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A Nonlinear Multigrid Eigenproblem Solver for the Complex Helmholtz Equation

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Abstract

The paper is motivated by the need for a fast robust adaptive multigrid method to solve complex Helmholtz eigenvalue problems arising from the design of optical chips. A nonlinear multigrid method is developed, which can be regarded as an extension of a previous adaptive Rayleigh quotient minimization method for selfadjoint Helmholtz eigenproblems. Since the complex Helmholtz operator is just a compact nonselfadjoint perturbation of a selfadjoint operator, linear algebra techniques like Schur decomposition can be extended from the finite dimensional case. The efficiency of the derived adaptive nonlinear multigrid method is illustrated by computations for a technologically relevant integrated optics component containing Multi Quantum Well Layers.

AMS Subject Classification: 65N25, 65N30, 65N55

Keywords: Eigenvalue problems, complex Helmholtz equation, multigrid methods, adaptive FEM, chip design

*Research supported by the BMBF under grant 03-DE7ZIB-5.

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1 Introduction

Eigenvalue problems for differential equations occur in many branches of science and engineering such as quantum mechanics, chemistry, acoustics, or optics. There are two basic approaches to be distinguished

- (I) the *discrete eigenproblem* approach: this approach *decouples* the discretization of the differential equations including boundary conditions (which comes *first*) and the numerical solution of the arising sparse linear algebra eigenproblem for given *fixed*, usually large dimension (which comes *second*),
- (II) the *continuous eigenproblem* approach: this approach *combines* the discretization and the numerical solution of a *sequence* of linear algebra eigenproblems with *increasing* dimension, performed by some *adaptive* multilevel or multigrid method.

For approach (I), there exists a large variety of well-established algorithms - see e.g. the recent survey paper by VAN DER VORST AND GOLUB [27] or the textbook by SAAD [24]. Among the most popular algorithms for large sparse *nonselfadjoint* eigenproblems are the Arnoldi-type method due to SORENSEN [26] as realized in the software package ARPACK or the Lanczos-type method with look-ahead strategies due to FREUND ET AL. [9]. Half-way towards the continuous approach lie multigrid or domain decomposition methods, when applied to the fixed dimension eigenproblem. Among the latter are the linear (multiplicative) multigrid method of HACKBUSCH [13], the preconditioned linear (additive) multigrid method due to BRAMBLE ET AL. [2], the nonlinear multigrid method of MANDEL AND MCCORMICK [19, 20], and the domain decomposition method due to CHAN AND SHARAPOV [4]. The first of these methods is constructed to apply to both the selfadjoint and the nonselfadjoint case, whereas the other methods are restricted to the selfadjoint case.

For approach (II), the above mentioned multigrid methods can, in principle, be implemented in their *nested* form. If, in addition, the construction of the successive nested grids is based on a-posteriori discretization *error estimators* or, at least, on *error indicators*, then the term *adaptive* multigrid method is justified. Examples of this kind have been worked out by DEUFLHARD ET AL. [6] as a modification and extension of the nonlinear multigrid method [19, 20] or by LEINEN ET AL. [17] as a hierarchical basis implementation of the preconditioned linear multigrid method [2]. In [6], the nonlinear multigrid method has been shown to be more robust for relatively coarse grids than the linear multigrid method - a feature, which is essential within adaptive implementations. For the design of optical chips, which has been treated in

[6], the restriction to selfadjoint eigenproblems means, that only *lossless* media could be modeled. It is the purpose of the present paper to get rid of this unrealistic restriction.

In the subsequent Section 2, a short description of the challenging problem class of component design in integrated optics is given, which motivated the present development. In particular, the necessity of an adaptive robust multigrid method for the nonselfadjoint multiscale Helmholtz eigenproblem is emphasized. In Section 3, the continuous eigenproblem approach is revisited in view of the well-established knowledge about the numerical solution of large nonselfadjoint eigenproblems in linear algebra. This leads to the idea of a *Schur decomposition* of the complex Helmholtz operator. On this basis, Section 4 deals with the construction of the nonlinear multigrid method for this eigenproblem as an extension of the method presented in [6] for the selfadjoint case. Finally, in Section 5, the performance of the herein developed algorithm is illustrated by the numerical treatment of a Multi Quantum Well (MQW) laser structure, which is out of the class of challenging problems introduced in the preceding Section 2. A more elaborate presentation of the contents of this paper will be given in a forthcoming (German) thesis [10].

2 A Challenging Problem Class: Design of Integrated Optics Components

Integrated optical components like semiconductor lasers, optical switches and filters are essential parts of modern fiber-optical networks. In general, these components are built again from sub-components. Optical waveguides are used to connect the various sub-components or they work as optical components themselves. Therefore, from the very beginning of integrated optics in the early seventies, the design of optical waveguides has been a central task. The analysis of optical waveguides is based on the knowledge of their eigenmodes and propagation constants. As an example, consider a typical integrated optical chip (Figure 1). The optical beam propagates in z-direction. The geometry of the chip itself is regarded as invariable (i. e. of infinite length) in this direction. The lateral confinement of the intensity distribution is caused by the rib-like structure above the beam. The task is to find modes that exhibit an intensity distribution invariant in z-direction and with finite lateral extension. This leads in a natural way to an eigenvalue problem, which will be derived here.

