{\mu^j} \leq \sqrt{\mu^{j-1}}.$$

Due to $\mu^j \geq 0$, we conclude the existence of a limit $\mu^* := \lim_{j\to\infty} \mu^j \geq 0$. This also implies the uniform bounds

$$\|\tilde{\boldsymbol{z}}^j\|_\beta = \sqrt{\mu^j} \leq \sqrt{\mu^0}, \qquad \|\boldsymbol{z}^j\|_\beta \lesssim C_{\mathcal{V}\hookrightarrow\mathcal{H}}\, \mu^{j-1} \leq C_{\mathcal{V}\hookrightarrow\mathcal{H}}\, \mu^0.$$

For the last estimate we have used the continuity of the embedding $\mathcal{V} \hookrightarrow \mathcal{H}$. Thus, there exist convergent subsequences and limits $\boldsymbol{z}^*, \tilde{\boldsymbol{z}}^* \in \mathcal{V}$, which satisfy (without relabeling) $\boldsymbol{z}^j \rightharpoonup \boldsymbol{z}^*, \tilde{\boldsymbol{z}}^j \rightharpoonup \tilde{\boldsymbol{z}}^*$ in $\mathcal{V}$. We emphasize that the two limits may only differ by a multiplicative constant, i.e., $\tilde{\boldsymbol{z}}^* = c\, \boldsymbol{z}^*$. A componentwise consideration with $\boldsymbol{z}^j = [u^j; \boldsymbol{x}^j]$, $\tilde{\boldsymbol{z}}^j = [\tilde{u}^j; \tilde{\boldsymbol{x}}^j]$, and $\boldsymbol{z}^* = [u^*; \boldsymbol{x}^*]$ then yields

$$u^j \rightharpoonup u^* \text{ in } V, \quad \tilde{u}^j \rightharpoonup c\, \tilde{u}^* \text{ in } V, \qquad \boldsymbol{x}^j \rightharpoonup \boldsymbol{x}^* \text{ in } X^L, \quad \tilde{\boldsymbol{x}}^j \rightharpoonup c\, \tilde{\boldsymbol{x}}^* \text{ in } X^L.$$

Using the compact embedding $V \hookrightarrow H$, we conclude that the first component converges strongly in $H$, i.e., $u^j \to u^*$ and $\tilde{u}^j \to c\, \tilde{u}^*$ in $\mathcal{H}$. We now show that the limit pair $(u^*, \lambda^*)$ with $\lambda^* := \mu^* - \beta$ solves the nonlinear eigenvalue problem (4.5). For this, we apply to (4.9) a test function $[v; 0] \in \mathcal{V}$ with arbitrary $v \in V$ and consider the limit $j \to \infty$,

$$\mathfrak{a}_\beta(\boldsymbol{z}^*, [v; 0]) \leftarrow \mathfrak{a}_\beta(\boldsymbol{z}^j, [v; 0]) = \mu^{j-1}\, \mathfrak{i}(\tilde{\boldsymbol{z}}^{j-1}, [v; 0]) \to \mu^*\, \mathfrak{i}(c\, \boldsymbol{z}^*, [v; 0]).$$

With the definitions of $\mathfrak{a}_\beta$ and $\mathfrak{i}$ we conclude that

$$\tfrac{1}{\mu_0}\mathcal{A}_{\mathbf{k}} u^* + \Xi\, \mathcal{I}_2 u^* = \mu^*\, c\, \mathcal{I}_\alpha u^* - \tilde{\beta}\, \mathcal{I}_\alpha u^* + \overline{\mathcal{I}}_2 \langle \mathbf{b}, \boldsymbol{x}^* \rangle \qquad \text{in } V^*.$$

On the other hand, taking the limit in (4.9) with a test function $[0; \boldsymbol{y}] \in \mathcal{V}$, we obtain

$$\big(\mathbf{A} + (\tilde{\beta} - \mu^* c)\, \mathbf{I}\big)\boldsymbol{x}^* = j_X^{-1} \mathbf{b}\, \overline{\mathcal{I}}_2^* u^* \qquad \text{in } X^L.$$

