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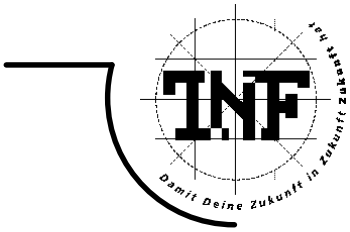

Eigenvalue Problems in SAW-Filter Simulations

Diplomarbeit

zur Erlangung des akademischen Grades

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Technische Mathematik

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Betreuung:

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For my parents

Abstract

This diploma thesis is concerned to the development of numerical solution methods in calculating so-called "dispersion diagrams" of periodic surface acoustic wave (SAW) filter structures. These piezoelectric devices are used in telecommunications for frequency filtering.
The mathematical problem is governed by two main points, the underlying periodic structure and the indefinite coupled field problem due to the properties of the used piezoelectric materials. Floquet-Bloch theory allows to restrict the infinite periodic computation domain to one reference cell by introducing quasi-periodic boundary conditions. Due to the Bloch-ansatz the dispersion context between "excitation frequency" and the "propagation constants" of the surface acoustic wave is described by parameter depending eigenvalue problems.
Three different solution approaches are developed for gaining these non-hermitian eigenvalue problems of generalized linear or quadratic form. Expanding the solution methods of periodic structures to the piezoelectric coupled field equations has the consequence that the eigenvalue problems get indefinite and worse-conditioned, i.e. special scaling methods, which ensure accurate numerical results, are required. A comprehensive collection of abstract theory and numerical solution methods for the occuring algebraic eigenvalue problems is provided.
Three different solvers for the numerical simulation of the dispersion context are developed and implemented. The used eigenvalue solver is concerned with the direct QZ-Method or the iterative Implicitly Restarted Arnoldi-Method, respectively.
The influence of periodic perturbations in the computation geometry is shown in numerical experiment for a pure mechanical model problem. Simulation results for the dispersion context of simplified periodic structures related to real-life TV- and GSM-filters are presented.

Zusammenfassung

Ziel der vorliegenden Diplomarbeit ist die Entwicklung numerischer Lösungsmethoden zur Berechnung sogenannter "Dispersionsdiagramme" von periodischen akustischen Oberfächenwellenfilter-Strukturen (SAW-Filter). Diese piezoelektrischen Bauteile werden in der Telekommunikation als Frequenzfilter eingesetzt.
Das dazugehörige mathematische Modell wird durch folgende zwei Hauptprobleme bestimmt, der Periodizität der zugrundeliegenden Geometrie und den gekoppelten Feldgleichungen zur Beschreibung der piezoelektrischen Eigenschaften des verwendeten Materials. Mit Hilfe der Floquet-Bloch-Theorie und Einführung quasi-periodischer Randbedingungen kann das ursprünglich unendlich (periodisch) angenommene Berechnungsgebiet auf eine Referenzzelle eingeschränkt werden, d.h. die Gleichungen müssen unter Erfüllung der speziellen Randbedingungen nur noch auf einer Periode gelöst werden. Die gesuchte Dispersionsbeziehung, die den funktionalen Zusammenhang zwischen Änregungsfrequenzünd Äusbreitungskonstanten"beschreibt, wird als Parameter-abhängiges Eigenwertproblem formuliert.
Es werden drei verschiedene Lösungsmethoden, die den Dispersionskontext beschreiben und auf nicht-hermitesche Eigenwertprobleme verallgemeinerter linearer beziehungsweise quadratischer Form führen, entwickelt. Nach Diskretisierung mittels der Methode Eine Erweiterung der vorgestellten Methoden auf piezoelektrische Feldgleichungen hat zur Konsequenz, dass die resultierenden Eigenwertproblem indefinit und schlecht-konditioniert werden. Letzteres erfordert spezielle Skalierungsalgorithmen, um numerisch zuverlässige Ergebnisse zu erhalten. Eine Zusammenstellung der abstrakten Theorie und der numerischen Lösung nicht-hermitescher algebraischer Eigenwertprobleme wird präsentiert und zur Lösung der modellierten Probleme angewendet und erweitert.
Drei alternative Löser werden entickelt und implementiert, wobei die auftretenden Eigenwertprobleme unter Verwendung der direkten QZ-Methode beziehungsweise der iterativen Implicit-Restarted-Arnoldi-Methode gelöst werden.
Der Einfluss periodischer Störungen des Material auf die Dispersionsbeziehung wird im numerischen Experiment anhand eines rein mechanisches Problems dargestellt. Abschliessend werden Dispersionsdiagramme von vereinfachten periodischen Strukturen, unter Verwendung der Daten von praktisch verwendeten TV-Filtern und GSM-Filtern, simuliert.

Acknowledgement

I want to express my thanks to Prof. Dr. Ulrich Langer for giving me the chance to write this thesis and for organizing some work shops about the treated problem.

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I want to thank Dipl. Ing. Manfred Hofer (University of Erlangen), who is writing his doctor thesis on the numerical simulation of SAW structures, for the collaborative and productive cooperation. I thank him for the patience of answering all the arising questions on the technical nature of the problem and for his implementational work.

I want to acknowledge EPCOS AG, Munich, for giving me the chance to work on a mathematically very interesting problem coming from applications and for their financial support. I thank Dr. Günter Kovacs for his support.

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Contents

List of Notations

Ω	domain in $\mathbb{R}^2$
Γ	$= \partial\Omega$, the boundary of a domain Ω in $\mathbb{R}^d$
Γ_D	part of boundary Γ according to Dirichlet conditions
Γ_N	part of boundary Γ according to Neumann conditions
$L_2(\Omega)$	space of over Ω quadratic-integrable functions
$H^m(\Omega)$	Sobolev-space of L_2-functions with quadratic-integrable derivations up to order m
$\|.\|_1$	$= \|.\|_{H^1(\Omega)}$ Sobolev-norm of order 1
$C(\Omega, \mathbb{C}^d)$	space of in Ω continuous functions mapping in $\mathbb{C}^d$
$C^k(\Omega, \mathbb{C}^d)$	space of in Ω k-times continuously differentiable functions mapping in $\mathbb{C}^d$
u_{tt}	$= \frac{d^2u}{dt^2}$
u_x	$= \frac{du}{dx}$
$\Re(z)$	real-part of a complex number $z \in \mathbb{C}$
$\Im(z)$	imaginary-part of a complex number $z \in \mathbb{C}$
ϵ_M	machine precision
	for a matrix A:
A^T	matrix transpose
A^*	conjugate transpose of A
A^{-1}	matrix inverse
A^{-T}	inverse of A^T
$Im(A)$	the image/range of the matrix A
$\mathcal{N}(A)$	the nullspace/kernel of the matrix A
$rk(A)$	the rank of the matrix A
$\sigma(A)$	the spectrum of A

Used Acronyms

SAW	surface acoustic wave
PBC	periodic boundary condition
ABC	absorbing boundary condition
EP	eigenvalue problem
EVP	eigenvalue problem
SC	Schur-Complement
INM-Method	Inner-Node-Matrix-Method (defined in Chapter 4)

Chapter 1

Introduction

This thesis deals with mathematical modeling and numerical simulation of periodic surface acoustic wave filters (briefly SAW-filters) and results in the computation of so-called "dispersion diagrams", which plays an important role in the telecommunication industry.
The principle of surface acoustic wave filters is based on the physical properties of piezoelelctric materials. The direct piezoelectric effect states that a mechanical deformation of a piezoelectric substrate evokes an electric field, which can be measured by charges on the surface. It always appears in combination with the converse effect, i.e. if a piezoelectric material is exposed to an electric field, the material shrinks or stretches. This implies that applying an electric signal on a piezoelectric substrate yields a mechanical (acoustic) wave. Due to the direct piezoelectric effect, this wave is always accompanied by an electric field. The main components of a SAW filter are a piezoelectric substrate and an input and an output interdigital transducer (IDT). An IDT is a comb of electrodes which is evaporated on the surface of the piezoelectric material. It is used for sending and receiving electric signals. If an electric field is applied at the input IDT, an acoustic wave is evoked on the surface of the material due to the piezoelectric effect. We are interested in waves which propagates along the surface. If such a wave, which is always accompanied by an electric field due to the direct piezoelectric effect, reaches the output IDT, the changing electric field evokes surface charges at the electrodes, i.e. an electric signal can be received.
The propagating surface wave is characterized by the frequency of the input signal, by the geometrical arrangements of the electrodes and by the material parameters of the piezoelectric substrate and electrodes. We will show that due to the underlying geometry no surface wave can propagate at special frequency intervals. Therefore these frequencies are missing in the output signal and the device can be used for frequency filtering. The frequency domain is parted into pass-bands, i.e. frequencies which get trough the piezoelectric device, and stop-bands, i.e. frequencies which get filtered out. For given geometry and material parameters the context between propagating/attenuated acoustic waves and the frequency can be read off so called "dispersion diagrams".

In this thesis we focus on surface acoustic wave devices used for frequency filtering in wireless communications, e.g. standard components in TV-sets and cellular phones. But one has to mention that there are many other application fields of SAW-devices as in radar and sensor technology and non-destructive evaluation.
We specialize on periodic SAW-filters, i.e. each IDT consists of some hundreds or even some thousands of electrodes, which are arranged periodically.
We assume time-harmonic excitation with the frequency $\frac{\omega}{2\pi}$, hence all field distributions are time-harmonic

$$f(x,t) = f(x)e^{i\omega t}. \tag{1.1}$$

The periodical arrangement of the electrodes implies that the mechanical field and the electric potential are *quasi-periodic* in space, i.e. they are of the form

$$f(x) = f_p(x)e^{(\alpha+i\beta)x}, \tag{1.2}$$

where p is the periodicity of the material and $f_p(.)$ denotes a p-periodic function. This means that all field distributions can be described by the frequency, a p-periodic function $f_p(.)$ and a complex propagation constant $\alpha + i\beta$. In this formulation α reflects the damping of the amplitude per period (electrode) and β the phase shift per period.
The graph presenting the functional context between the excitation frequency and the propagation constant is called the diagram of dispersion. This context is very important in SAW-filter design and its computation is the task of this thesis.

A fundamental and recommendable introduction to acoustic field problems, various (surface) wave modes and piezoelectricity is provided by Auld in [4] and [5]. The numerical solution of piezoelectric systems via the finite element method is treated by Lerch in [27]. An overview of the historical development of SAW-devices is given in [29]. The principles of periodic SAW-devices are treated by some IEEE papers like [17], but it has to be mentioned that in most papers damping effects ($\alpha \neq 0$) are not considered.

The mathematical justification for the quasi-periodic field distribution (1.2) is given by Floquet-Bloch theory, which analyze the spectral properties of ordinary and partial differential operators in periodic structures. This theory was developed for solving special problems in quantum mechanics, where one deals with periodic Schrödinger operators, by Bloch and for ordinary differential equations by Floquet. A description by physicists can be found in Madelung [28] and in Ashcroft and Mehrmin [3]. A functional analytic consideration is provided by Simon and Reed [30]. The generalization to partial differential equations with periodic coefficients is done by Bensoussan,Lions and Papanicolaou in [9] for real and elliptic problems and by Kuchment [19], who applied the theory for scalar equations on photonic and acoustic band-gap devices in [6].
Bloch-Floquet theory implies that the solution on periodic structures can be decomposited in quasi-periodic functions so-called Bloch waves. Therefore the problem can be restricted

to the unit-cell, i.e. the domain including one electrode. Repeating this unit-cell one gets the original geometry. In order to describe the original periodic system, appropriate quasi-periodic boundary conditions have to be established.
The one cell problem turns out to be a coupled-field parameter-depending (on propagation constant or frequency) eigenvalue problem, which we want to solve numerically by the method of finite elements. We introduce a detailed stepwise mathematical modeling for the problem of periodic structures, i.e. formulating appropriate boundary conditions and according discretization methods. We start with a Helmholtz-type problem and establish three different solution methods for computing the dispersion context. All these methods result in non-hermitian eigenvalue problems of linear or quadratic form. Applying the established methods to periodic structures on piezoelectric problems, is formally equivalent to the Helmholtz-model case, but the matrices get indefinite and worse conditioned due to piezoelectric properties, which requires special numerical treatment.
Mathematical modeling results in two reasonable variants of frequency-depending eigenvalue problems, one of quadratic form and the other one of generalized linear form. This requires special theory and numerics of algebraic eigenvalue problems.
An overview of and motivation for solving eigenvalue problems is provided in [37]. In [8] a recommendable collection of state-of-the-art direct and iterative methods for large-scale eigenvalue problems is given, the book includes description of improvement tools and implementational details. Tisseur [36] specializes on quadratic eigenvalue problems and Lehouqh et al. [23] and Sorensen [35] on Arnoldi and Implicit Restarted Arnoldi methods. Mehrmann provides a collection of structure-preserving methods in [11].
The stated eigenvalue problems are solved numerically by using the open-source software packages Lapack [2] (direct method) and Arpack [13] (iterative Implicite Restarted Arnoldi method).