We start from the well-known time-harmonic Maxwell equations for the electric and magnetic fields \mathbf{E} and \mathbf{H} , respectively, in isotropic, nonmagnetic and

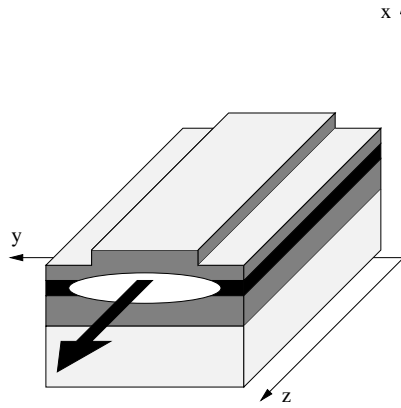


Figure 1: Typical integrated optical chip.

sourceless media with permittivity ϵ , permeability μ , conductivity σ and the optical angular frequency ω :

$$\begin{aligned} \text{curl } \mathbf{H} &= (i\omega\epsilon + \sigma)\mathbf{E}, & \text{div } \mathbf{H} &= 0, \\ \text{curl } \mathbf{E} &= -i\omega\mu\mathbf{H}, & \text{div } \epsilon\mathbf{E} &= 0 \quad . \end{aligned}$$

Taking the curl of the first equation to eliminate the electrical field via the third equation, employing the definition of the vectorial Laplace operator Δ applied to twice continuously differentiable vector valued functions \mathbf{V}

$$\Delta \mathbf{V} = \text{grad}(\text{div } \mathbf{V}) - \text{curl } \text{curl } \mathbf{V}$$

and using the divergence condition for \mathbf{H} shows that the magnetic field satisfies the vector Helmholtz equation

$$-\Delta \mathbf{H} - \omega^2 \tilde{\epsilon} \mu \mathbf{H} = \nabla \log \tilde{\epsilon} \times \text{curl } \mathbf{H} \quad . \quad (1)$$

Here we have introduced the complex permittivity $\tilde{\epsilon} = \epsilon - i\sigma/\omega$. In the problem class under consideration the variation of $\tilde{\epsilon}$ is in general very weak, therefore the term on the right-hand side of (1) can be neglected. We obtain a simplified version of (1)

$$-\Delta \mathbf{H} - \omega^2 \tilde{\epsilon} \mu \mathbf{H} = 0 \quad .$$

Now we fix the 3D cartesian coordinate system as shown in Figure 1. In cartesian coordinates the vectorial Laplace operator simplifies to the usual scalar one, applied to each coordinate independently. Further, because the vectorial coupling term has been neglected, we do not need to differentiate

between the vector components of \mathbf{H} . Let $H(x, y, z)$ be any component of the vector $\mathbf{H}(x, y, z)$. Then, for each H , we have the scalar Helmholtz equation

$$-\Delta H - \omega^2 \tilde{\epsilon} \mu H = 0 \quad . \quad (2)$$

This equation may be regarded as a scalar approximation of the field description given by the full Maxwell's equations. The modes to be determined will come out of the separation ansatz

$$H(x, y, z) = u(x, y)e^{-ikz}$$

in terms of a lateral amplitude function $u(x, y)$ and a complex propagation constant k . With the imaginary part $\Im(k) = 0$ the propagation is loss-free, for $\Im(k) < 0$ the mode is damped, for $\Im(k) > 0$ it is amplified. The real part $\Re(k)$ represents the phase velocity and determines the lateral confinement of $u(x, y)$. If $\Re(k)$ becomes larger than some cut-off value k_c , we have $\lim_{(x,y) \rightarrow \infty} |u(x, y)| \neq 0$ and therefore that mode will not be confined to bounded region around the waveguide. For the physical problem under investigation, however, we need to know the modes with bounded support. This means, that we have to look for modes in the region $\Re(k) \leq k_c$, i. e. for the modes with lowest real parts.

Finally, inserting the above separation ansatz into (2) yields the eigenproblem for the example under consideration: determine functions $u(x, y)$ and complex numbers k such that

$$-\Delta u(x, y) - \omega^2 \tilde{\epsilon} \mu u(x, y) = -k^2 u(x, y) \quad .$$

For the subsequent investigation we slightly extend this example to the general *Helmholtz eigenproblem*: given a piecewise continuous, complex valued function $f(x, y)$, find eigenfunctions $u(x, y)$ and eigenvalues λ such that

$$\begin{aligned} -\Delta u(x, y) - f(x, y)u(x, y) &= \lambda u(x, y), & (x, y) \in \Omega \\ u(x, y) &= 0, & (x, y) \in \partial\Omega \end{aligned} \quad . \quad (3)$$

In view of a numerical treatment, this type of eigenvalue problems exhibits three main difficulties:

- The geometry and the material jumps of the optical semiconductor devices lead to multiscale ratios of up to 10^3 .
- The eigenvalue problem is nonselfadjoint, if losses or gain are included in the model - which is the realistic case.
- Clusters of neighboring eigenvalues may occur, mainly due to geometrical symmetries, and must be resolved (sometimes to a relative accuracy of the eigenvalues down to 10^{-6} or 10^{-8}).

3 Schur Decomposition of the Complex Helmholtz Operator

In general, the numerical discretization of (3) leads to a large algebraic eigenvalue problem. For the algebraic problem, canonical matrix decompositions like the Jordan decomposition and the Schur decomposition are used to construct numerical algorithms. The purpose of this section is to establish an appropriate decomposition for the continuous case.

The general approach to solving eigenproblems of the considered type is to determine invariant subspaces of small dimension. It is known from the perturbation analysis of matrices [12], that an invariant subspace, spanned by sensitive eigenvectors, may nevertheless be insensitive to perturbations in the given matrix, if the corresponding cluster of eigenvalues is separated. This insight suggests a simultaneous computation of eigensolutions.

For the representation of invariant subspaces we need suitable bases. It is natural to choose these bases as subsets of bases of the entire space. In the finite dimensional case there are two obvious choices.

The first is in terms of eigenvectors. For selfadjoint problems it is well known that the eigenvectors form an orthonormal basis of the underlying space. However, for nonselfadjoint problems this property can not be guaranteed. But from the Jordan canonical decomposition we know that the set of eigenvectors supplemented with possibly arising generalized eigenvectors is complete. This canonical form possesses an enormous meaning in theoretical analysis, e. g. stability analysis etc. Unfortunately, the numerical determination of this basis may be and often is ill-conditioned. The reason for this occurrence is that the set of diagonalizable matrices is dense in the set of all matrices, and hence small perturbations of a defective matrix may effectively destroy its Jordan form.

The alternative choice is based on the Schur canonical decomposition. Since this involves a unitary similarity transformation of a given matrix to an upper triangular matrix, the computation of the corresponding orthonormal basis is well-conditioned. Such a reduction is *always* possible and forms the foundation of many commonly used algorithms for solving the general eigenproblem. We conclude that the knowledge of the Schur vectors as an orthonormal basis related to a given matrix is an essential prerequisite for the construction of numerical algorithms.