These two equations together then give with $\zeta := \mu^* c - \tilde{\beta}$,

$$\tfrac{1}{\mu_0}\mathcal{A}_{\mathbf{k}}u^* + \Xi\,\mathcal{I}_2 u^* = \zeta\,\mathcal{I}_\alpha u^* + \mathbf{b}^*(\mathbf{A} - \zeta\,\mathbf{I})^{-1}\mathbf{b}\,\mathcal{I}_2 u^* \qquad \text{in } V^*.$$

Thus, the pair $(u^*, \zeta)$ is an eigenpair of the nonlinear eigenvalue problem (4.5). □

This result shows that the convergence in maintained for this particular case coming from the linearization of a nonlinear eigenvalue problem. In contrast to Section 3, however, we only showed the convergence in $H$ and not in $V$ due to a lack of compactness.

## 5. The Full Drude-Lorentz model

Similarly as in Section 4, we consider an extension of Example 2.8 where the electric permittivity $\varepsilon$ is frequency-dependent and has the form (4.1). However, we allow here for a more general class of models for the electric permittivity $\varepsilon_2(\omega)$. Indeed, the simplified Drude-Lorentz model considered in Section 4 has the particular property that it can be linearized in a way that ensures Assumption 2.3. But other – more realistic – models may not have this nice property. We are especially interested in the general causality-preserving model described in [GVDZ17] and the full Drude-Lorentz model, see e.g. [LL10] or [Jac99, Ch. 7.5]. Here we restrict ourselves to the real part of $\varepsilon_2(\omega)$ in order to preserve the Hermitian structure of the eigenvalue problem. The information about the imaginary part can be included later through perturbation theory as a post-processing step, see [RF11]. After presenting the considered class of models in more detail, we show in this section how the resulting nonlinear eigenvalue problem can be solved with a Newton-type iteration, provided some a priori knowledge on the eigenpair of interest is given.

### 5.1. **Definition of the eigenvalue problem.**

In the remainder of this section, we assume that $\varepsilon_1(\omega) \equiv \alpha_1 \in \mathbb{R}^+$, $\varepsilon_2$ is holomorphic and bounded on an open connected set $D \subset \mathbb{C}$, and $\varepsilon_2(\omega) \in \mathbb{R}^+$ for all $\omega \in D$. Moreover, we assume the derivatives $\varepsilon_2'(\omega), \varepsilon_2''(\omega)$ to be bounded for all $\omega \in D$. As usual, $\mathcal{L}(X,Y)$ denotes the set of bounded linear operators mapping from the vector space $X$ into $Y$.

We consider the nonlinear eigenvalue problem

$$\mathcal{T}(\omega)u := \mathcal{A}u - \mathcal{B}(\omega)u = 0 \qquad \text{in } \mathcal{V}^* \tag{5.1}$$

where $\mathcal{A}\colon \mathcal{V} \to \mathcal{V}^*$ is defined by the sesquilinear form (2.2) via $\langle \mathcal{A}u, v\rangle_{\mathcal{V}^*,\mathcal{V}} = a(u,v)$ for all $u, v \in \mathcal{V}$ and $\mathcal{B}(\omega)\colon D \to \mathcal{L}(\mathcal{V}, \mathcal{V}^*)$ is defined by

$$\langle \mathcal{B}(\omega)u, v\rangle_{\mathcal{V}^*,\mathcal{V}} := \int_\Omega \big(\alpha_1\chi_1(x) + \varepsilon_2(\omega)\chi_2(x)\big)\, u(x)\overline{v(x)}\,\mathrm{d}x$$

for all $u, v \in \mathcal{V}$. We denote by $(u^*, \omega^*) \in \mathcal{V} \times D$ an eigenpair of (5.1), which we assume to be of algebraic multiplicity equal to 1.