On the tasks of this thesis
The conceptual formulation of this thesis is based on a part of the doctor thesis on Finite-Element calculations of SAW-structures [14] (to appear) by Manfred Hofer , Department of Sensor Technology at the University of Erlangen. We cooperate in a joint project on SAW filters. Two conference papers [16], [15] were published by M. Hofer et al. during the work on this problem. (co-authorship)
The main tasks of this thesis consist in the following points:

1. Due to the quasi-periodical field distribution one can restrict the computation domain to one cell. This requires to introduce appropriate quasi-periodical boundary conditions.

2. In most common models only pure imaginary propagation constants are considered, i.e. $\alpha = 0$ in (1.2), which has the effect that one only simulates non-attenuated waves. In real life problems the incident surface wave is mostly transmitted in each

cell, but the amplitude of the propagating wave gets decreased by reflection at the electrode, material damping, conversion to volume waves and thermal losses. In this thesis material damping and attenuation through reflection at periodically arranged electrodes are considered.

3. The aim is to compute the *diagram of dispersion*, which gives the context between the constant of propagation $\alpha + i\beta$ and the frequency ω for a given cell geometry.

On the organization of this thesis

- Chapter 2
  The physical characteristics of the problem are provided. The principles of SAW devices are quoted, the terms stop-band diagram of dispersion are explained in detail. At the end of the chapter the piezoelectric effect and its governing equations are posted.

- Chapter 3
  The principle concepts and results of the finite element method for elliptic and coupled field problems are given. Moreover, the basic ideas, results and an error analysis for solving eigenvalue problems by the finite elment method are sketched.

- Chapter 4
  We provide a detailed mathematical modeling, separated in three main points, i.e. in the theory of periodic structures for Helmholtz-type problems, in the consideration of damping effects and in expansion of the modeled approaches to piezoelectric coupled field problems. The steps of mathematical modeling provide two reasonable methods, which yield in frequency-depending complex non-hermitian eigenvalue problems of linear or quadratic form.

- Chapter 5
  We provide the theoretical background and numerical solution methods for large-scaled non-hermitian linear and quadratic algebraic eigenvalue problems and finally introduce open-source software packages, which are used in numerical simulation.

- Chapter 6
  This chapter combines the methods introduced in Chapter 5 with the problems stated in Chapter 4. The spectral properties of the various solution methods are analyzed. Three alternative solution algorithms using the available software packages Arpack and Lapack are stated. At the end, scaling methods for eigenvalue problems, which are necessary for the convergence of piezoelectric problems, are treated and some implementional aspects are discussed.

- Chapter 7
  Numerical results for periodically perturbed model problems (Laplace and plane strain problem) and for piezoelectric real life problems (GSM-filter and TV-filter) are presented. Finally, the three implemented solvers are compared to each other via the simulation of a piezoelectric problem, which is just capable for all three methods.

- Chapter 8
  The presented models, theories, methods and algorithms are reviewed. Open problems, on which further work can be done, are discussed.

- Appendix A
  The material data used in numerical simulation are cited.

Chapter 2

Problem formulation and governing equations

2.1 Problem description

We study a *surface acoustic wave* (*SAW, Rayleigh-wave*) device consisting of a piezoelectric substrate and evaporated electrodes (see Figure 2.1). If an electric signal is applied on the transmitter electrodes, an acoustic wave is excited on the surface of the piezoelectric medium (converse piezoelectric effect). The propagating surface wave is accompanied by an electric field on its travel trough the material (direct piezoelectric effect). This electric field can be measured at the receiver electrodes.

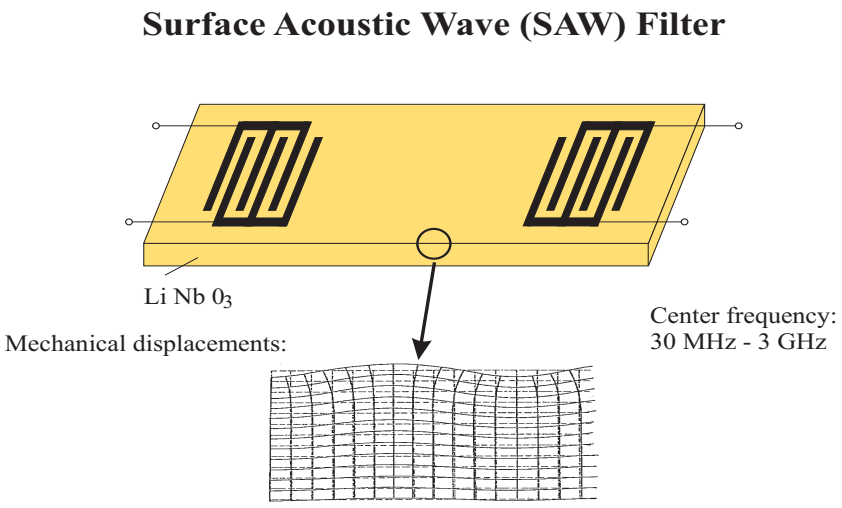

Figure 2.1: SAW filter [26]

We are interested in the propagation of Rayleigh-waves at the electrodes. These waves live near the surface, the amplitude decreases rapidly with depth and becomes negligibly small within the depth of a few wavelengths.
In general, surface waves are 3 dimensional, but Rayleigh-waves polarize (particle displacement) only in the plane spanned up by the direction of propagation (x) and the surface normal (y). This plane is called the sagittal plane. Therefore displacement and electric fields only depend on x and y coordinates and we can restrict the computational geometry to the sagittal plane.

Since in devics used in practise there are some hundred electrodes, extending the electrodes periodically to infinity is a suitable approximation. We get an infinite domain of a piezoelectric substrate with periodically arranged electrodes. See Figure 2.2.

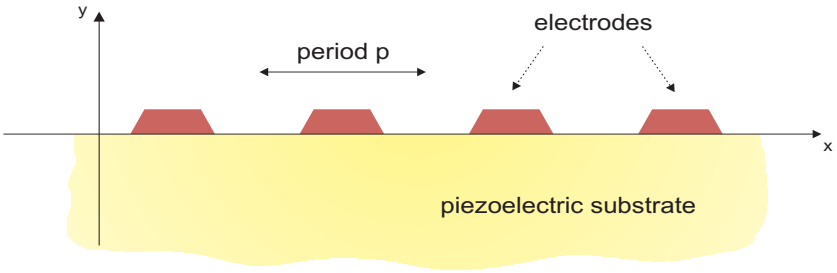

Figure 2.2: Periodic geometry

Properties of waves in a periodic geometry We assume a time-harmonic excitation of the wave. This implies harmonic field quantities (mechanical displacement and electric potential).
Due to the periodicity of the material the field distribution is *quasi-periodical*, that means periodical irrespective damping

$$u(x+p) = u(x)e^{(\alpha+i\beta)p}. \tag{2.1}$$

The following notation is used:
p ... period of the material (i.e. the distance between the centers of two successive electrodes),
α ... attenuation of the propagating wave per period,
β ... phase shift per period.
The condition (2.1) is equivalent to the existence of a p-periodic function $u_p(x) = u_p(x+p)$ such that

$$u(x) = u_p(x)e^{(\alpha+i\beta)x}. \tag{2.2}$$

The diagram of dispersion The aim is to compute the *diagram of dispersion*, which gives the context between the constants of propagation α, β and the frequency ω for a given cell geometry. See Figure 2.3.

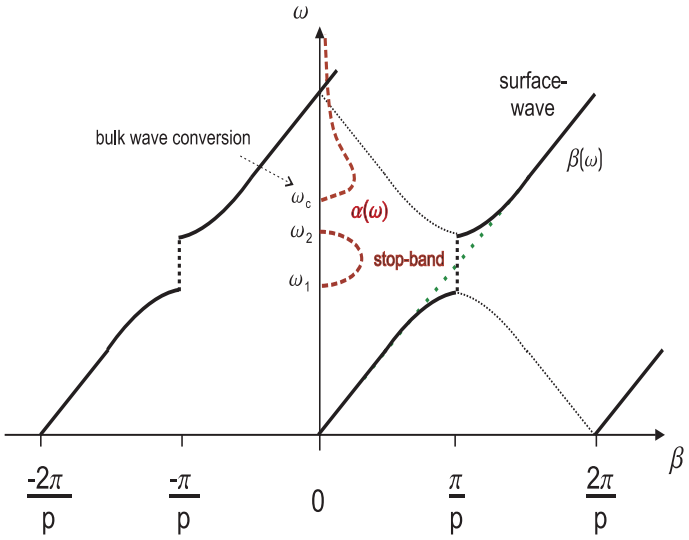

Figure 2.3: Diagram of dispersion: structure with periodical arranged electrodes [16], [15]

In this diagram we are mainly interested in the stopband regions (ω_1, ω_2), see stop band attenuation. The damping term starting at the frequency (ω_c) is produced by the fact that above a particular frequency a part of the reflected wave is converted to volume waves. This loss of energy implies a damping of the surface wave. This effect will not be considered in the model presented here (see Chapter 8).
The doted straight green line in Figure 2.3 shows the dispersion context, if there are no periodic disturbances.

Stop-band attenuation A wave traveling in x-direction will be partially reflected at the electrodes. If p is a multiple of $\frac{\lambda}{2}$ with λ denoting the wavelength, the reflected amplitudes are all in phase and can interfere constructively. For a huge number of fingers there are many waves adding constructively and the sum of reflected waves interacts with the propagating wave. Then even if the reflected part per cell is small and it impedes the propagation.
If the length of period of the material is equal the wavelength of the wave propagating in x-direction, the wave cannot propagate. Moreover it turns out that the wave cannot propagate in a whole frequency interval. This interval is called the *stop-band*. The width of this stop-band gives information on the quantity of the reflection at the electrodes.
This effect occurs independently of the consideration of material damping in the model.

2.2 The piezoelectric effect and governing equations

A material possesses piezoelectric properties, if it produces an electrical polarization under the application of mechanical stress or deformations. The polarization is measurable by produced charges on the surface. This phenomenon is called the *direct piezoelectric effect*. The effect is reversible, it is always accompanied by the *converse piezoelectric effect*. If an electric field is applied to a piezoelectric medium, there is an elastic deformation.
Piezoelectric effects result from special asymmetries occurring in some crystalline materials (e.g. in quartz by nature or in industrial produced ceramics). These effects cannot exist in isotropic media. For more details see [4] pages 102–103.

The piezoelectric effect is described by a coupling of elastic and electric field quantities in a medium. We can assume this coupling to be linear since nonlinear coupling terms are negligible small. To get the governing equations we state the uncoupled field properties and equations first:

2.2.1 The equations of elasticity

Let $\Omega \subset \mathbb{R}^d$ with $d = 1, 2, 3$ be a bounded domain which describes the reference configuration (original state) of a deformable body, and let $\partial\Omega$ be the boundary of Ω which is supposed to be sufficiently smooth (polygonal in our applications).
The deformation of the body is represented by the mapping

$$\begin{aligned} P : \bar{\Omega} \times \mathbb{R}_0^+ &\rightarrow \mathbb{R}^d \\ (x, t) &\rightarrow P(x, t), \end{aligned}$$

which is assumed to be injective, sufficiently smooth, orientation preserving.
At $t = 0$ the body is in reference configuration,i.e. $P(x, 0) = x \quad \forall x \in \Omega$.