We now turn to a discussion of the continuous problem (3). When passing from the finite to infinite dimensional case, two questions arise naturally. The first question concerns the structure of the spectrum. Since in the present case the region Ω and the function f under consideration are bounded and

Dirichlet boundary conditions are prescribed, we know that the spectrum is discrete. The second question to be studied is whether there exists a basis of (generalized) eigenfunctions or Schur functions or a combination of both (like the block diagonal decomposition in the algebraic case). In the selfadjoint case the minimax principle of COURANT shows the existence of an orthonormal basis of eigenfunctions. In the nonselfadjoint case, however, the structure is more complicated. It can be shown that any union of orthonormal bases of invariant subspaces forms a basis of the whole space. The resulting basis, however, need not to be orthonormal. For this reason, a careful analysis is included here.

In what follows, we will consider the eigenvalue problem (3) in its variational form. Let Ω be an open, bounded, and connected subset of \mathbb{R}^2 , and $f \in L^\infty(\Omega)$. Then problem (3) reads as follows: Determine *eigenfunctions* $u \in H_0^1(\Omega) \setminus \{0\}$ and *eigenvalues* $\lambda \in \mathbb{C}$, such that

$$a(v, u) = \lambda (v, u) \quad \forall v \in H_0^1(\Omega) \quad (4)$$

holds. The sesquilinear form $a(\cdot, \cdot)$ is defined by

$$a(v, u) = (\nabla v, \nabla u) - (v, fu) \quad , \quad (5)$$

and the inner product (\cdot, \cdot) is the usual L^2 product

$$(v, u) = \int_{\Omega} \overline{v(x, y)} u(x, y) \, d(x, y) \quad .$$

For *selfadjoint* eigenvalue problems, i. e. for real valued functions f , we have an equivalent formulation of the eigenproblem by means of the well-known COURANT minimax principle

$$\lambda_j = \min_{\substack{W_j \subset H_0^1(\Omega) \\ \dim W_j = j}} \max_{u \in W_j \setminus \{0\}} R(u) = R(u_j), \quad j = 1, 2, \dots, \quad (6)$$

in terms of the *Rayleigh quotient*

$$R(u) = \frac{a(u, u)}{(u, u)} \quad .$$

In this case the eigenfunctions are known to form an orthonormal basis of $L^2(\Omega)$.

For the *nonselfadjoint* case there exists a completeness result due to KATSNELSON [15], which we want to recall briefly here. For this purpose we will construct the natural representation operator of the sesquilinear form $a(\cdot, \cdot)$.

Consider the *grad* term in (5) first. From the representation theorem of FRIEDRICHS [22] we know that there exists a unique linear, selfadjoint, and positive operator $L : D_L \rightarrow L^2(\Omega)$ with domain D_L dense in $L^2(\Omega)$, such that the relation

$$(\nabla v, \nabla u) = (v, Lu) \quad \forall u \in D_L, v \in H_0^1(\Omega)$$

holds. Next, from the theorem of FRECHÉT-RIESZ we represent the second right hand term in (5) as

$$(v, fu) = (v, Mu) \quad \forall u, v \in L^2(\Omega) \quad .$$

The operator $M : L^2(\Omega) \rightarrow L^2(\Omega)$ is linear and continuous, since f is bounded. Hence the representation operator $A : D_A \rightarrow L^2(\Omega)$ of the sesquilinear form $a(\cdot, \cdot)$ is simply given by $A = L - M$ with domain $D_A = D_L$. In lieu of (4) we may therefore investigate the alternate eigenvalue problem

$$Au = \lambda u \quad ,$$

where $u \in D_A \setminus \{0\}$ and $\lambda \in \mathbb{C}$. Now we are ready to apply the basic

Theorem 1 (KATSNELSON [15]). *Let T be a closed operator in a Hilbert space H , L a positive selfadjoint operator in H with discrete spectrum and domain $D_L \subset\subset D_T$, and $A = L + T$. Let for some p , $0 < p \leq 1$, the following conditions be satisfied:*

1. *The operator $L^{\frac{p-1}{2}} T L^{\frac{p-1}{2}}$ is bounded.*
2. $\overline{\lim}_{n \rightarrow \infty} n \cdot \mu_n^{-p} < \infty$,

where $\mu_1 \leq \mu_2 \leq \dots$ is the sequence of all eigenvalues of the operator L . Then the spectrum of the operator A is discrete, and the set $\Lambda = \{\lambda_n\}_{n=1}^{\infty}$ of all eigenvalues of the operator A can be subdivided into finite subsets Λ_k , such that the system $\{S_k\}_{k=1}^{\infty}$ of spectral subspaces of the operator A which correspond to the subsets Λ_k forms a basis for the space H , which is equivalent to an orthogonal base.

We identify $p = 1$, $T = -M$ and $D_T = H = L^2(\Omega)$. The operator T is continuous with domain $L^2(\Omega)$ and hence closed and bounded. Moreover, L has a compact and selfadjoint inverse. From spectral theory [8] we thus have the discreteness of the spectrum of L^{-1} and hence of L . The domain D_L is compactly embedded in $L^2(\Omega)$, and the asymptotic behaviour of the eigenvalues of L is described by the following formula of COURANT AND HILBERT [5]:

$$\lim_{n \rightarrow \infty} \frac{n}{\mu_n} = \frac{|\Omega|}{4\pi} \quad ,$$

where $|\Omega|$ is the area of the bounded region Ω . Therefore, from Theorem 1 we know that any $v \in L^2(\Omega)$ can be uniquely expanded in a series of the form

$$v = \sum_{k=1}^{\infty} v_k \quad ,$$

where $v_k \in S_k$.