The eigenvalue problem (5.1) was already addressed in [Eng10], but formulated in terms of operators mapping from $\mathcal{V}$ into itself. From the results of that paper, an important property of the operator-valued function $\mathcal{T}(\omega)$ can be directly derived.

**Lemma 5.1.** *For all $\omega \in D$, the operator $\mathcal{T}(\omega)\colon \mathcal{V} \to \mathcal{V}^*$ is Fredholm with index 0.*

*Proof.* In [Eng10] it is shown that the operator $T(\omega)\colon \mathcal{V} \to \mathcal{V}$ defined by $(T(\omega)u, v)_{\mathcal{V}} := \langle \mathcal{T}(\omega)u, v\rangle_{\mathcal{V}^*,\mathcal{V}}$ for all $u, v \in \mathcal{V}$ is Fredholm with index 0. Denoting by $j_{\mathcal{V}}$ the Riesz isomorphism between $\mathcal{V}$ and $\mathcal{V}^*$, it follows that $\mathcal{T}(\omega) = j_{\mathcal{V}}\, T(\omega)$ is a composition of two Fredholm operators with index 0 and thus, $\mathcal{T}(\omega)$ is Fredholm with index 0 itself. □

5.2. **A Newton-type iteration.** In this subsection, we aim to extend the results of [Sch08, Ch. 4] to the infinite-dimensional problem (5.1). To this end, we adopt ideas from [AR68], where operators mapping from $\mathcal{V} \to \mathcal{V}$ are considered. We follow the reasoning of [Sch08] and start by rewriting the eigenvalue problem as

$$\mathcal{F}_y(u,\omega) := \begin{bmatrix} \mathcal{T}(\omega)u \\ (y,u)_{\mathcal{V}} - 1 \end{bmatrix} = 0,$$

where the normalizing vector $y \in \mathcal{V}$ has to be chosen such that $(y,u^*)_{\mathcal{V}} \neq 0$. By assumption, $\varepsilon_2$ is holomorphic in $D$, which implies that $\mathcal{F}_y(u,\omega)$ is twice continuously differentiable in $u$ and in $\omega$. A Taylor expansion of $\mathcal{F}_y(u,\omega)$ in the eigenpair $(u^*,\omega^*)$ yields

$$\begin{aligned}\mathcal{F}_y(u,\omega) =& \mathcal{F}_y(u^*,\omega^*) + \partial\mathcal{F}_y(u^*,\omega^*)\begin{bmatrix} u-u^* \\ \omega-\omega^* \end{bmatrix} \\ &+ \frac{1}{2}\partial^2\mathcal{F}_y(u^*,\omega^*)\left(\begin{bmatrix} u-u^* \\ \omega-\omega^* \end{bmatrix}, \begin{bmatrix} u-u^* \\ \omega-\omega^* \end{bmatrix}\right) + \mathcal{O}\left(\left\|\begin{pmatrix} u-u^* \\ \omega-\omega^* \end{pmatrix}\right\|_{\mathcal{W}}^3\right)\end{aligned}$$

where $\mathcal{W} := \mathcal{V} \times \mathbb{C}$ and $\|\,[u-u^*;\ \omega-\omega^*]\,\|_{\mathcal{W}}^2 := \|u-u^*\|_{\mathcal{V}}^2 + |\omega-\omega^*|^2$. The corresponding Jacobian is given by

$$\partial\mathcal{F}_y(u,\omega) = \begin{bmatrix} \mathcal{T}(\omega) & \mathcal{T}'(\omega)u \\ \mathcal{P}_y & 0 \end{bmatrix},$$

where $\mathcal{T}'$ denotes the derivative with respect to $\omega$ and $\mathcal{P}_y \colon \mathcal{V} \to \mathbb{C}$ is defined by $\mathcal{P}_y u := (y,u)_{\mathcal{V}}$ for all $u \in \mathcal{V}$. In order to shorten the notation, we introduce the variables $\Delta u := u - u^*$ and $\Delta\omega := \omega - \omega^*$. The second derivative of $\mathcal{F}_y$ along the direction $[\Delta u;\ \Delta\omega]$ reads

$$\partial^2\mathcal{F}_y(u,\omega)\big([\Delta u;\ \Delta\omega],[\Delta u;\ \Delta\omega]\big) = \Delta\omega \begin{bmatrix} 2\mathcal{T}'(\omega)\Delta u + \mathcal{T}''(\omega)\Delta u\Delta\omega \\ 0 \end{bmatrix}.$$