Let a volume force

$$f(., t) : P(\Omega, t) \rightarrow \mathbb{R}^d$$

and a surface traction

$$g(., t) : P(\Gamma_1, t) \rightarrow \mathbb{R}^d \quad \text{with } \Gamma_1 \subset \partial\Omega$$

be given in the domain Ω and at the Neumann part Γ_1 of the boundary $\partial\Omega$, respectively.

The fundamental axiom of continuum mechanics states the existence of a stress field $t(x, n)$ (acting on the surface $\partial P(A, t)$ with according normal vector n for any subdomain $A \subset \Omega$), which satisfies conservation of momentum and angular momentum in A.

One of the main results in continual mechanics (Ciarlet [12]) states that the stress vector is linear in n and can be represented by a (differentiable) *stress tensor* $T(x) \in \mathbb{R}^d_d$ of the form

$$t(x,n) = T(x).n \quad \forall\, x \in P(\Omega,t) \tag{2.3}$$

satisfying the *Cauchy equations of motion*

$$\begin{array}{rcll} div_x T(x,t) + f(x,t) & = & \rho(x,t)\frac{\partial^2 u}{\partial t^2}(x,t) & t \in I,\ x \in P(\Omega,t) \\ T(x,t) & = & T^T(x,t) & t \in I,\ x \in P(\Omega,t) \\ T(x,t).n & = & g(x,t) & t \in I,\ x \in P(\Gamma_1,t) \end{array} . \tag{2.4}$$

$\rho(x,t)$ denotes the mass density and $I = [0,t_e]$ the time-interval in $\mathbb{R}^+_0$.

We assume elastic deformation i.e. releasing the external forces the medium returns completely in its original reference state. Deformations imply strains in the deformed medium. Let $u(x)$ describe the displacement vector of a particle through deformation, i.e.

$$u(x,t) := P(x,t) - x \qquad \forall\, x \in \Omega \tag{2.5}$$

Green's strain tensor describes the change in lengths between two particles:

$$\varepsilon_{ij} := \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} + \sum_{k=1}^{d} \frac{\partial u_k}{\partial x_j}\frac{\partial u_k}{\partial x_i}\right) \qquad \forall\, i,j = 1,\ldots,d \tag{2.6}$$

If we assume small deformations $|\frac{\partial u_k}{\partial x_j}| \ll 1$, we get negligible quadratic terms. In linear elastic theory we use the *(linearized) Cauchy-Green strain tensor* by

$$\begin{array}{rcll} S_{ij} & := & \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) & \forall\, i,j = 1,\ldots,d \\ S & := & \frac{1}{2}(\nabla u + (\nabla u)^T) =: Bu & \end{array} . \tag{2.7}$$

Hook's law states that in linear elastic materials there is a linear connection between stresses and strains of the form

$$\begin{array}{rcll} T_{ij} & = & \sum_{k,l=1}^{d} c_{ijkl} S_{kl} & \forall\, i,j = 1,\ldots,d \\ T & = & cS & \end{array} . \tag{2.8}$$

There are 81 elastic stiffness coefficients c_{ijkl} which describe the elastic properties of the material. The material is called homogeneous if $c_{ijkl} \neq c_{ijkl}(x)$.

It turns out that only 21 elastic stiffness coefficients are independent. Under special material properties the number of independent coefficients can be further decreased:

1. Isotropic materials are materials characterized by possessing equal properties in all directions. It turns out that there are only two independent coefficients $\lambda(x), \mu(x) > 0$ known as Lamé-constants with

$$c_{ijkl} = \lambda\delta_{ij}\delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \tag{2.9}$$

   and Hook's law simplifies to

$$T_{ij} = \lambda \sum_{k=1}^{d} S_{kk}\delta_{ij} + 2\mu S_{ij} \qquad \forall\, i,j = 1,\ldots,d \tag{2.10}$$

2. Anisotropic materials have in general 21 independent stiffness coefficients. Some crystals possess symmetry axes or two different directions which have equal material properties. Therefore the number of independent coefficients reduces as well in such crystals.

The linearized strain tensor S and the according stress tensor T are symmetric.

2.2.2 The electrostatic field in a dielectric medium

We assume a dielectric medium which has the properties to be polarizable and is insulating, i.e. there are no free volume charges. Applying an electric field to a dielectrica implies a distortion of the dipoles within the material resulting in a surface charge. Internal the dipoles sum up to zero, ie. inside it is neutral. The polarization P acts against the electric field E which leads to the dielecitric displacement field D (the field was initially introduced to explain the fact that the electric field of a capacitor decreases if a dielectric is put in between). Since the polarization depends on the electric field as well one gets:

$$D = \varepsilon_0 E + P = \varepsilon E \tag{2.11}$$

with ε_0 the dielectric permittivity of vacuum and ε the dielectric permittivity tensor of the material.

The fourth law of Maxwell equations (Gauss law of dielectric fields) states in integral form

$$\int_{\partial A} D^T n \, ds = \int_A q_{free}(x) \, dx \qquad \forall \text{ proper } A \subset \Omega \tag{2.12}$$

or, in differential form,

$$div_x D(x) = q_{free}(x) \qquad \forall \, x \in \Omega, \tag{2.13}$$

where $q_{free}(x)$ denotes the free volume charge density in x.
We consider an insulating material, i.e. $q_{free} = 0$ in Ω, and we get

$$div_x D(x) = 0. \tag{2.14}$$

In electrostatics, the electric field can be expressed by the scalar potential field $\Phi(x)$ as

$$E(x) = -\nabla\Phi(x). \tag{2.15}$$

2.2.3 The piezoelectric equations

The piezoelectric effect states a liner coupling between strain field and electric field. The linearity is described by a coupling coefficient tensor e which is equal for direct and converse effect.
Expansion of Hook's law and the electrostatic equation by the direct and the converse piezoelectric effect gives the constitutive piezoelectric equations:

$$\begin{aligned} T &= c^E S - e^T E \\ D &= eS + \varepsilon^S E \end{aligned} \quad . \tag{2.16}$$

c^E ... mechanical stiffness matrix (measured at constant electric field E)
ε^S ... permittivity matrix (measured at constant mechanical strain $\mathbf{S}$)
e ... piezoelectric coupling coefficient matrix
The mechanical stiffness matrix and the permittivity matrix are symmetric matrices.

The displacement field u and the potential field Φ in a piezoelectric material (with no impressed volume forces) are governed by

$$\boxed{\begin{aligned} div_x[(c^E S - e^T E)(x,t)] &= \rho(x,t)\tfrac{\partial^2 u}{\partial t^2}(x,t) \\ div_x[(eS + \varepsilon^S E)(x,t)] &= 0 \end{aligned} \quad \text{with} \quad \begin{aligned} S &= \tfrac{1}{2}(\nabla u + (\nabla u)^T) \\ E &= -\nabla\Phi \end{aligned}} \tag{2.17}$$

with still open boundary conditions (stated in the section of mathematical modeling).

We refer the readet to [4] and [5] for more detailed information.

Chapter 3

The Finite Element Method

The finite elment method is a powerful method for solving partial differential equations numerically.
In this chapter the main results of finite element analysis, which are required in mathematical modeling of chapter 4, are provided. We start with FEM for elliptic source problems, which occur in model problems for periodic structures. Then mixed FE-approximation, which is required for solving piezoelectric problems, i.e. coupled field problems, is introduced.

Modeling the dispersion relation will lead to variational eigenvalue problems. FE-solutions of these problems are connected to source problems, but need a separate (error-) analysis. Therefore, we finish this chapter with a brief sketch of finite element methods for eigenvalue problems.

3.1 The method of finite elements

The Finite Element Method (FEM) is used to approximate the solution of second order problems, which are posed in variational form in some subspace V_0 of the Sobolev space $H^1(\Omega)$.
We start with the weak formulation coupled with the fundamental theorem of Lax-Milgram for elliptic problems, introduce the Galerkin-method and then specialize on FEM.

The weak formulation Let $\Omega \subset \mathbb{R}^d$ be a bounded sufficiently smooth domain. We assume a given problem in weak formulation, which is already homogenised, i.e. the Dirichlet conditions on $\Gamma_D \subset \partial\Omega$ are homogeneous. We define $V_0 := \{v \in V : v|_{\Gamma_D} = 0\} \subset H^1(\Omega)$.

We state the weak problem in abstract form as follows

$$\text{Find } u \in V_0 : \quad a(u,v) = F(v) \quad \forall\, v \in V_0. \tag{3.1}$$

For elliptic problems existence and uniqueness of a weak solution is provided by the theorem of Lax-Milgram.

Theorem 3.1.1 (Lax-Milgram) *[10]*
Let $V_0 \subset H^1(\Omega)$. If the bilinear form $a(.,.) : V_0 \times V_0 \to \mathbb{R}$ is

1. *elliptic, i.e. there is a constant $\mu_1 > 0$ such that*

$$a(v,v) \geq \mu_1 \|v\|_1^2 \qquad \forall\, v \in V_0, \tag{3.2}$$

   where $\|.\|_1 = \|.\|_{H^1(\Omega)}$ denotes the norm of H^1 on Ω.

2. *continuous, i.e. there is a constant $\mu_2 > 0$ such that*

$$|a(w,v)| \leq \mu_2 \|w\|_1 \|v\|_1 \qquad \forall\, w, v \in V_0, \tag{3.3}$$

and the linear form $F : V_0 \to \mathbb{R}$ is continuous, i.e. there is a constant $c > 0$ such that

$$|\tilde{F}(v)| \leq c\|v\|_1 \qquad \forall\, v \in V_0, \tag{3.4}$$

then there exists a unique solution $u \in V_0$ which solves

$$a(u,v) = F(v) \qquad \forall v \in V_0.$$

The Galerkin Method - Discretization The Galerkin method states the approximative solution of the weak problem by solving the problem only over finite-dimensional subspaces $V_h \subset V$. The index h is the discretization parameter and denotes that with $h \to 0$ we want to achieve convergence of the approximate solution $u_h \in V_h$ against the exact solution $u \in V$.

We state the discrete problems in $V_h \subset V$

$$\text{Find } u_h \in V_{0h} : \quad a(u_h, v_h) = F(v_h) \quad \forall\, v_h \in V_{0h}. \tag{3.5}$$

with the finite-dimensional subspace $V_{0h} := V_0 \cap V_h$.

Due to $V_{0h} \subset V_0$ the *Lax-Milgram theorem* still holds for the discrete problem, i.e. there is a unique $u_h \in V_{0h}$ solving (3.5).

We choose a base $(p^{(i)})_{i\in\overline{\omega}_h}$ of V_h such that

$$V_{0h} = span\{p^{(i)}, i \in \omega_h\},$$

i.e. $u_h \in V_{0h}$ is represented by the linear combination $u_h = \sum_{i\in\omega_h} u^{(i)} p^{(i)}$ with $u^{(i)} \in \mathbb{R}$. By $\overline{\omega_h}$ and ω_h we denote index sets for the chosen bases of V_h and V_{0h}. The discrete problem is fulfilled, if (3.5) holds forall $p^{(j)}$ with $j \in \omega_h$. Choosing $v_h = p^{(j)}$ for all $j \in \omega_h$ leads to the **Galerkin system**

$$\boxed{\text{Find } \underline{u}_h = (u^{(i)})_{i\in\omega_h} \in \mathbb{R}^{N_h} : \qquad K_h \underline{u}_h = \underline{f}_h} \tag{3.6}$$

with $N_h = dim\,\omega_h$ and $K_{h,ij} = a(p^{(i)}, p^{(j)}), \forall\, i,j \in \omega_h$, $\underline{f}_{h\,j} = f(p^{(j)}), \forall\, j \in \omega_h$.