So far, we can represent any function from $L^2(\Omega)$ in terms of the invariant subspaces of the operator A . The relation between a basis of subspaces and a vector basis is established by the following

Lemma 2 (GOHBERG, KREĬN [11], P. 344). *If the sequence of subspaces $\{S_k\}_{k=1}^{\infty}$ is a basis of the space H equivalent to an orthogonal one, then any sequence $\{u_j\}_{j=1}^{\infty}$, obtained as the union of orthonormal bases of all the subspaces S_k , is a basis of the space H equivalent to an orthonormal one.*

Next, we consider the restriction A_k of A on the invariant subspace S_k . This mapping is an endomorphism that is a linear mapping from S_k into itself. The subsets Λ_k are given by $\Lambda_k = \{\lambda \in \sigma(A) : t_{k-1} < \Re(\lambda) \leq t_k\}$ in terms of a sequence $\{t_k\}_{k=1}^{\infty}$ with $t_k < t_{k+1}$, $t_0 = -\infty$ and $t_k \rightarrow \infty$. Since these subsets are all finite and every eigenvalue of A has finite multiplicity, the dimension $d_k = \dim(S_k)$ of S_k is finite. Hence we can represent A_k by some $(d_k \times d_k)$ -matrix. Via the *Schur decomposition* [12] of this matrix, we can find an orthonormal basis $\{u_{k,l}\}_{l=1}^{d_k}$ of S_k such that the equations

$$Au_{k,l} = \lambda_{k,l}u_{k,l} + \sum_{m=1}^{l-1} \tau_{k,ml}u_{k,m}, \quad l = 1, \dots, d_k,$$

and the inequalities $\Re(\lambda_{k,1}) \leq \dots \leq \Re(\lambda_{k,d_k})$ hold. Using Lemma 2, we see that the sequence

$$\{u_1, u_2, \dots\} = \{u_{1,1}, \dots, u_{1,d_1}, u_{2,1}, \dots, u_{2,d_2}, \dots\} \quad ,$$

obtained from the above determined bases $\{u_{k,l}\}$ of S_k by renumbering, is a basis of $L^2(\Omega)$. In a similar way, the corresponding eigenvalues are renumbered such that

$$\{\lambda_1, \lambda_2, \dots\} = \{\lambda_{1,1}, \dots, \lambda_{1,d_1}, \lambda_{2,1}, \dots, \lambda_{2,d_2}, \dots\}$$

and

$$\Re(\lambda_1) \leq \Re(\lambda_2) \leq \dots \rightarrow \infty \quad .$$

We thus arrive at the relation

$$Au_j = \lambda_j u_j + \sum_{k=k_j}^{j-1} \tau_{kj} u_k$$

for the basis $\{u_j\}_{j=1}^\infty$, where $1 \leq k_j \leq j$ and $k_j \leq k_{j+1}$.

Remark 1. Although the basis $\{u_j\}_{j=1}^\infty$ is the union of finite dimensional orthonormal bases, this basis itself is not necessarily orthonormal. The equivalence to an orthonormal basis $\{w_j\}_{j=1}^\infty$ means that there exists a continuous and bijective linear transformation $B : L^2(\Omega) \rightarrow L^2(\Omega)$ with $u_j = Bw_j$ for all $j \in \mathbb{N}$. The deviation of the basis $\{u_j\}_{j=1}^\infty$ from an orthonormal basis is measured by the condition number

$$\kappa = \|B\| \|B^{-1}\| \quad .$$

This quantity measures a characteristic spectral property of the operator A and does not describe the particular behaviour of certain eigensolutions.

Summarizing, we get for the variationally formulated problem the following theorem, which will serve as the starting point for our construction of a numerical algorithm.

Theorem 3. *Let the region $\Omega \subset \mathbb{R}^2$ be bounded and the function $f : \Omega \rightarrow \mathbb{C}$ be an element of the function space $L^\infty(\Omega)$. Then there exists a basis $\{u_j\}_{j=1}^\infty$ of $L^2(\Omega)$, such that the relation*

$$a(v, u_j) = \lambda_j (v, u_j) + \sum_{k=k_j}^{j-1} \tau_{kj} (v, u_k) \quad \forall v \in H_0^1(\Omega) \quad ,$$

with $1 \leq k_j \leq j$ and $k_j \leq k_{j+1}$, holds. For the eigenvalues λ_j we have the inequalities $\Re(\lambda_1) \leq \Re(\lambda_2) \leq \dots \rightarrow \infty$.

With these careful considerations, we are now perfectly legitimated to pose the continuous eigenproblem exactly like algebraic eigenproblems.

For selfadjoint problems, i. e. for real valued functions f , the basis $\{u_j\}_{j=1}^\infty$ is orthonormal. It consists only of eigenfunctions, i. e. all τ_{kj} vanish. In the nonselfadjoint case we will refer to the functions u_j as *Schur functions*. If we do not distinguish between these two cases, the functions u_j are called eigensolutions. In contrast to the finite dimensional nonselfadjoint case, where the Schur decomposition is based on a *totally* orthonormal basis, in the continuous case, we obtain only a *partially* orthonormal system.

Finally, we look at the *sensitivity* of the eigensolutions with respect to *perturbations in f* . Using Theorem 3, we can carry out a perturbation analysis just as for matrices [12]. As in the finite dimensional case, the sensitivity of eigensolutions is dependent on one hand upon the *spectral gap* of the interesting eigenvalues from the remaining part of the spectrum, and on the other hand upon the condition of the underlying basis $\{u_j\}_{j=1}^{\infty}$ of $L^2(\Omega)$. *As in the finite dimensional case, the invariant subspace spanned by sensitive eigensolutions can be insensitive, if only the corresponding eigenvalues are sufficiently separated from the rest of the spectrum.* We will therefore attack the eigenproblem by the computation of invariant subspaces, that is by *simultaneous* computation of several eigensolutions corresponding to *eigenvalue clusters*.

4 Adaptive Nonlinear Multigrid FEM

From now on we will consider the eigenproblem in the following variational form: Determine functions $u_j \in H_0^1(\Omega) \setminus \{0\}$ and values $\tau_{kj} \in \mathbb{C}$ satisfying

$$a(v, u_j) = \sum_{k=1}^j \tau_{kj} (v, u_k) \quad \forall v \in H_0^1(\Omega) \quad , \quad (7)$$

where $\tau_{jj} = \lambda_j$ and $j = 1, \dots, q$ (q is the number of desired eigensolutions). As discussed in Section 2, we are interested in those eigenvalues with lowest real parts. The subspace spanned by the corresponding eigensolutions may be viewed as a subset of the invariant subspace S_1 (see Theorem 1). Hence the functions u_j form an orthonormal system in $L^2(\Omega)$.