Following the strategy of the standard formulation of Newton's method, we define the following iterative process: Given an initial vector $[u_0;\ \omega_0] \in \mathcal{W}$ satisfying $(y,u_0)_{\mathcal{V}} = 1$, the iterates are defined by $u_{j+1} := u_j + s_j$, $\omega_{j+1} := \omega_j + \nu_j$ with

$$\begin{bmatrix} \mathcal{T}(\omega_j) & \mathcal{T}'(\omega_j)u_j \\ \mathcal{P}_y & 0 \end{bmatrix}\begin{bmatrix} s_j \\ \nu_j \end{bmatrix} = -\begin{bmatrix} \mathcal{T}(\omega_j)u_j \\ 0 \end{bmatrix} \tag{5.2}$$

for $j = 0,1,2,\ldots$. Clearly, $\mathcal{T}(\omega)$ is not invertible in $\omega = \omega^*$. Nevertheless, we show in the following subsection that equation (5.2) is uniquely solvable for $[u_j;\ \omega_j]$ in a neighbourhood of the eigenpair $[u^*;\ \omega^*]$.

5.3. **Convergence of the Newton-type iteration.** This subsection is devoted to the proof of local convergence of the iteration introduced in (5.2). For $v \in \mathcal{V}$, we denote by $B_\tau(v) \subset \mathcal{V}$ the open ball of radius $\tau$ centered at $v$.

**Lemma 5.2.** *Let $\omega^*$ be an isolated eigenvalue of $\mathcal{T} \colon D \to \mathcal{L}(\mathcal{V},\mathcal{V}^*)$, where the corresponding eigenvector $u^*$ is normalized such that $\mathcal{P}_y u^* = 1$. Then there exist $\tau_1, \delta_1 > 0$ such that $\partial\mathcal{F}_y(u,\omega)$ is invertible for all $\omega \neq \omega^*$ satisfying $|\omega-\omega^*| < \delta_1$ and all $u \in B_{\tau_1}(u^*)$ satisfying $\mathcal{P}_y u = 1$. In this case, $\partial\mathcal{F}_y(u,\omega)^{-1}$ is bounded.*

*Proof.* Let us prove the bijectivity of $\partial\mathcal{F}_y(u,\omega)$ by showing that the equation

$$\partial\mathcal{F}_y(u,\omega)\begin{bmatrix} s \\ \nu \end{bmatrix} = \begin{bmatrix} f \\ g \end{bmatrix} \tag{5.3}$$

has a unique solution for all $f \in \mathcal{V}^*,\ g \in \mathbb{C}$. Since $\omega^*$ is an isolated eigenvalue, there exists a $\tilde{\delta} > 0$ such that $\mathcal{T}(\omega)$ is invertible for all $\omega \neq \omega^*$ satisfying $|\omega - \omega^*| = |\Delta\omega| < \tilde{\delta}$. Thus, the upper row of equation (5.3) implies

$$s = \mathcal{T}^{-1}(\omega)(f - \nu\, \mathcal{T}'(\omega)u)$$

whereas the lower row implies

$$g = \mathcal{P}_y s = \mathcal{P}_y \mathcal{T}^{-1}(\omega)(f - \nu \mathcal{T}'(\omega)u).$$