Cea's Lemma states [10] that the discretization error can be bounded by the approximation error, i.e. under the assumptions of the theorem of Lax-Milgram the estimate

$$\|u - u_h\|_1 \leq \frac{\mu_2}{\mu_1} \inf_{w_h \in V_{0h}} \|u - v_h\|_1 \tag{3.7}$$

holds for the solution $u \in V_0$ of (3.1) and its approximation u_h satisfying (3.5) .

Finite element subspaces The finite element method is a special case of the Galerkin method, i.e. a special choice of the subspaces V_h. There are three main aspects in constructing such a subspace V_h:

1. The triangulation τ_h of the given geometry Ω in subdomains (called elements) $T \in \tau_h$ satisfies

   (a) $\forall T \in \tau_h : T = \overline{\overset{\circ}{T}}$ and $\overset{\circ}{T} \neq \emptyset$,

   (b) $\bigcup_{T\in\tau_h} T = \overline{\Omega}$,

   (c) for $T_1, T_2 \in \tau_h : T_1 \neq T_2 \Rightarrow T_1 \cap T_2 = \begin{cases} \emptyset \\ \text{vertex} \\ \text{edge} \\ \text{face} \quad (\text{if d=3}) \end{cases}$

2. All $v_h \in V_h$ are piecewise polynomials, i.e. $P_T = \{v_h|_T : v_h \in V_h\}$ is a polynomial set. is set of polynomials of degree k.

3. A base of V_h with base functions having small support exist.

Concerning the model problem, which will be stated in Chapter 4, Ω is defined on $\mathbb{R}^2$ and triangles or rectangles are used for triangulation. The set of vertices of all T in τ_h is described by the nodes $\{x^{(i)}, i \in \overline{\omega}_h\}$. We will use linear elements, i.e. the ansatz functions $v_h|_T$ are linear for triangles and bilinear for rectangles.

For the construction of the base functions $p^{(i)}$ of V_h we choose

$$p^{(j)}(x^i) = \delta_{ij} \qquad \forall\, i, j \in \overline{\omega}_h, \tag{3.8}$$

which are well-defined for $p^{(i)}|_T$ linear or respectively bilinear.

Since $a(p^{(i)}, p^{(j)}) = 0$ if $\text{meas}_{\mathbb{R}^2}(supp(p^{(i)}) \cap supp(p^{(j)})) \neq 0$, choosing base functions with small support (which will lead to nodal basis functions) implies that the stiffness matrix K_h in the Galerkin system (3.6) becomes sparse.

3.2 FEM for coupled field problems

The weak formulation of piezoelectric problems yields in a mixed variational problem of the form:

Find $u \in X$ and $\phi \in M$ which satisfy

$$\begin{array}{rcrcll} a(u,v) & + & b(v,\phi) & = & f(v) & \forall\, v \in X \\ b(u,\psi) & - & c(\phi,\psi) & = & g(\psi) & \forall\, \psi \in M \end{array}$$

Theorem 3.2.1 *Let us assume that*

f and g are bounded linear forms, i.e. $f \in X^*$, $g \in M^*$,

2. *the bilinear forms* $a(.,.) : X \times X \to \mathbb{R}$ *and* $b(.,.) : X \times M \to \mathbb{R}$ *are continuous,i.e.*

$$\begin{array}{lrcll} \exists \alpha_2 > 0 : & |a(w,v)| & \leq & \alpha_2 \|w\|_X \|v\|_X & \forall\, w,v \in X \\ \exists \beta_2 > 0 : & |b(v,\psi)| & \leq & \beta_2 \|v\|_X \|\psi\|_M & \forall\, v \in X, \forall\, \psi \in M, \end{array}$$

3. *the bilinear form* $b(.,.)$ *fulfills the inf-sup-condition, i.e.*

$$\exists \beta_1 > 0 : \; inf_{\substack{\psi \in M \\ \psi \neq 0}} sup_{\substack{v \in X \\ v \neq 0}} \frac{b(v,\psi)}{\|v\|_X \|\psi\|_M} \geq \beta_1.$$

4. $a(.,.)$ *is elliptic on* $V_0 = Ker\, b = \{v \in X | b(v,\psi) = 0 \, \forall \psi \in M\}$,*i.e.*

$$\exists \alpha_1 : a(v,v) \geq \alpha_1 \|v\|_X \qquad \forall\, v \in V_0,$$

5. $a(.,.)$ *is non-negative on* X , *i.e.*

$$a(v,v) \geq 0 \qquad \forall\, v \in X,$$

6. *The bilinear form* $c(.,.) : M \times M \to \mathbb{R}$ *fulfills the conditions*

$$\begin{array}{rcll} c(\psi,\psi) & \geq & 0 & \forall\, \psi \in M, \\ c(\psi,\phi) & = & c(\phi,\psi) & \forall\, \psi,\phi \in M.. \end{array}$$

Then the weak coupled-field problem

Find $u \in X$ *and* $\phi \in M$ *such that*

$$\begin{array}{rcrcll} a(u,v) & + & b(v,\phi) & = & f(v) & \forall\, v \in X \\ b(u,\psi) & - & c(\phi,\psi) & = & g(\psi) & \forall\, \psi \in M \end{array} \tag{3.9}$$

has a unique solution $(u,\phi) \in X \times M$.

Proof: see Remark 10.8 in [31] p.572-573.

Remark 3.2.2 *Theory of problems of the form (3.9) are derived form the theory of saddle point problems (c(.,.)=0). The assumption (1)-(4) are nothing but the assumptions of Brezzi's theorem.*

Discretization of mixed problems Choosing finite-dimensional subspaces $X_h \subset X$ and $M_h \subset M$ the discrete mixed problem reads as follows:

Find $u_h \in X_h, \phi_h \in M_h$ such that

$$\begin{array}{rcrcll} a(u_h, v_h) & + & b(v_h, \phi_h) & = & f(v_h) & \forall\, v_h \in X_h \\ b(u_h, \psi_h) & - & c(\phi_h, \psi_h) & = & g(\psi_h) & \forall\, \psi_h \in M_h. \end{array} \tag{3.10}$$

In contrast to elliptic problems, the assumptions posed for existence and uniqueness results are not all automatically implied on the discrete spaces. Since in general $V_{0h} := \{v_h \in X_h \mid b(v_h, \psi_h) = 0 \,\forall\, \psi_h \in M_h\} \not\subset V_0$, the ellipticity of $a(.,.)$ has to be explicitly required for the discrete problem as well as the discrete inf-sup-condition.

Theorem 3.2.3 *Under the assumptions of theorem 3.2.1 and the discrete conditions*

1. *$a(.,.)$ is V_{0h}-elliptic,*
2. *the discrete inf-sup-condition is fulfilled, i.e.*

$$\exists \tilde{\beta}_1 \neq \tilde{\beta}_1(h) > 0 : \; inf_{\substack{\psi_h \in M_h \\ \psi \neq 0}} sup_{\substack{v_h \in X_h \\ v \neq 0}} \frac{b(v_h, \psi_h)}{\|v_h\|_{X_h} \|\psi_h\|_{M_h}} \geq \tilde{\beta}_1,$$

the discrete problem (3.10) has one and only one solution $u_h \in X_h, \psi_h \in M_h$.

Finite Element Discretisization We assume two finite element subspaces $X_h \subset X$ and $M_h \subset M$ with the nodal bases $p^{(i)}$ of X_h and $\Psi^{(i)}$ of M_h according to the node $x^i \in \omega_h$, i.e. $p^{(i)}(x^j) = \delta_{ij}$ and $\Psi^{(i)}(x^j) = \delta_{ij}$.
With $u_h = \sum_{i=1}^n \underline{u}_h^i p^{(i)}$ and $\phi_h = \sum_{i=1}^n \underline{\phi}_h \Psi^{(i)}$ we achieve the Galerkin-problem

$$\begin{pmatrix} A & B^* \\ B & -C \end{pmatrix} \begin{pmatrix} \underline{u}_h \\ \underline{\phi}_h \end{pmatrix} = \begin{pmatrix} \underline{f}_h \\ \underline{g}_h \end{pmatrix}, \tag{3.11}$$

where the matrices are defined by $A_{ij} = a(p^{(i)}, p^{(i)})$, $B_{i,j} = b(p^{(i)}, \Psi^{(i)})$, $B^* = B^T$ and $C_{ij} = c(\Psi^{(i)}, \Psi^{(i)})$.
The system matrix $\begin{pmatrix} A & B^* \\ B & -C \end{pmatrix}$ is regular, but indefinite. Due to the small support of the base functions, the system matrix is sparse.

For further information we refer the reader to [10] and [31].

3.3 Finite element method for eigenvalue problems

In this section the following questions will be sketched : What happens if one solves eigenvalue problems via finite-element method? Which eigenvalues will be approximated, how are the convergence properties adn how accurate is this approximation?

The statements and results of the following section stem from "Finite Element Methods - Eigenvalue problems" by Babuska and Osborn [7] and can be found there with proofs.

Since we want to apply finite element techniques on eigenvalue problems we assume a given eigenvalue problem of weak form. The theroy of approximating variational formulated eigenvalue problems will be traced back on spectral theroy of compact operators. Then finite element techniques are applied analogous to the source variational problems. The discretized eigenvalue problems can be again traced back on compact operators. Then an error estimate for the approximated eigenvalues will be given.
More detailed spectral analysis is known for self-adjoint elliptic problems. Since in Chapter 4 we will state self-adjoint elliptic problems in the first phases of modeling, some results for these special type of eigenvalue problems will be given.
Detailed spectral theory for coupled field problems (especially piezoelectric problems) will be left open within this thesis, for further information and references see [7].

Abstract eigenvalue problem We start with a *variationally posed eigenvalue problem* on complex Hilbert-spaces $(H_1, \|.\|_1, (.,.)_1), (H_2, \|.\|_2, (.,.)_2)$: A scalar $\lambda \in \mathbb{C}$ is called an *eigenvalue of the bilinar form a with respect to the bilinear form b* if there is an eigenvector $u \neq 0 \ \in H_1$ fulfilling

$$a(u,v) = \lambda b(u,v) \qquad \forall v \in H_2. \tag{3.12}$$

Let $a(.,.)$ be a bilinear form on $H_1 \times H_2$ which continuous

$$\exists \alpha_2 > 0 : \quad |a(w,v)| \leq \alpha_2 \|w\|_1 \|v\|_2 \, \forall \, w \in H_1 \, \forall \, v \in H_2 \tag{3.13}$$

and satisfies the *inf-sup conditions*

$$\inf_{\substack{u \in H_1, \\ \|u\|_1 = 1}} \sup_{\substack{v \in H_2, \\ \|v\|_2 = 1}} |a(u,v)| \ = \ \alpha > 0, \tag{3.14}$$

$$\sup_{u \in H_1} |a(u,v)| \ > \ 0 \qquad \forall v \neq 0 \ \in H_2. \tag{3.15}$$

The bilinear form $b(.,.)$, defined on $W_1 \times W_2$ with $H_1 \ \subset \ W_1$ compact and $H_2 \ \subset \ W_2$ bounded, is assumed to be continuous in $W_1 \times W_2$, i.e.

$$\exists \beta_2 > 0 : \quad |b(w,v)| \leq \beta_2 \|w\|_{W_1} \|v\|_{W_2} \qquad \forall \, w \in W_1 \, \forall \, v \in W_2. \tag{3.16}$$

The main idea of spectral theory of variationally posed eigenvalue problems
The assumptions (3.13)-(3.16) for $a(.,.), b(.,.)$ imply the the existence of *unique compact operators*

$$T : H_1 \to H_1 \text{ and } T_* : H_2 \to H_2,$$

which hold

$$\begin{array}{rcll} a(Tu, v) & = & b(u, v) & \forall\, u \in H_1 \forall\, v \in H_2 \\ a(u, T_* v) & = & b(u, v) & \forall\, u \in H_1 \forall\, v \in H_2 \\ \|Tu\|_1 & \leq & \frac{\beta_2}{\alpha}\|u\|_{W_1} & \forall\, u \in H_1. \end{array} \tag{3.17}$$

Theorem 3.3.1 *(λ, u) is an eigenpair of (3.12) if and only if $(\frac{1}{\lambda}, u)$ is an eigenpair of T, i.e. $Tu = \frac{1}{\lambda}u$.*

Therefore the analysis of variationally formulated eigenvalue problems is given by spectral theory of compact operators.