Discretization of (7) by finite elements leads to the generalized matrix problem

$$AU = BUT \quad , \quad (8)$$

wherein the system matrix A and the mass matrix B are sparse $(N \times N)$ -matrices defined as

$$A = (a(v_m, v_l))_{m,l=1,\dots,N} \quad \text{and} \quad B = ((v_m, v_l))_{m,l=1,\dots,N} \quad .$$

The functions v_l are the basis functions of the finite element space $V_h \subset H_0^1(\Omega)$ with $N = \dim(V_h)$, the subscript h is a meshsize parameter indicating the underlying triangulation of the region Ω . By definition, B is selfadjoint and positive definite. The matrices U and T are the matrices of unknowns. The matrix U is a full $(N \times q)$ -matrix consisting of the coefficients of the discrete eigensolutions $u_{j,h} \in V_h$ with respect to the basis functions v_l , whereas the

matrix T is an upper triangular $(q \times q)$ -matrix formed by the approximate values $\tau_{kj,h}$.

Upon using the Cholesky factorization $B = R^*R$, we may rewrite problem (8) in standard form

$$CX = XT \quad , \quad (9)$$

where $C = R^{-*}AR^{-1}$ and $X = RU$. From the Schur decomposition of matrices we know that there *always* exists a unitary $(N \times q)$ -matrix X , such that (9) holds and the diagonal of T consists of the q desired approximate eigenvalues $\lambda_{j,h}$ with lowest real parts. We see that the functions $u_{j,h}$, formed by the coefficients from the solution $U = R^{-1}X$ of equation (8), are an orthonormal system in V_h with respect to the scalar product in $L^2(\Omega)$.

After these preliminaries, we now turn to the description of multigrid methods for the discrete problem (8). Any of these methods needs a hierarchy of meshes, say a sequence of triangulations. In view of the difficulties arising in the problem class (as described at the end of Section 2), we construct a sequence of meshes by *adaptive* mesh refinement. For convenience, we will restrict our attention to conforming elements only, which means

$$V_{h_0} \subset V_{h_1} \subset \dots \subset V_{h_{i_{\max}}} \subset H_0^1(\Omega) \quad .$$

4.1 Selfadjoint case

For the convenience of the reader we start with a brief outline of our German paper [6], which treats the selfadjoint case only. In this case, the matrix T reduces to a real diagonal matrix Λ . Without loss of generality, we can choose all eigenfunctions to be real valued. Thus we have to solve

$$AU = BUA \quad , \quad U^T BU = I \quad ,$$

where A, B, U are real and Λ is diagonal.

First, we want to describe a generalization of the Rayleigh quotient multigrid minimization of MANDEL, MCCORMICK [19, 20] to invariant subspace computation. As all multigrid methods, this method consists of two parts, the smoothing algorithm and the coarse grid correction procedure. For both parts, the discrete analogue of the Courant minimax principle (6) provides the foundation. The task is to find the q minimal stationary points of the Rayleigh quotient in a subspace of \mathbb{R}^N , spanned by vectors u_1, \dots, u_q and vectors p_1, \dots, p_r . This is equivalent to the computation of the q lowest eigenvalues of the projected problem

$$(V^T AV)Q = (V^T BV)Q\Lambda \quad , \quad Q^T (V^T BV)Q = I \quad (10)$$

with $V = (u_1 \cdots u_q \ p_1 \cdots p_r)$. Here the vectors u_j are eigenvector approximations whereas the vectors p_k denote search directions. In the smoothing process the vectors p_k are formed in our case by generalized conjugate gradients corresponding to the approximate eigenvectors. In the coarse grid correction procedure the vectors p_k come from the coordinate representation of the coarse grid basis functions with respect to the fine grid basis functions, which form the prolongation matrix P from the coarse to the fine grid.

As for the smoothing algorithm we apply the simultaneous conjugate gradient method of DÖHLER [7]. The significant feature of this method is the simultaneous determination of the conjugate gradients by solving a Sylvester equation (in contrast to the procedures suggested e. g. by LONGSINE, MCCORMICK [18] or SARTORETTO ET AL. [25], where the search directions are computed sequentially). For reasons of clarity, we omit iteration subscripts.

Algorithm 1. Smoother/Selfadjoint Eigenproblem

- Initialization:

- * given a $(N \times q)$ -matrix U with

$$U^T B U = I$$

$$U^T A U = \Lambda_U = \text{diag}(\lambda_1 \cdots \lambda_q)$$

- * set $P = G = -(AU - BU\Lambda_U)$

- Iteration:

- * set $V = (U \ P)$

- * solve (10) with eigenvalue order $\lambda_1 \leq \dots \leq \lambda_q < \lambda_{q+1} \leq \dots \leq \lambda_{2q}$

- * set $(U \ P) = VQ$

- * compute $G = -(AU - BU\Lambda_U)$

- * determine X from

$$X\Lambda_U - \Lambda_P X = P^T(AG - BG\Lambda_U)$$

$$\text{with } \Lambda_P = P^T A P = \text{diag}(\lambda_{q+1} \cdots \lambda_{2q})$$

- * set $P = G + PX$

A theoretical convergence analysis of this method is a recent research topic, see e. g. KNYAZEV [16]. Numerical experience, however, shows that the convergence rates depend not only on the spectral gap, which is unavoidable,

but also on the meshsize h of the underlying triangulation of the region Ω , which is certainly undesirable. One idea to overcome the mesh dependence is to apply *linear preconditioning*, i. e. to replace the gradient G in Algorithm 1 by

$$G = -C^{-1}(AU - BU\Lambda_U) \quad ,$$

where C^{-1} is an approximate inverse of the (possibly shifted) system matrix $A(+\mu B)$. For an exposition of this method, especially in conjunction with linear multigrid methods, see for example JUNG ET AL. [14], BRAMBLE ET AL. [2] and LEINEN ET AL. [17]. An alternative approach is the nonlinear multigrid method presented in this subsection.