Thus $\nu \in \mathbb{C}$ is uniquely defined by

$$\nu = \frac{\mathcal{P}_y \mathcal{T}^{-1}(\omega) f - g}{\mathcal{P}_y \mathcal{T}^{-1}(\omega)\mathcal{T}'(\omega)u}$$

if the condition $\mathcal{P}_y \mathcal{T}^{-1}(\omega)\mathcal{T}'(\omega)u \neq 0$ is satisfied. In this case, $\partial\mathcal{F}_y(u, \omega)$ is linear, bijective, and bounded which implies the existence of a bounded inverse. It remains to show that $\mathcal{P}_y \mathcal{T}^{-1}(\omega)\mathcal{T}'(\omega)u \neq 0$ in a neighbourhood of $(u^*, \omega^*)$ with $\mathcal{P}_y u = 1$.

Note that $\mathcal{V}$ can be decomposed into $\mathcal{V} = \operatorname{span}\{u^*\} \oplus \ker(\mathcal{P}_y)$, since $\mathcal{P}_y u^* = 1$. Indeed, for any $v \in \mathcal{V}$ it holds that

$$v = u^*(\mathcal{P}_y v) + (v - u^*(\mathcal{P}_y v))\,.$$

Moreover, the Taylor expansion of first order of $\mathcal{T}$ around $\omega$ with the remainder written in Lagrange form gives

$$\mathcal{T}(\omega^*) = \mathcal{T}(\omega) - \mathcal{T}'(\omega)\Delta\omega + \frac{\mathcal{T}''(\xi)}{2}\Delta\omega^2$$

for some $\xi \in [\min(\omega, \omega^*), \max(\omega, \omega^*)]$. Therefore,

$$\begin{aligned}
\mathcal{P}_y \mathcal{T}^{-1}(\omega)\mathcal{T}'(\omega)u &= \frac{1}{\Delta\omega}\mathcal{P}_y\left(u - \mathcal{T}^{-1}(\omega)\mathcal{T}(\omega^*)u + \frac{\Delta\omega^2}{2}\mathcal{T}^{-1}(\omega)\mathcal{T}''(\xi)u\right)\\
&= \frac{1}{\Delta\omega}\mathcal{P}_y\left(u^*\mathcal{P}_y u - \mathcal{T}^{-1}(\omega)\mathcal{T}(\omega^*)(u - u^*\mathcal{P}_y u) + \frac{\Delta\omega^2}{2}\mathcal{T}^{-1}(\omega)\mathcal{T}''(\xi)u\right).
\end{aligned}$$

When $\mathcal{P}_y u = 1$, the continuity of the functional $\mathcal{P}_y$ implies that $\mathcal{P}_y \mathcal{T}^{-1}(\omega)\mathcal{T}'(\omega)u \neq 0$ if $\|\mathcal{T}^{-1}(\omega)\mathcal{T}(\omega^*)(u - u^*) - \frac{\Delta\omega^2}{2}\mathcal{T}^{-1}(\omega)\mathcal{T}''(\xi)u\|_{\mathcal{V}} < \varepsilon$ for a certain threshold $\varepsilon > 0$. Choosing $\tau_1 < 0.5\,\varepsilon\,\|\mathcal{T}^{-1}(\omega)\mathcal{T}(\omega^*)\|_{\mathcal{V}}^{-1}$ and $\delta_1 < \min(\tilde{\delta}, \varepsilon\,\|\mathcal{T}^{-1}(\omega)\mathcal{T}''(\xi)u\|_{\mathcal{V}}^{-1/2})$ finishes the proof. □

**Lemma 5.3.** *Let $\omega^*$ be an isolated eigenvalue of $\mathcal{T}\colon D \to \mathcal{L}(\mathcal{V}, \mathcal{V}^*)$ with algebraic multiplicity equal to 1, where the corresponding eigenvector $u^*$ is normalized such that $\mathcal{P}_y u^* = 1$. Then there exists $\tau_2 > 0$ such that $\partial\mathcal{F}_y(u, \omega^*)$ has a bounded inverse for all $u \in B_{\tau_2}(u^*)$.*

*Proof.* Let us prove the bijectivity of $\partial\mathcal{F}_y(u, \omega^*)$ by showing that equation (5.3) with $\omega = \omega^*$ and $u \in B_{\tau_2}(u^*)$ has a unique solution for all $f \in \mathcal{V}^*$, $g \in \mathbb{C}$.