Definition 3.3.2 *The eigenvalue λ of the variational eigenvalue problem is of multiplicity m by definition, if λ^{-1} is a m-multiple eigenvalue of T.*

The finite element method for approximating eigenproblems
The finite element method of eigenvalue problems is formally equal to FEM of source problems. We choose finite element spaces $H_{1h} \subset H_1$ and $H_{2h} \subset H_2$ of equal dimension, i.e. $dim H_{1,h} = dim H_{2,h} = N$, for which

$$\inf_{\substack{u \in H_{1h}, \\ \|u\|_1 = 1}} \sup_{\substack{v \in H_{2,h}, \\ \|v\|_2 = 1}} |a(u, v)| = \alpha_h = \alpha(h) > 0 \tag{3.18}$$

and

$$\lim_{h \to 0} \alpha_h^{-1} \inf_{w_h \in H_1} \|u - w_h\|_1 = 0 \tag{3.19}$$

is valid.
Then we formulate the weak eigenvalue problem (3.12) on the FE-subspaces and get the finite element *Galerkin eigenvalue problem*

$$\text{Search } (\lambda_h, u_h) \in (\mathbb{C}, H_{1h}), u_h \neq 0 : \quad a(u_h, v_h) = \lambda_h b(u_h, v_h) \quad \forall\, v_h \in H_{2h}. \tag{3.20}$$

Let $(\Phi_1, ...\Phi_N)$ and $(\Psi_1, ..., \Psi_N)$ be bases of the subspaces H_{1h} and H_{2h} .
By choosing $A_{ij} = a(\Phi_i, \Psi_j)$, $B_{ij} = b(\Phi_i, \Psi_j)$ and $\underline{u}_h = (u_i)_{i=\overline{1,N}}$ with $u_h = \sum_{i=1}^N u_i \Phi_i$, we get the *algebraic eigenvalue problem*

$$\text{Search } \lambda_h \in \mathbb{C} \text{ and } \underline{u}_h \in \mathbb{C}^N : \quad A\underline{u}_h = \lambda_h B \underline{u}_h, \tag{3.21}$$

which is equivalent the Galerkin eigenvalue problem (3.20).

The analysis of Galerkin eigenvalue problems can be again reduced to spectral theory of compact operators.
For every h we define an operator $T_h : H_1 \to H_{1h}$ by

$$a(T_h u, v_h) = b(u, v_h) \quad \forall\, u \in H_1 \forall\, v_h \in H_{2h}.$$

T_h can be written as $P_h T$ with P_h denoting the projection of H_1 on H_{1h},i.e.

$$a(P_h u, v_h) = a(u, v_h) \qquad \forall\, u \in H_1\, \forall\, v_h \in H_{1h}.$$

The compactness of T and the projection property of P_h imply that $T_h = P_h T \to T$ in $\|.\|_1$.
Again (λ_h, u_h) is an eigenpair of (3.20) if and only if (λ_h^{-1}, u_h) is an eigenpair of T_h.

Error analysis Before giving a result on the quality of eigenvalue aproximation by the finite element method some notational work is required.
The (generalized) eigenspaces according to an eigenvalue λ of (3.12) are denoted by

$$\begin{aligned} E(\lambda) &:= \{u|(\lambda, u) \text{ solves (3.12) with } \|u\|_1 = 1\}, \\ E^*(\lambda) &:= \{v|(\lambda, v) \text{ adjoint eigenpair of (3.12) with } \|u\|_2 = 1\}. \end{aligned}$$

If (λ) is of multiplicity m, there are m corresponding eigenvalues $\lambda_1(h), ..., \lambda_m(h)$ for each finite element subspaces H_{1h}, H_{2h} with $\lambda_j(h) \to \lambda$ for $h \to 0$, since $T_h \to T$.
The eigenspace of (3.20) according to λ of (3.12),i.e. $\lambda_j(h) \to \lambda$, is the sum of the m eigenspaces of $\lambda_j(h)$, $(j = 1, ..., m)$. We denote this eigenspace with $E_h(\lambda)$ and assume the eigenvectors of $E_h(\lambda)$ be normalized in $\|.\|_1$.

Moreover, we define the approximation error in respect to the eigenspaces by

$$\begin{aligned} \varepsilon_h(\lambda) &:= \sup_{u \in E(\lambda)} \inf_{w_h \in H_{1h}} \|u - w_h\|_1, \\ \varepsilon_h^*(\lambda) &:= \sup_{u \in E^*(\lambda)} \inf_{w_h \in H_{2h}} \|v - w_h\|_2. \end{aligned}$$

Theorem 3.3.3 *Error estimate for approximative eigenvalues*
Let λ be an eigenvalue of (3.12) of multiplicity m and $\lambda_j(h)$ $(j = 1, ..., m)$ the m according eigenvalues of the discrete problem (3.20) satisfying $\lambda_j(h) \to \lambda$.
Then the following estimate holds

$$\exists c_1 > 0 : \qquad |\lambda - \hat{\lambda}(h)| \le c_1(\beta(h)\varepsilon_h \varepsilon_h^*) \qquad \text{with } \hat{\lambda}(h) := \frac{1}{m}\sum_{j=1}^{m} \lambda_j(h). \tag{3.22}$$

Stronger estimates can be given for the special case of self-adjoint elliptic eigenvalue problems,i.e. T, T_h is self-adjoint and elliptic.

3.3.1 Self-adjoint elliptic eigenvalue problems

We view the eigenvalue problems (3.12) and its FE-approximations (3.20) under the following assumptions:

1. $H = H_1 = H_2$.
2. The bilinearform $a(.,.)$ is

$$\begin{array}{lrcll} \text{symmetric:} & a(u,v) & = & a(v,u) & \forall\, u \in H \forall\, v \in H, \\ \text{continuous:} & a(u,v) & \leq & \alpha_2 \|u\| \|v\| & \forall\, u \in H \forall\, v \in H, \\ \text{elliptic:} & a(u,u) & \geq & \alpha_1 \|u\|^2 & \forall\, u \in H. \end{array}$$

3. $W = W_1 = W_2 \supset H$ is a compact embedding.
4. The bilinearform $b(.,.)$ is

$$\begin{array}{lrcll} \text{symmetric:} & b(u,v) & = & b(v,u) & \forall\, u \in W \forall\, v \in W, \\ \text{continuous:} & b(u,v) & \leq & \beta_2 \|u\| \|v\| & \forall\, u \in W \forall\, v \in W, \\ \text{positive:} & b(u,u) & \geq & 0 & \forall\, u \neq 0 \ \in H. \end{array}$$

Remark: The energetic norm $\|.\|_a = \sqrt{a(.,.)}$ is an equivalent norm to $\|.\|_H =: \|.\|$.

The assumptions on spaces and bilinear forms imply that $T = T_* = T^*$ is a compact and self-adjoint operator, where T^* denotes the adjoint of T.
Due to spectral theory of operators T has countable sequence of positive eigenvalues converging to zero. Therefore the variational eigenproblem (3.12) has a countable sequence of eigenvalues with

$$0 < \lambda_1 \leq \lambda_2 \leq ... \nearrow \infty. \tag{3.23}$$

The corresponding eigenvectors $u_1, u_2, ...$ can be chosen the way they satisfy

$$a(u_i, u_j) = \lambda_j \, b(u_i, u_j) = \delta_{ij} \tag{3.24}$$

Moreover, these eigenvectors form a base of H, i.e. $\forall\, u \in H: \quad u = \sum_i^\infty a(u, u_i) u_i$.

Finite element discretization
Let $V_h \subset H$ denote a finite-element subspace of H.
The eigenvectors u_j $(j = 1, ..., N)$ of of the associated Galerkin eigenvalue problem (3.20) corresponding to the eigenvalues

$$0 < \lambda_{1,h} \leq \lambda_{2,h} \leq ... \leq \lambda_{N,h} \qquad \text{with } N = dim V_h$$

can be chosen the way

$$a(u_i, u_j) = \lambda_{j,h} \, b(u_i, u_j) = \delta_{ij}. \tag{3.25}$$

holds.

Theorem 3.3.4 *Error estimates*
If λ_k has geometric multiplicity m_k, i.e. $\lambda_k = ... = \lambda_{k+m_k-1}$, then

$$\lambda_{k+j,h} \searrow \lambda_k \quad \text{for } j = 0, ..., m_k - 1$$

with the estimate

$$\exists C > 0: \quad \lambda_k \leq \lambda_{j,h} \leq \lambda_k + C\varepsilon^2(\lambda_k) \qquad j = 0, ..., m_k - 1 \tag{3.26}$$

holds.
Concerning the approximation of eigenvectors there are two estimates:

1. *Let $u_{k+j,h}$ be an eigenvector of (3.20) corresponding to $\lambda_{k+j,h}$ for $j = 0, ..., m_k - 1$. Then there is a unit eigenvector in $E(\lambda_k)$ which satisfies*

$$\exists C > 0: \quad \|u - u_{j,h}\|_1 \leq C\varepsilon_h(\lambda_k). \tag{3.27}$$

2. *If u is a unit eigenvector of (3.12) corresponding to λ_k, i.e. $u \in E(\lambda_k)$ then there is a vector $\tilde{u}_h \in E_h(\lambda_k)$ such that*

$$\exists C > 0: \quad \|u - \tilde{u}_h\|_1 \leq C\varepsilon_h(\lambda_k). \tag{3.28}$$

If $m_k = 1$, i.e. λ_k is simple, then

$$\exists C > 0: \quad \|u_k - u_{k,h}\|_1 \leq C\varepsilon_h(\lambda_k) \tag{3.29}$$

holds.

Further analysis and estimates for self-adjoint ellitpic variational eigenvalue problems can be found in [7].

Remark 3.3.5 *On the "well-approximated part" of the spectrum*
Due to Babuska and Osborn [7] the finite element method give reasonable approximations for low eigenvalues. The dimension of the finite element subspaces and according the dimension of the algebraic eigenvalue problem will be much larger than the number of well approximated eigenvalues and eigenvectors.
The solver for the algebraic eigenvalue problem should be designed to find low eigenvalues of large sparse generalized eigenvalue problems.

Chapter 4

Mathematical modeling

Before starting with a stepwise construction of the mathematical model we have to precise the problem formulation, i.e. stating the boundary conditions and the geometry of the desired final model.

4.1 Problem-based assumptions, geometry and boundary conditions

Harmonic approach To reduce the space-time problem to a spatial one, we assume all field quantities to be time-harmonic, i.e.

$$v(x,t) = v_1(x)\cos(\omega t) + v_2(x)\sin(\omega t). \tag{4.1}$$

Using a complex formulation $\hat{v}$ of v with $\Re(\hat{v}(x)) = v_1(x)$ and $\Im(\hat{v}(x)) = v_2(x)$ leads to the simplification that derivations in time are multiplications $\frac{\partial}{\partial t} \rightarrow i\omega t.$ and $\frac{\partial^2}{\partial t^2} \rightarrow -\omega^2$. Therefore we consider the complex function $\hat{v}$ during the computation and take the real part afterwards.

$$\begin{aligned} \hat{v}(x,t) &= \hat{v}(x)e^{i\omega t} \\ v(x,t) &= \Re(\hat{v}(x,t)) \end{aligned} \tag{4.2}$$

Due to the linearity of the applied operations this is valid. For easier notation the hat marker is be suppressed.

Electrodes In order to get the propagation parameter caused by periodic perturbations (electrodes), we need not to simulate the sending or receiving state at the electrodes. It is sufficient to simulate the problem with short-circuited electrodes (i.e. the potential field is zero in the electrode domain Ω_{el}) or floating electrodes (i.e. the potential field is constant within each electrode, but the constant can differ between the electrodes). We will restrict ourselves to the first problem.