The final result of [6] is, that the computation of the coarse grid corrections in the nonlinear multigrid method can be performed also with the help of an eigenvalue problem of the form (10). As mentioned above, the vectors p_k are the columns of the prolongation matrix P which describes the transition between the coarse and the fine grid. If the dimension of the finite element space corresponding to the coarse grid is equal to n , then the coarse grid correction eigenvalue problem is of dimension $q+n \ll N$. Since this correction problem is of the same type as the original problem, we can solve it using the same fine grid-coarse grid scheme. The resulting multigrid V-cycle is then given in

Algorithm 2. Multigrid V-cycle/Selfadjoint Eigenproblem
 $[U_l, \Lambda_l] = \text{MGM}(A_l, B_l, U_l, \Lambda_l, l)$

1. presmoothing using Algorithm 1: $U_l \rightarrow \tilde{U}_l, \Lambda_l \rightarrow \tilde{\Lambda}_l$
2. coarse grid correction: $\tilde{U}_l \rightarrow \hat{U}_l, \tilde{\Lambda}_l \rightarrow \hat{\Lambda}_l$
 - compute $A_{l-1} = V_l^T A_l V_l$ and $B_{l-1} = V_l^T B_l V_l$, where in case
 - * $l = l_{\max}$: $V_l = \begin{pmatrix} \tilde{U}_l & P_l \end{pmatrix}$
 - * $l < l_{\max}$: $V_l = \begin{pmatrix} \tilde{U}_l & 0 \\ & P_l \end{pmatrix}$
 - if
 - * $l > 1$: $[U_{l-1}, \Lambda_{l-1}] = \text{MGM}(A_{l-1}, B_{l-1}, \begin{pmatrix} I \\ 0 \end{pmatrix}, \tilde{\Lambda}_l, l-1)$
 - * $l = 1$: solve

$$\begin{aligned} A_0 U_0 &= B_0 U_0 \Lambda_0 \\ U_0^T B_0 U_0 &= I \end{aligned}$$

- set $\widehat{U}_l = V_l U_{l-1}$, $\widehat{\Lambda}_l = \Lambda_{l-1}$

3. postsmoothing using Algorithm 1: $\widehat{U}_l \rightarrow U_l$, $\widehat{\Lambda}_l \rightarrow \Lambda_l$

The matrices A_l and B_l are the (augmented) system and mass matrix corresponding to the triangulation with meshsize h_l . The matrix U_l (with q columns) and the diagonal matrix Λ_l are the matrices of unknowns. For $l < l_{\max}$, the matrices U_l are initialized, such that each current eigenvector approximation gets the coefficient 1, whereas each coarse grid search direction gets the coefficient 0. The matrix P_l is the prolongation matrix for the interpolation between the meshes with sizes h_l and h_{l-1} . The number of pre- and postsmoothing steps, i. e. the number of iterations in Algorithm 1, is chosen empirically, say $\nu \in \{1, 2, 3\}$. Summarizing, the multigrid procedure is then given as

Algorithm 3. Multigrid Procedure/Selfadjoint Eigenproblem

- Initialization:
 - * given a $(N \times q)$ -matrix U with $U^T B U = I$, $U^T A U = \Lambda$
- Iteration:
 - * while $\|AU - BUA\|_{\text{diag}(B)^{-1}} > \text{tol}$: $[U, \Lambda] = \text{MGM}(A, B, U, \Lambda, l_{\max})$

An important feature of this multigrid method is its *monotonicity*. To see this note that the matrices A_{l-1} and B_{l-1} can be expressed as

$$A_{l-1} = W_l^T A W_l \quad , \quad B_{l-1} = W_l^T B W_l$$

with $W_l = V_{l_{\max}} V_{l_{\max}-1} \dots V_{l+1} V_l$. This means, that in every step and at every stage of the above algorithm we solve a projected eigenvalue problem of the form (10). As shown in DÖHLER [7], the matrix $U = W_l Q_{l-1}$ formed by the solution of this problem gives the minimal value of the functional

$$F(U) = \text{trace}((U^T B U)^{-1} (U^T A U)) \quad (11)$$

with respect to all possible choices $U' = W_l Q'_{l-1}$. Hence the sequence of functional values decreases monotonically in every step and at every stage of the algorithm. Especially, the algorithm for a single vector ($q = 1$) recovers the monotone Rayleigh quotient multigrid minimization of MANDEL, MCCORMICK [19, 20].

Since the functional (11) is bounded from below, the sequence is *always* convergent. This property is the reason for the numerical robustness of the method.

First optimal complexity results for a variant of the described method (with a different smoothing procedure) were given by MCCORMICK [21] and CAI ET AL. [3]. A simple, but illustrative numerical comparison (1D) between this method and the multigrid method of HACKBUSCH [13] in the context of adaptive meshes may be found in [6], which shows that the above method is more robust. A proof of optimality, which is different from [3], has been suggested by CHAN, SHARAPOV [4] in connection with domain decomposition methods.

Remark 2. Numerical experiments show that the convergence speeds up significantly, if we replace the simple gradient G in Algorithm 1 by a modified gradient with Jacobi preconditioning. This means, that the matrix G is now computed by

$$\text{diag}(A)G - \text{diag}(B)G\Lambda_U = -(AU - BU\Lambda_U) \quad .$$

This choice of gradient corresponds to a basis transformation, adapted to each iteration vector, in the underlying finite element space. In correspondence with Algorithm 2 we use this formula for $l < l_{\max}$ only for the computation of rows with index greater than q . The rows of G with index less or equal q are set to zero.