Since $\mathcal{P}_y u^* = 1$ by assumption on $y$, the vector $s$ can be decomposed as $s = \alpha u^* + s_{\ker}$ for some scalar $\alpha \in \mathbb{C}$ and some $s_{\ker} \in \ker(\mathcal{P}_y)$. Therefore, the lower row of equation (5.3) implies $g = \mathcal{P}_y s = \alpha$. The Hermiticity of $\mathcal{T}$ implies that $\langle \mathcal{T}(\omega^*)v, u^*\rangle_{\mathcal{V}^*,\mathcal{V}} = \langle \mathcal{T}(\omega^*)u^*, v\rangle_{\mathcal{V}^*,\mathcal{V}} = 0$ for all $v \in \mathcal{V}$. Therefore, the upper row of equation (5.3) tested with $u^*$ yields

$$\langle f, u^*\rangle_{\mathcal{V}^*,\mathcal{V}} = \langle \mathcal{T}(\omega^*)s, u^*\rangle_{\mathcal{V}^*,\mathcal{V}} + \langle \nu\mathcal{T}'(\omega^*)u, u^*\rangle_{\mathcal{V}^*,\mathcal{V}} = \nu\langle \mathcal{T}'(\omega^*)u, u^*\rangle_{\mathcal{V}^*,\mathcal{V}},$$

from which it follows that

$$\nu = \frac{\langle f, u^*\rangle_{\mathcal{V}^*,\mathcal{V}}}{\langle \mathcal{T}'(\omega^*)u, u^*\rangle_{\mathcal{V}^*,\mathcal{V}}}$$

if the condition $\langle \mathcal{T}'(\omega^*)u, u^*\rangle_{\mathcal{V}^*,\mathcal{V}} \neq 0$ holds. Moreover, we note that the restriction of $\mathcal{T}(\omega^*)$ to $\ker(\mathcal{P}_y)$ is bijective as mapping from $\ker(\mathcal{P}_y)$ to its range. Indeed,

$$\ker(\mathcal{T}(\omega^*)|_{\ker(\mathcal{P}_y)}) = \ker(\mathcal{T}(\omega^*)) \cap \ker(\mathcal{P}_y) = \{0\}$$

implies the injectivity, and the surjectivity is obvious. Therefore we obtain from the upper row of equation (5.3) that

$$f = \mathcal{T}(\omega^*)s + \nu\mathcal{T}'(\omega^*)u = \mathcal{T}(\omega^*)|_{\ker(\mathcal{P}_y)}s_{\ker} + \nu\mathcal{T}'(\omega^*)u,$$

which implies

$$s_{\ker} = \mathcal{T}(\omega^*)|^{-1}_{\ker(\mathcal{P}_y)}(f - \nu\mathcal{T}'(\omega^*)u).$$