Geometry We start with an infinite piezoelectric substrate with periodical arranged electrodes on its surface. Due to the fact that we are mainly interested in Rayleigh-waves, we can restrict the computation domain to the sagittal plane. In the mathematical model we denote this plane with the (x_1, x_2)-plane. With these assumption we achieve the domain shown in Figure 4.1.

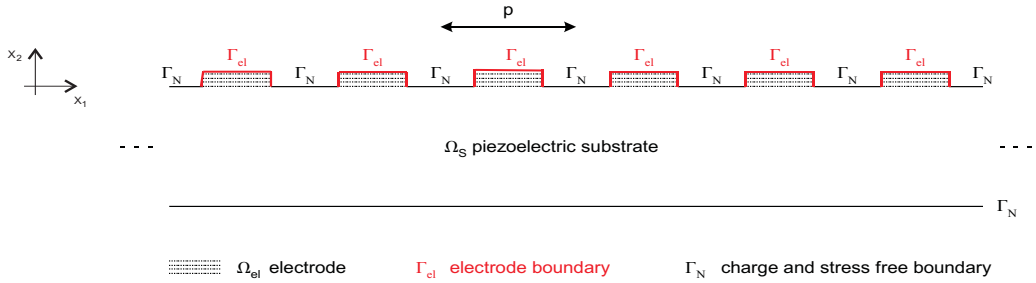

Figure 4.1: Infinite model geometry for piezoelectric problem

Two piezoelectric model cases $u \in \mathbb{R}^d$

1. d=2: We assume that there is no displacement in the x_3-direction and displacement and potential are not depending on the x_3-coordinate, i.e. $u(x_1, x_2, t) \in \mathbb{R}^2$ and $\Phi(x_1, x_2, t) \in \mathbb{R}$.

$$Bu := S = \begin{pmatrix} S_{x_1x_1} & S_{x_1x_2} \\ S_{x_2x_1} & S_{x_2x_2} \end{pmatrix} = \begin{pmatrix} \frac{\partial u_1}{\partial x_1} & \frac{1}{2}\left(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1}\right) \\ \frac{1}{2}\left(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1}\right) & \frac{\partial u_2}{\partial x_2} \end{pmatrix}, \tag{4.3}$$

$$-B\Phi = E = \begin{pmatrix} -\frac{\partial \Phi}{\partial x_1} \\ -\frac{\partial \Phi}{\partial x_2} \\ 0 \end{pmatrix}. \tag{4.4}$$

2. d=3: Due to the anisotropy of the material wave components in the z-direction can occur in practical applications. The deviation of the ideal case is considered by allowing constant behavior of the fields in x_3-direction:

$$\begin{matrix} \frac{\partial u_i}{\partial x_3} \\ \frac{\partial \Phi}{\partial x_3} \end{matrix} \begin{matrix} = \\ = \end{matrix} \begin{matrix} 0 \\ 0 \end{matrix} \qquad \text{for } u = (u_1, u_2, u_3)^T \in \mathbb{R}^3 \quad . \tag{4.5}$$

This implies the differential operators in Ω by

$$Bu = S = \begin{pmatrix} S_{x_1x_1} & S_{x_1x_2} & \frac{1}{2}\frac{\partial u_3}{\partial x_1} \\ S_{x_2x_1} & S_{x_2x_2} & \frac{1}{2}\frac{\partial u_3}{\partial x_2} \\ \frac{1}{2}\frac{\partial u_3}{\partial x_1} & \frac{1}{2}\frac{\partial u_3}{\partial x_2} & 0 \end{pmatrix}, \tag{4.6}$$

$$-B\Phi = E = \begin{pmatrix} -\frac{\partial \Phi}{\partial x_1} \\ -\frac{\partial \Phi}{\partial x_2} \\ 0 \end{pmatrix}. \tag{4.7}$$

We treat the electrodes as piezoelectric material with coupling coefficients set to zero and achieve the behaviour of non-piezoelectric material avoiding an explicit change of the governing equations. This leads to the problem of *partial differential equations with periodical coefficients* and will lead to *Bloch theory*.

The boundary conditions The surface excluding the electrodes (denoted with Γ_N in Figure 4.1) piezoelectric substrate is stress- and charge-free , i.e.

$$T.n = 0 \text{ and } D.n = 0 \text{ on } \Gamma_N.$$

Setting potential Φ to zero simulates short-circuited electrodes, i.e.	$\Phi = 0$ in Ω_{el}.
The mechanical field is again stress-free on Γ_{el}, i.e.	$T.n = 0$ on Γ_{el}.

4.2 The main steps of modeling

We have three main points to be considered in the construction of a mathematical model

- the periodical geometry, i.e. partial differential equations with periodic coefficients
- the physical properties of piezoelectric media
- damping effects

We want to construct the model step by step. To get a first impression of modeling and possible solution methods we initially concentrate on the first item, i.e. wave propagation in periodical perturbed media. We search for modeling and solution approaches for the wave equation with periodic coefficients. We start in 1 dimension and then upgrade to 2 dimension.
In this state of modeling we restrict only to pure propagating mode ($\alpha = 0$), since this simplification leads to self-adjoint problems.

In the second step we also permit stop band attenuation and consider material damping in the model and solution approaches for the wave equation. Including damping effects to our model implies that the operators get complex.

After coming up with the problem of periodic geometry and damping for the wave equation, finally we extend the developed methods to the system of piezoelectric equations.

4.3 Modeling wave equation with periodic coefficients in 1 D

We simplify the infinite periodical geometry to one dimension,i.e. $\Omega := \mathbb{R}$, and state the strong problem as searching a solution $u \in C^2(\Omega, \mathbb{R})$ of the periodic wave equation:

$$\boxed{\forall\, x \in \Omega\, \forall\, t \in \mathbb{R}: \qquad (a(x)u_X(x,t))_x = u_{tt}(x,t) \quad \text{with } a(x+p) = a(x).} \tag{4.8}$$

Let $p > 0 \in \mathbb{R}$ be a given, fixed period.
The positive periodic coefficient $a \in C^1(\Omega)$ describes the periodical properties of the material. We remark that for the weak formulation of the problem the condition $a \in L^\infty(\Omega) : 0 < \underline{a} \leq a(.) \leq \overline{a}$ almost everywhere (a.e.) in Ω will be sufficient.

The first step is using a harmonic approach as explained in (4.2)

$$\hat{u}(x,t) = \hat{u}\,(x)e^{i\omega t} \tag{4.9}$$

with $\hat{u}(.)$ in $C^2(\Omega, \mathbb{C})$. The hat marker will be suppressed furtheron.

Applying this approach to problem (4.8) leads to the *Helmholtz-type* equation

$$\text{Find } u \in C^2(\Omega, \mathbb{C}): \quad -(a(x)u'(x))' - \omega^2 u(x) = 0. \tag{4.10}$$

In order to give a formulation of the problem in operator form, we define the elliptic differential operator

$$\begin{aligned} A : C^2(\Omega, \mathbb{C}) &\rightarrow C(\Omega, \mathbb{C}) \\ u(.) &\rightarrow -(a(.)u'(.))'. \end{aligned}$$

and get the operator eigenvalue problem

$$\boxed{\text{Find u} \in C^2(\Omega, \mathbb{C}), \omega \in \mathbb{R}: \quad Au = \omega^2 u.} \tag{4.11}$$

The periodicity of the coefficient function $a(.)$ can be expressed in the operator equation via the shift operator

$$\begin{array}{rcccl} T_p & : & C(\Omega,\mathbb{C}) & \rightarrow & C(\Omega,\mathbb{C}) \\ & & u(.) & \rightarrow & T_p u(.) := u(.+p) \end{array} \tag{4.12}$$

by the fact that the operator A is invariant over translation of period p (the operators commute)

$$T_p A = A T_p. \tag{4.13}$$

In this case Bloch's theorem (introduced afterwards) states that the solution of problem (4.10) can be fully described via quasi-periodic eigenfunctions of the form

$$\exists \alpha, \beta \in \mathbb{R}: \quad u(x+p) = u(x) e^{(\alpha+i\beta)p}, \tag{4.14}$$

which is equivalent to

$$\exists\, u_p \in C^2(\Omega,\mathbb{C}) \text{ periodic with period p such that } \quad u(x) = u_p(x)\, e^{(\alpha+i\beta)x}. \tag{4.15}$$

4.3.1 Blochs Theorem

Theorem 4.3.1 (Bloch's Theorem 1D)
Let A be a linear (differential) operator mapping $C^2(\Omega,\mathbb{C})$ into $C(\Omega,\mathbb{C})$ which is invariant over T_p defined in (4.12), i.e.

$$T_p A = A T_p.$$

Then for each eigenspace $\mathcal{E}_A(\lambda) := \{v \in V \mid Av = \lambda v\}$ (with $dim(\mathcal{E}_A(\lambda) =: m$), there is a base of eigenfunctions $\tilde{\Phi} = (\tilde{\phi}_1, ..., \tilde{\phi}_m)$ satisfying

$$A\tilde{\phi}_j = \lambda \tilde{\phi}_j \;\; \textit{and} \;\; T_p \tilde{\phi}_j = e^{(\alpha_j + i\beta_j)p} \tilde{\phi}_j.$$

Proof: See "Asymptotic analysis of periodic structures, Spectral theory of differential operators with periodic coefficients" in Lions [9].

In terms of above theorem the following equivalences of quasi-periodicity hold

$$T_p \Phi = e^{(\alpha+i\beta)p}\Phi \;\Leftrightarrow\; \Phi(x) = \Phi_p(x) e^{(\alpha+i\beta)x} \;\Leftrightarrow\; \Phi(x+p) = e^{(\alpha+i\beta)p}\Phi(x) \tag{4.16}$$

.

4.3.2 Restriction to the unit cell

Bloch's theorem implies that we can restrict the problem on searching eigenfunctions in the space of quasi-periodic functions, i.e. we can assume $u(x) = u_p(x)\, e^{\alpha+i\beta x}$ with a complex pure-periodic function $u_p(.)$. Due to this periodicity the problem is fully described by a solution on the unit cell.

It is sufficient to solve problem (4.10) only on the unit cell $\Omega_p := [0, p]$, if the quasi-periodicity (4.14) is considered in the boundary conditions of left and right bound of the unit cell.

Notation 4.3.2 *For briefer notation we define* $\gamma := e^{(\alpha+i\beta)p}$.

In the starting phase of modeling we will concretize on pure propagating,i.e. not-attenuated solutions, i.e. we primarily assume $\alpha = 0$, which implies that $|\gamma| = 1$.

Classical formulation Search $u \in C^2(\Omega_p, \mathbb{C})$ satisfying

$$-(a(x)u'(x))' = \omega^2 u(x) \qquad \forall x \in \Omega_p. \tag{4.17}$$

Quasi-periodicity plus its derivation impose the boundary conditions:

$$u(p) = \gamma u(0), \tag{4.18}$$

$$\left.\begin{array}{l} w_l := -a(0)u'(0). \\ w_r := a(p)u'(p) = a(0)u'(0)e^{i\beta p} \end{array}\right\} \quad \rightarrow \quad w_r = -\gamma w_l. \tag{4.19}$$

Weak formulation Through integration by parts we get

$$\int_{\Omega_p} a(x)u'(x)v'(x)\, dx - \int_{\Omega_p} \omega^2 u(x)v(x)\, dx - a(x)u'(x)v(x)|_0^p = 0. \tag{4.20}$$

Using the flux notation defined in (4.19) leads to the variatonal formula

Search for a solution $u \in H^1(\Omega_p, \mathbb{C})$ satisfying $\forall v \in H^1(\Omega_p, \mathbb{C})$:

$$\underbrace{\int_{\Omega_p} a(x)u'(x)v'(x)\, dx}_{=: a_1(u,v)} - \omega^2 \underbrace{\int_{\Omega_p} u(x)v(x)\, dx}_{=: a_0(u,v)} - \underbrace{w_l v(0) + w_r v(p)}_{=: <w,v>_{\Gamma_b}} = 0. \tag{4.21}$$

For given ω we define the bilinear form $a(u, v) = a_1(u, v) - \omega^2 a_0(u, v)$ for $u, v \in V := H^1(\Omega_p)$ and claim the the quasi-periodicity of u explicitely.