4.2 Nonselfadjoint case

We are now ready to construct a multigrid method for the nonselfadjoint case. Starting point is our basic formulation (8) for the computation of an invariant subspace. From the analysis in Section 3 we know that we can represent this subspace in terms of an orthonormal basis, i. e. we have to solve the problem

$$AU = BUT \quad , \quad U^*BU = I \quad .$$

The structure of this general problem is the same as for the special selfadjoint case, except that Λ is now replaced by T . Forced by this similarity, we expect that the principal structure of the selfadjoint algorithm can be maintained in the nonselfadjoint case.

The essential idea is to replace the projected eigenvalue problems (10) of the selfadjoint algorithm by projected *Schur problems* of the form

$$(V^*AV)Q = (V^*BV)QT \quad , \quad Q^*(V^*BV)Q = I \quad . \quad (12)$$

The matrix V here consists of approximate Schur vectors u_j and additional vectors p_k which are chosen analogously to the selfadjoint case.

The smoothing algorithm for the nonselfadjoint multigrid method then reads:

Algorithm 4. Smoother/Nonselfadjoint Eigenproblem

- Initialization:
 - * given a $(N \times q)$ -matrix U with $U^*BU = I$, $U^*AU = T_U$, where T_U is upper triangular with eigenvalues $\Re(\lambda_1) \leq \dots \leq \Re(\lambda_q)$
 - * set $P = R = -(AU - BUT_U)$
- Iteration:
 - * set $V = \begin{pmatrix} U & P \end{pmatrix}$
 - * solve (12) with $\Re(\lambda_1) \leq \dots \leq \Re(\lambda_q) < \Re(\lambda_{q+1}) \leq \dots \leq \Re(\lambda_{2q})$
 - * set $\begin{pmatrix} U & P \end{pmatrix} = VQ$
 - * compute $R = -(AU - BUT_U)$
 - * determine X from

$$XT_U - T_P X = P^*(AR - BRT_U)$$

with $T_P = P^*AP$ upper triangular

- * set $P = R + PX$

The sorting of the eigenvalues in each iteration step needs a careful consideration, since we have to sort the diagonal elements of an upper triangular matrix. Our implementation applies an algorithm given by RUHE [23]. Since the matrices T_U and T_P are upper triangular with disjoint spectra, the solution of the Sylvester equation for the determination of X is easy.

Remark 3. Note that this algorithm is not based on a minimization principle. Nevertheless, numerical experiments support the expectation that it has also some smoothing property. In fact, the method may be interpreted as a kind of one step *block Arnoldi algorithm*.

The associated multigrid V-cycle may be derived along the lines of 4.1, merely replacing the eigenvalue problems in Algorithm 2 by appropriate Schur problems.

Algorithm 5. Multigrid V-cycle/Nonselfadjoint Eigenproblem

$[U_l, T_l] = \text{MGM}(A_l, B_l, U_l, T_l, l)$

1. presmoothing using Algorithm 4: $U_l \rightarrow \tilde{U}_l, T_l \rightarrow \tilde{T}_l$
2. coarse grid correction: $\tilde{U}_l \rightarrow \hat{U}_l, \tilde{T}_l \rightarrow \hat{T}_l$

- compute $A_{l-1} = V_l^* A_l V_l$ and $B_{l-1} = V_l^* B_l V_l$, where in case
 - * $l = l_{\max}$: $V_l = \begin{pmatrix} \tilde{U}_l & P_l \end{pmatrix}$
 - * $l < l_{\max}$: $V_l = \begin{pmatrix} \tilde{U}_l & 0 \\ & P_l \end{pmatrix}$
- if
 - * $l > 1$: $[U_{l-1}, T_{l-1}] = \text{MGM}(A_{l-1}, B_{l-1}, \begin{pmatrix} I \\ 0 \end{pmatrix}, \tilde{T}_l, l-1)$
 - * $l = 1$: solve

$$\begin{aligned} A_0 U_0 &= B_0 U_0 T_0 \\ U_0^* B_0 U_0 &= I \end{aligned}$$

- set $\hat{U}_l = V_l U_{l-1}$, $\hat{T}_l = T_{l-1}$

3. postsmoothing using Algorithm 4: $\hat{U}_l \rightarrow U_l$, $\hat{T}_l \rightarrow T_l$

The meaning of the arising matrices is the same as in Algorithm 2. Finally, we end up with the following multigrid procedure:

Algorithm 6. Multigrid Procedure/Nonselfadjoint Eigenproblem

- Initialization:
 - * given a $(N \times q)$ -matrix U with $U^* B U = I$, $U^* A U = T$
- Iteration:
 - * while $\|AU - BUT\|_{\text{diag}(B)^{-1}} > \text{tol}$: $[U, T] = \text{MGM}(A, B, U, T, l_{\max})$

Since we can write the matrices A_{l-1} and B_{l-1} according to

$$A_{l-1} = W_l^* A W_l \quad , \quad B_{l-1} = W_l^* B W_l \quad ,$$

where $W_l = V_{l_{\max}} V_{l_{\max}-1} \dots V_{l+1} V_l$, this method is an *orthogonal* projection method. In the case of a selfadjoint problem it reduces to the algorithm of 4.1. The theoretical investigation of this method and, in particular, any proof of optimal complexity is an open topic for future research.

Remark 4. As for selfadjoint problems we observe a considerable improvement of the convergence rates, if we replace the residue matrix R in Algorithm 4 by the modified matrix determined by

$$\text{diag}(A)R - \text{diag}(B)RT_U = -(AU - BUT_U) \quad .$$

Again, for $l < l_{\max}$, only the rows with index greater than q are considered.

5 Numerical Results

For the illustration of the performance of our multigrid procedure (Algorithm 6) we return to the integrated optical structure shown in Figure 2. The permittivity is complex valued and parameter dependent in the Multi Quantum Well (MQW) layers (the narrow stripes in the zoom of Figure 2), complex valued in the metal layer, and real valued otherwise. The exact parameters of the structure are technologically relevant and therefore not documented here.