It is left to show that the condition $\langle \mathcal{T}'(\omega^*)u, u^*\rangle_{\mathcal{V}^*,\mathcal{V}} \neq 0$ holds. Since $\omega^*$ is an eigenvalue with algebraic multiplicity equal to 1, $\mathcal{T}'(\omega^*)u^* \notin \operatorname{im}(\mathcal{T}(\omega^*))$, see e.g. [LGMC07]. Moreover, since $\mathcal{T}'(\omega^*)$ is a linear operator, the statement stays true in a neighbourhood of $u^*$, i.e., there exists $\tau_2 > 0$ such that $\mathcal{T}'(\omega^*)u \notin \operatorname{im}(\mathcal{T}(\omega^*))$ for all $u \in B_{\tau_2}(u^*)$. From Lemma 5.1, $\mathcal{T}(\omega^*)$ is Fredholm with index 0, which implies that $\operatorname{codim}(\operatorname{im}(\mathcal{T}(\omega^*))) = \dim(\ker(\mathcal{T}(\omega^*))) = 1$, since the geometric multiplicity of the eigenvalue $\omega^*$ is 1. Thus, we consider the decomposition $\mathcal{V}^* = \operatorname{im}(\mathcal{T}(\omega^*)) \oplus \operatorname{span}\{\mathcal{T}'(\omega^*)u\}$ and observe that due to $u^* \neq 0$, there must exist some $h \in \mathcal{V}^*$, $h = \alpha\mathcal{T}'(\omega^*)u + \mathcal{T}(\omega^*)v$ for some $\alpha \in \mathbb{C}, v \in \mathcal{V}$ such that $0 \neq \langle h, u^*\rangle_{\mathcal{V}^*,\mathcal{V}} = \langle \alpha\mathcal{T}'(\omega^*)u + \mathcal{T}(\omega^*)v, u^*\rangle_{\mathcal{V}^*,\mathcal{V}} = \alpha\langle \mathcal{T}'(\omega^*)u, u^*\rangle_{\mathcal{V}^*,\mathcal{V}}$, and thus $\langle \mathcal{T}'(\omega^*)u, u^*\rangle_{\mathcal{V}^*,\mathcal{V}} \neq 0$. □

**Theorem 5.4.** *Let $\omega^*$ be an isolated eigenvalue of $\mathcal{T}\colon D \to \mathcal{L}(\mathcal{V}, \mathcal{V}^*)$ with algebraic multiplicity equal to 1, where the corresponding eigenvector $u^*$ is normalized such that $\mathcal{P}_y u^* = 1$. Let $\delta$ and $\tau$ be such that $\mathcal{T}'(\omega^*)u \notin \operatorname{im}(\mathcal{T}(\omega^*))$ and $\mathcal{P}_y\mathcal{T}^{-1}\mathcal{T}'(\omega)u \neq 0$ for all $u \in B_\tau(u^*)$ and all $\omega$ satisfying $0 < |\omega - \omega^*| < \delta$. Then, given an initial vector $(u_0, \omega_0) \in \mathcal{W}$ satisfying $\mathcal{P}_y u_0 = 1$, $u_0 \in B_\tau(u^*)$ and $|\omega_0 - \omega^*| < \delta$, the iteration* (5.2) *is well defined and the errors satisfy*

$$\|[u_{j+1} - u^*; \omega_{j+1} - \omega^*]\|_{\mathcal{W}} \leq |\omega_j - \omega^*| \left(K_1\|u_j - u^*\|_{\mathcal{V}} + K_2|\omega_j - \omega^*|\right)$$

*for some uniform constants $K_1$, $K_2$.*

*Proof.* It follows from Lemmas 5.2 and 5.3 that there exist $0 < \tau < \min(\tau_1, \tau_2)$ and $0 < \delta < \delta_1$ such that the Jacobian $\partial\mathcal{F}_y$ is uniformly bounded with a certain constant $C_1$ in a closed ball of radius $\min(\tau, \delta)$ around $(u^*, \omega^*)$. For the sake of readability, we introduce the notation $z_j := [u_j; \omega_j] \in \mathcal{W}$ and $z^* := [u^*; \omega^*] \in \mathcal{W}$. Then, using the Taylor expansion of first order of $\mathcal{F}_y(z^*)$ around $z_j$ and writing the remainder in Lagrange form yields

$$\begin{aligned} z_{j+1} - z^* &= z_j - \partial\mathcal{F}_y(z_j)^{-1}\mathcal{F}_y(z_j) - z^* \\ &= \partial\mathcal{F}_y(z_j)^{-1}\left(\partial\mathcal{F}_y(z_j)(z_j - z^*) - \mathcal{F}_y(z_j) + \mathcal{F}_y(z^*)\right) \\ &= \partial\mathcal{F}_y(z_j)^{-1}\left(\frac{1}{2}\partial^2\mathcal{F}_y(\zeta)(z_j - z^*, z_j - z^*)\right) \end{aligned}$$