Discretization and the Galerkin-FE-system We choose a finite element mesh with n nodes $(x_1, ..., x_n)$, a FE-subspace $V_h = span\{\, p^{(i)} \mid i = \overline{1,n} \,\} \subset V = H^1(\Omega_p)$ with $(p^{(i)})_{i=\overline{1,n}}$ denoting the finite elment base of V_h with $p^{(i)}(x^{(j)}) = \delta_{ij}$.
Moreover we split up the set of nodes in three disjoint subsets according to Figure 4.2, the set of inner (subscript i), of left boundary (subscript l) and of right boundary (subscript r) nodes with $x_i := (x_1, ..., x_{n-2})$, $x_l := x_{n-1}$, $x_r := x_n$. The periodical boundary nodes are denoted separately with the subscript b: $x_b := (x_l, x_r)$.

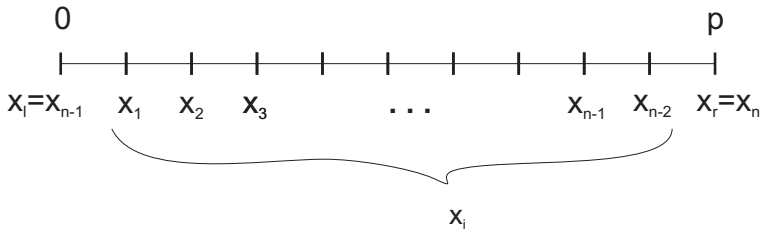

Figure 4.2: Splitting in inner, left and right vertices

By setting $K_{i,j} = a(p^{(i)}, p^{(j)})$ and $u_h(x) = \sum_{i=1}^{n} u_i p^{(i)}(x)$ with $\underline{u}_h = (u_i)_{i=\overline{1,n}} \in \mathbb{C}^n$ we get a linear system with unknown right side

$$K\underline{u}_h - \underline{w}_h = 0 \tag{4.22}$$

$$\text{with } \underline{u}_h = \begin{pmatrix} u_1 \\ \vdots \\ u_{n-1} \\ u_l \\ u_r \end{pmatrix} \text{ and } \underline{w}_h := (< w, p^{(i)} >_{\Gamma_b})_{i=\overline{1,n}} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ w_l p^{(l)}(0) \\ w_r p^{(r)}(p) \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ w_l \\ w_r \end{pmatrix}.$$

In the next step we split the system in inner and boundary nodes. We achieve

$$\left(\begin{array}{c|c} K_i & K_{ib} \\ \hline K_{bi} & K_b \end{array}\right) \begin{pmatrix} \underline{u}_i \\ \underline{u}_b \end{pmatrix} = \begin{pmatrix} 0 \\ w_b \end{pmatrix}. \tag{4.23}$$

Due to the sparse right side we can eliminate the inner nodes u_i. Eliminating $\underline{u}_i$ from the first equation and putting it into the second one gives the smaller Schur-complement system

$$\underbrace{(-K_{bi}K_i^{-1}K_{ib} + K_b)}_{=: S \in \mathbb{R}_2^2 \text{ Schur-complement}} u_b = w_b. \tag{4.24}$$

Considering the quasi-periodic boundary conditions

$$\underline{u}_b = \begin{pmatrix} u_l \\ u_l\,\gamma \end{pmatrix}, \quad \underline{w}_b = \begin{pmatrix} w_l \\ -w_l\,\gamma \end{pmatrix}$$

leads to 2 equations in 3 variables $(u_l, w_l, \gamma = e^{i\beta p})$

$$\left.\begin{array}{rcl} S_{11}u_l + \gamma S_{12}u_l &=& w_l \\ S_{21}u_l + \gamma S_{22}u_l &=& -\gamma w_l \end{array}\right\} \quad \Rightarrow \quad S_{12}\gamma^2 u_l + (S_{11}+S_{22})\gamma u_l + S_{21}u_l = 0 \tag{4.25}$$

with the notation $S = (S_{ij})_{i,j=1,2}$.
If u_l does not vanish identically, we get a **quadratic equation in $\boldsymbol{\gamma}$**

$$S_{12}\gamma^2 + (S_{11}+S_{22})\gamma + S_{21} = 0. \tag{4.26}$$

Remark 4.3.3 *Since $S_{12} = S_{21} \neq 0$, the eigenvalues occur in the pair $\{\gamma, \frac{1}{\gamma}\}$, if γ solves (4.26).*

Conclusion:
In 1 dimension the model for the wave equation leads to a quadratic equation. With given ω the the dispersion context between ω and γ can be easily evaluated as a function $\gamma(\omega)$. The next question is how the evaluation of this context changes if we go up to two dimensions.

4.4 Model of wave equation with periodical coefficients in 2D

Modeling the 2D problem is comparable to the way we have done it in the 1D case. We present 3 variants of solution methods, they all result in eigenvalue problems (generalized linear and nonlinear). Two of them evaluate the dispersion relation as searching the propagation constant depending on given frequency, i.e. $\gamma(\omega)$, and the other the inverse mapping via given propagation constant, i.e. $\omega(\gamma)$. Since we want to get an idea of the whole diagram of dispersion, there is initially no advantage of any of the three methods.

4.4.1 Periodic geometry and Floquet-Bloch theorem

We chose the strip $\Omega := \mathbb{R} \times [0, H]$ as underlying geometry.
We want to solve the 2 dimensional harmonic wave equation with periodic coefficients in direction of propagation (x_1-direction) in Ω with boundary conditions according to Figure 4.3:

Search for a solution $u(x,t) \in C^2(\Omega \times \mathbb{R})$

$$\boxed{\operatorname{div}_x \left(a(x)\nabla_x u(x,t)\right) = u_{tt}(x,t) \quad \text{with } \; a(x_1+p, x_2) = a(x_1, x_2).} \tag{4.27}$$

The positive function $a \in C^1(\mathbb{R}^2)$ describes the periodical properties of the material in x_1-direction, i.e.

$$a(x_1 + p, x_2) = a(x_1, x_2) \;\forall\, x_1 \in \mathbb{R},\; \forall\, x_2 \in [0, H]. \tag{4.28}$$

We note that for the later derived weak formulation periodic $a \in L^\infty(\Omega)$ with $0 < \underline{a} \leq a(x) \leq \overline{a}$ for almost all $x \in \Omega$ will be sufficient.
We use again a harmonic ansatz of the form

$$\hat{u}(x_1, x_2, t) = \hat{u}(x_1, x_2)\, e^{i\omega t}. \tag{4.29}$$

Suppressing the hat marker, we get the partial differential equations only in space:

Search for $u \in C^2(\Omega, \mathbb{C})$

$$-div(a\nabla u(x)) = \omega^2 u(x) \quad \forall x \in \Omega. \tag{4.30}$$

Remark on the choice of boundary conditions:
The periodic coefficient already simulates the periodic geometry. We choose periodical arranged homogenous Dirichlet boundary conditions due to the fact that in the piezoelectric model, we want to achieve in the final step, an equivalent boundary condition is claimed on the potential.

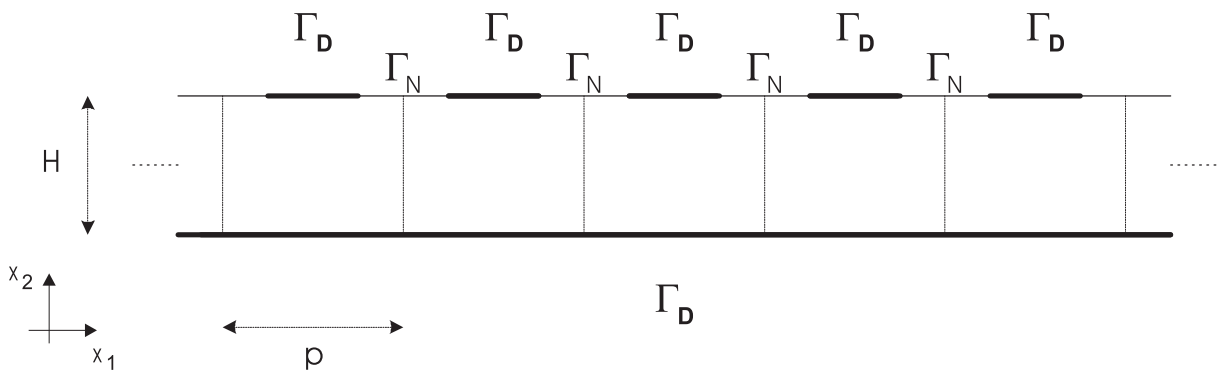

Figure 4.3: Infinite periodical cluster 2D (Ω)

Since the propagation of surface waves should be negligible within depth of a few wavelength we set also zero-Dirichlet conditions on the bottom.

Theorem 4.4.1 (Bloch's Theorem 2D)
Assume a given operator $A : C^2(\Omega, \mathbb{C}) \to C(\Omega, \mathbb{C})$, which is invariant over translation T_p of period p in x_1-direction, i.e.

$$T_p A = A T_p \quad with \quad \begin{array}{rccc} T_p : & C^2(\mathbb{R}^2, \mathbb{C}) & \to & C^2(\mathbb{R}^2, \mathbb{C}) \\ & f(.,.) & \to & f(.+p,.) \end{array} .$$

Then the eigenfunction of A can be chosen quasi-periodicly in x_1-direction :

$$\exists\, \alpha, \beta \in \mathbb{R} \forall\, (x_1, x_2) \in \Omega \; : \; u(x_1, x_2) = u_p(x_1, x_2) e^{(\alpha + i\beta) x_1} \tag{4.31}$$

with periodic function $u_p(x_1 + p, x_2) = u_p(x_1, x_2) \;\; \forall\, (x_1, x_2) \in \Omega$,
this is equal to

$$\exists\, \beta \in \mathbb{R} \forall\, (x_1, x_2) \in \Omega \; : \; u(x_1 + p, x_2) = u(x_1, x_2) e^{i(\alpha + i\beta) p} \tag{4.32}$$

Implying that for each eigenspace $\mathcal{E}_A(\lambda) := \{v \in \; | Av = \lambda v\}$ (with $dim(\mathcal{E}_A(\lambda) =: m$), there is a base of eigenfunctions $\tilde{\Phi} = (\tilde{\phi}_1, ..., \tilde{\phi}_m)$ satisfying

$$A\tilde{\phi}_j = \lambda \tilde{\phi}_j \;\; and \;\; T_p \tilde{\phi}_j = e^{(\alpha_j + i\beta_j) p} \tilde{\phi}_j . \tag{4.33}$$

Proof: A proof for $\alpha = 0$ is given in Lions [9]. The general case is treated in Kuchment [19].

Remark 4.4.2 *on theorem 4.4.1*
Bloch's theorem states that every eigenvector of the eigenvalue-problem $Av = \lambda v$ can be decomposited into so called Bloch-waves of the form (4.33).
Therefore the solution is fully described by quasi-periodic functions and we can restrict the solution set to this special form :
Search eigenvectors $u \in C^2(\Omega)$ solving $Au = \lambda u$ of the form

$$u(x_1 + p, x_2) = e^{(\alpha_j + i\beta_j)p} u(x_1, x_2) \qquad \forall (x_1, x_2) \in \Omega, \tag{4.34}$$

or of the equivalent form

$$u(x_1, x_2) = e^{(\alpha_j + i\beta_j)x_1} u_p(x_1, x_2) \qquad \forall (x_1, x_2) \in \Omega \tag{4.35}$$

with $u_p \in C^2(\Omega, \mathbb{C})$ periodic in x_1-coordinate, i.e. $u_p(x_1, x_2) = u_p(x_1 + p, x_2)\, \forall (x_1, x_2) \in \Omega$.