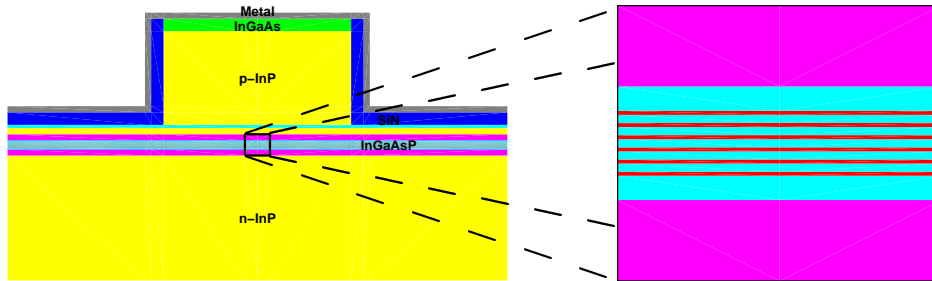


Figure 2: Cross section of an integrated optical structure with zoom.

In a first experiment, we were interested in the two eigenvalues with lowest real part and their corresponding Schur functions. A difficulty of this problem was to find a proper starting triangulation. Since we must resolve the very thin MQW layers with normally sized triangles, the coarsest mesh (shown in Figure 3 a) consists of 2515 nodes and 4956 triangles. For the construction of

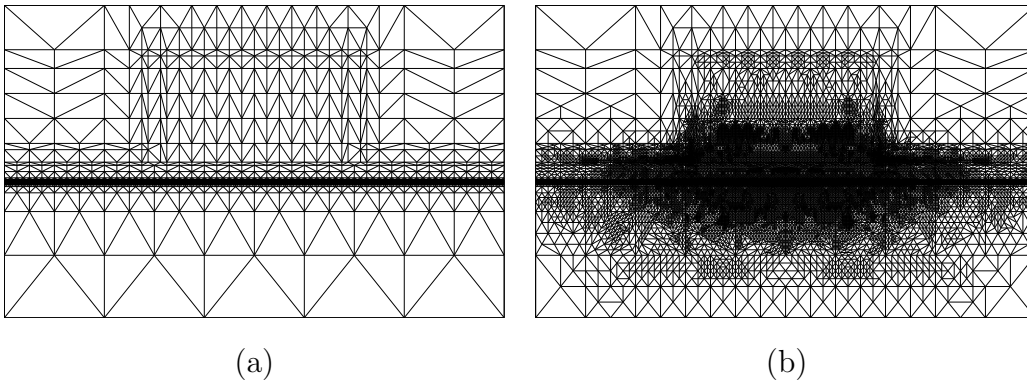


Figure 3: Starting and final triangulation.

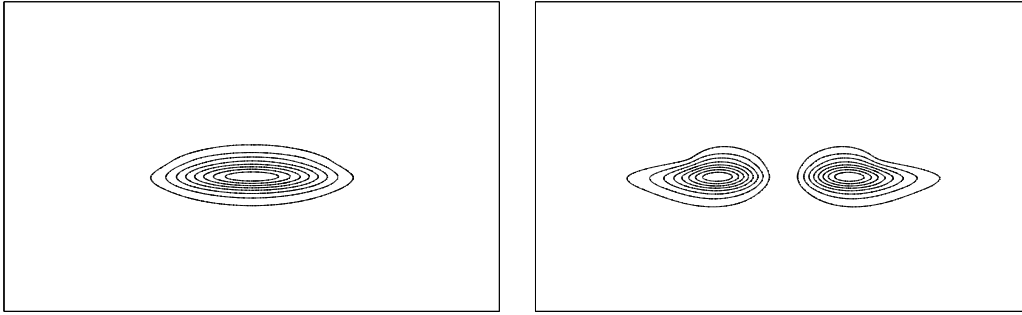


Figure 4: Contour plots of $|u_1|^2$ and $|u_2|^2$.

the hierarchy of meshes we use a nested iteration technique in connection with a usual error indicator. The final triangulation with 15246 nodes and 30396 triangles reached after 6 refinements is given in Figure 3 b. As suggested in [1], the numerical experiments have been performed with a *common* tolerance $\text{tol} = 10^{-3}$ for all multigrid levels. The whole computation with a MATLAB program took 16 minutes on a SUN ULTRA 1 workstation. The coarsest grid problems were solved with the usual Block Arnoldi procedure (see e. g. SAAD [24]). Contour plots for the resulting Schur functions on the final mesh are represented in Figure 4. The convergence history of the full multigrid run is given in Table 1.

Grid	1	2	3	4	5	6
Inner points	2564	2888	3987	5536	9422	15152
MG Iterations	3	3	4	4	4	4

Table 1: Number of inner points and number of multigrid iterations per grid.

In a second experiment, we carried out a parameter study to demonstrate the dependence of the eigenvalues on the imaginary part of the permittivity in the MQW layers. We computed eigensolutions for the parameter values $\alpha = 0, 0.25, 0.5, 0.75, 1$ corresponding to the four eigenvalues with lowest real part - see Figure 5. The two lowest eigenvalues from the above computation are marked with arrows. This type of diagram is of technological interest.

Acknowledgment. The authors wish to thank Dr. Reinhard März from Siemens AG, Corporate Research and Development, Munich for stimulating

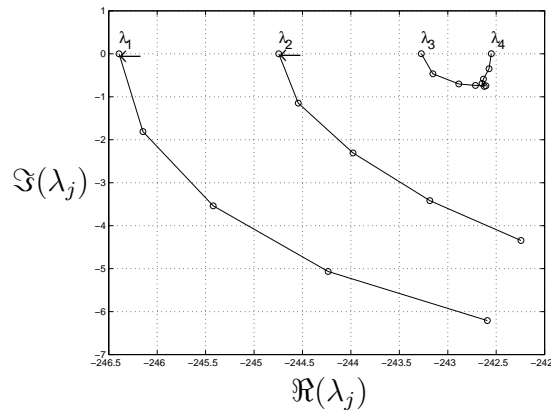


Figure 5: Dependence of the eigenvalues on the imaginary part of the permittivity in the Multi Quantum Well layers.

discussions and a fruitful cooperation. Moreover, they gratefully acknowledge helpful discussions on the functional analytic aspects of Schur decomposition by Dirk Werner, Free University of Berlin, and David E. Edmunds, University of Sussex at Brighton.

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