where $\zeta = z^* + t(z_j - z^*) \in \mathcal{W}$ for some $t \in [0, 1]$. Thus, with $\zeta =: [u_\zeta; \omega_\zeta]$ we obtain

$$\begin{aligned} \|z_{j+1} - z^*\|_{\mathcal{W}} &= \frac{1}{2}\left\|\partial\mathcal{F}_y(z_j)^{-1}\left(\partial^2\mathcal{F}_y(\zeta)(z_j - z^*, z_j - z^*)\right)\right\|_{\mathcal{W}} \\ &\leq \frac{C_1}{2}\left\|\partial^2\mathcal{F}_y(\zeta)(z_j - z^*, z_j - z^*)\right\|_{\mathcal{W}^*} \\ &\leq \frac{C_1}{2}|\omega - \omega^*|\left(2\left\|\mathcal{T}'(\omega_\zeta)\right\|_{\mathcal{V}^*}\|u_j - u^*\|_{\mathcal{V}} + \left\|\mathcal{T}''(\omega_\zeta)\right\|_{\mathcal{V}^*}\|u_\zeta\|_{\mathcal{V}}|\omega - \omega^*|\right) \end{aligned}$$

By assumption, $\varepsilon'(\omega)$ and $\varepsilon''(\omega)$ are bounded for all $\omega$ in $D$ which implies that $\|\mathcal{T}'(\omega_\zeta)\|_{\mathcal{V}^*}$ and $\|\mathcal{T}''(\omega_\zeta)\|_{\mathcal{V}^*}$ are bounded with some constants $C_2$ and, respectively, $C_3$. Setting $K_1 = C_1C_2$ and $K_2 = \frac{1}{2}C_1C_3(\|u^*\| + \tau)$ terminates the proof. $\square$

Theorem 5.4 implies that the iterates $(u_j, \omega_j)$ converge strongly to the eigenpair $(u^*, \omega^*)$ if the starting pair was chosen close enough. Indeed, if $(u_0, \omega_0)$ satisfies $\|u_0 - u^*\|_{\mathcal{V}} \le \delta_0$ and $|\omega - \omega_0| \le \delta_0$ for some $\delta_0 \le \frac{1}{2}(K_1 + K_2)^{-1}$, then $\|[u_1 - u^*;\, \omega_1 - \omega^*]\|_{\mathcal{W}} \le (K_1 + K_2)\, \delta_0^2$, and thus $\|u_1 - u^*\|_{\mathcal{V}} < \frac{1}{2}\delta_0$ and $|\omega_1 - \omega^*| < \frac{1}{2}\delta_0$. By induction it follows that

$$\|u_j - u^*\|_{\mathcal{V}} \le (K_1 + K_2)\, \|u_{j-1} - u^*\|_{\mathcal{V}}^2 \le (K_1 + K_2)^{2j-1}\, \delta_0^{2j} \le \left(\frac{1}{2}\right)^{2j-1} \delta_0,$$

and similarly

$$|\omega_j - \omega^*| \le \left(\frac{1}{2}\right)^{2j-1} \delta_0.$$

## 6. Conclusion

In this paper, we have considered iterative methods for linear Hermitian as well as specific nonlinear eigenvalue problems arising in photonic crystal modeling. In case the electric permittivity is given by a Drude-Lorentz model with real coefficients and no dissipation, we are able to linearize the problem to obtain a linear and Hermitian eigenvalue problem. For this, we show the convergence of the inverse power method.

For more realistic models taking dissipation into account, the same procedure would lead to a linear but non-Hermitian eigenvalue problem. Thus, instead of a linearization we directly apply Newton's method, for which we prove local convergence.

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