Remark 4.4.3 *on Bloch decomposition*
Due to Bloch's theorem every eigenvector can be written as a discrete sum of quasi-periodic Bloch waves. The parameter α of each Bloch wave describes the attenuation per period. If $\alpha > 0$ the parameter describes the attenuation of "forward-running" waves, i.e. propagation in x_1-direction is positive, and $\alpha < 0$ the attenuation of "backward-running" waves, i.e. propagation in x_1-direction is negative. Since we view a periodic medium and are mainly interested in waves which propagate in the whole periodic geometry, we can restrict the numerical calculation on pure propagating modes ($\alpha = 0$) and Bloch-waves with attenuation parameter α smallest in magnitude.
We will first solve the problem of pure propagating modes and then extend the problem to attenuated Bloch-waves, where we are interested in solutions according to α smallest in magnitude.

4.4.2 Restriction to the unit cell

Due to the validity of Bloch's theorem, we can restrict the problem (4.30) to the unit cell $\Omega_p := [0, p] \times [0, H]$. Bloch waves on the unit-cell fully describes the solutions on the infinite strip.

We use the notation $\gamma := e^{(\alpha + i\beta)p}$ and primarly consider only non-attenuated (pure-propagating) waves, i.e. $\alpha = 0$.

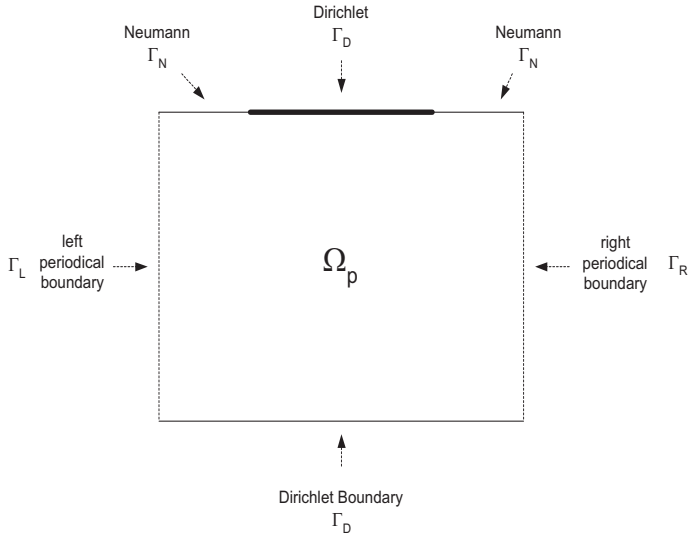

Figure 4.4: Restriction to the unit cell 2D (Ω_p)

Classical formulation Search for a function $u \in C^2(\Omega_p, \mathbb{C})$ which solves $\forall\, x \in \Omega_p$:

$$-div(a(x)\nabla u(x)) - \omega^2 u(x) = 0 \tag{4.36}$$

with $a \in C^1(\Omega_p)$ and $a(0) = a(p)$ satisfying the boundary conditions (see Figure 4.4)

$$\begin{array}{lll} \text{Dirichlet boundary:} & u(x) = 0 & \text{on } \Gamma_D \\ \text{Neumann boundary:} & \frac{\partial u}{\partial N}(x) := a(x)\frac{\partial u}{\partial n}(x) = 0 & \text{on } \Gamma_N \\ \text{Periodic boundary:} & \Gamma_L\,,\ \Gamma_R & \\ & u(p, x_2) = \gamma u(0, x_2) & \forall x_2 \in [0, H] \\ & \frac{\partial u}{\partial N}(p, x_2) = -\gamma \frac{\partial u}{\partial N}(0, x_2) & \forall x_2 \in [0, H] \end{array} \tag{4.37}$$

$$\left.\begin{array}{l} \forall x \in \Gamma_L: \quad \tilde{w}_l(x) := \frac{\partial u}{\partial N}(x) \\ \forall x \in \Gamma_R: \quad \tilde{w}_r(x) := \frac{\partial u}{\partial N}(x) \end{array}\right\} \quad \tilde{w}_r(x) = -\gamma \tilde{w}_l(x)$$

with $\frac{\partial u}{\partial n}(x)$ for $x \in \Gamma$ describing the partial derivation in direction of the normal vector (pointing to the exterior of Ω_p) of the according boundary Γ.
The conditions stated on the quasi-periodic boundaries stem from applying and differentiating equation (4.34).

Variational formulation We start with the classical problem and test it with functions v of the testspace V_0 (specified later)

$$\int_{\Omega_p} div_x(a(x)\nabla u(x))\,.\,v(x)\,dx - \int_{\Omega_p} \omega^2 u(x)v(x)\,dx = 0.$$

Integration by parts leads to

$$\int_{\Omega_p} a(x)\nabla u(x)\nabla^T v(x)\,dx - \int_{\Gamma_D\cup\Gamma_N} \frac{\partial u}{\partial N}(x)v(x)\,ds - \int_{\Omega_p} \omega^2 u(x)v(x)\,dx - \int_{\Gamma_L\cup\Gamma_R} \frac{\partial u}{\partial N}(x)v(x)\,ds = 0.$$

By choosing test-functions which vanish on the Dirichlet-boundary (essential boundary condition), i.e.

$$V_0 := \{v \in H^1(\Omega_p, \mathbb{C}) : v(x) = 0 \text{ on } \Gamma_D\} \tag{4.38}$$

the boundary integral over Γ_D gets zero. Under consideration of the Neumann-conditions (natural boundary condition) we get

$$\int_{\Omega_p} a(x)\nabla u(x)\nabla^T v(x)\,dx - \int_{\Omega_p} \omega^2 u(x)v(x)\,dx - \int_{\Gamma_L\cup\Gamma_R} \frac{\partial u}{\partial N}(x)v(x)\,ds = 0.$$

Since the solution has to satisfy the stated boundary conditions (in the weak sense) we choose the search space as

$$V_p := V_0 \cap \{u \in V = H^1(\Omega_p) \,|\, u(x_1, x_2) = \gamma u(x_1 + p, x_2)\}.$$

Under condition (4.37) for the flux $\tilde{w}_l$,$\tilde{w}_r$ over the periodic boundaries, we get the **weak formulation:**

Search for a solution $u \in V_p$: $\quad \forall v \in V_0$

$$\underbrace{\int_{\Omega_p} a(x)\nabla u(x)\nabla^T v(x)\,dx}_{=:a_1(u,v)} - \omega^2 \underbrace{\int_{\Omega_p} u(x)v(x)\,dx}_{=:a_0(u,v)} - (\underbrace{\int_{\Gamma_L} \tilde{w}_l(x)v(x)\,ds \int_{\Gamma_R} \tilde{w}_r(x)v(x)\,ds}_{=:<\tilde{w},v>_{\Gamma_b}}) = 0. \tag{4.39}$$

Remark 4.4.4 *Properties of the stated bilinear forms* $a_0(.,.), a_1(.,.) : \; H^1 \times H^1 \to \mathbb{R}$: *Both are* symmetric *and* continuous. *Moreover,* $a_1(.,.)$ *is* elliptic *for* $a(.) \in L_\infty(\Omega_p)$ *with* $0 < \underline{a} \le a(x) \le \overline{a}$ *for* x *a.e. in* Ω_p *and* $a_0(.,.)$ *is positive.*

Supplementary, we define the bilinear form $a(u,v) := a_1(u,v) - \omega^2 a_0(u,v)$ for given ω in $\mathbb{R}_0^+$.

Remark 4.4.5 *The problem arises that the chosen test space in the weak formulation is bigger than the search space. If we treat the flux over the left boundary as independent function of* u *and extend the serach space with* w_l *the spaces become isomorph.*
$V_{wph} = \{(u,w) \in H^1(\Omega), L^2(\Gamma_L \cup \Gamma_R) \,|\, u \in V_{0p}, w = \sum_{i=1}^{n_l} w^{l(i)}(p^{l(i)} - \gamma p^{r(i)}) \,,\, w^{(\,l(i)} \in \mathbb{C}\}$
For easier notation/assembling we choose u *in* V_{0h} *and incorporate the quasi-periodicity explicitely in the discretized matrix equation.*

FE-Discretization and Galerkin problem We choose a regular triangulation with following supplementary properties: We have a mesh of n nodes which we split up in $n = n_i + n_d + n_l + n_r$ with n_d denoting the nodes according to Dirichlet boundary, n_l, n_r according to the left and right boundary (quasi-periodical boundaries) excluding Dirichlet nodes and n_i denoting all remaining nodes (including the nodes on the Neumann boundary).
Morover, we assume a grid, in which right and left boundary have an identical connection. We introduce the index mappings $d(.), l(.), r(.), i(.) : \{1, ..., n_*\} \rightarrow \{1, ..., n\}$ and supplementary $x_{r(i)} = x_{l(i)} + (0, p)$ for $i = \overline{1, n_l}$.

We choose the FE-subspaces

$$\begin{aligned}
V_h &:= span\{p^{(j)}\, j = \overline{1,n} \,:\, p^{(j)} \text{ base function acc. to node } x_j\} && \subset V = H^1(\Omega_p),\\
V_{0h} &:= \{u_h = \textstyle\sum_{j=1}^{n} u^{(j)} p^{(j)} \mid u^{(j)} \in \mathbb{C} \text{ with } u_{d(i)} = 0 \text{ for } i = \overline{1, n_d}\} && \subset V_h,\\
V_{ph} &:= \{u_h \in V_{0h} \text{ with } u^{r(i)} = \gamma u^{l(i)} \text{ for } i = \overline{1, n_l}\} &&\\
&= \{\textstyle\sum_{j=1}^{n_i} u^{i(j)} p^{i(j)} + \sum_{j=1}^{n_l} u^{l(j)} (p^{l(j)} + \gamma p^{r(j)})\} && \subset V_{0h} \subset V_h
\end{aligned}$$

The discretization is done by formulating the weak problem within search space and test space both V_{0h}. We get $N := n - n_d$ according to the setting $v_h = p^{(i)}$ for $i \in \{1, ..., n\} \setminus \text{range}(d(.))$.
During the computation we treat the flux $\tilde{w}_l, \tilde{w}_r = -\gamma \tilde{w}_l$ over the quasi-periodical boundaries as unknown from the displacement u independent functions. We will see that in the discretized equation one can drop the flux vector after consideration of their quasi-periodicity.

We get the **Galerkin-FE-system** (note that $\underline{w}$ is also unknown)

$$\boxed{\text{Search } \underline{u} \in \mathbb{C}^N \text{ and } (\gamma \text{ or } \omega) : \quad (K - \omega^2 M)\,\underline{u} - \underline{w} = 0,} \tag{4.40}$$

or in more detail

$$\begin{pmatrix} K_{ii} & K_{il} & K_{ir} \\ K_{li} & K_{ll} & K_{lr} \\ K_{ri} & K_{rl} & K_{rr} \end{pmatrix} \begin{pmatrix} u_i \\ u_l \\ u_r \end{pmatrix} - \omega^2 \begin{pmatrix} M_{ii} & M_{il} & M_{ir} \\ M_{li} & M_{ll} & M_{lr} \\ M_{ri} & M_{rl} & M_{rr} \end{pmatrix} \begin{pmatrix} u_i \\ u_l \\ u_r \end{pmatrix} - \begin{pmatrix} 0 \\ w_l \\ -\gamma w_l \end{pmatrix} = 0 \tag{4.41}$$

under the quasi-periodic condition

$$\boxed{u_r = \gamma u_l\ .} \tag{4.42}$$

The system is defined by following notations:

$$\begin{aligned}(K_{ii})_{kj} &= a_1(p^{i(k)}, p^{i(j)}) \quad \forall\, k = \overline{1,n_i},\ j = \overline{1,n_i}\\ (K_{il})_{kj} &= a_1(p^{i(k)}, p^{i(j)}) \quad \forall\, k = \overline{1,n_i},\ j = \overline{1,n_l}\end{aligned}$$

analogous for $K_{rr}, K_{ri}, K_{rl}, K_{ir}, K_{li}, K_{lr}$

$$\begin{aligned}(M_{ii})_{kj} &= a_0(p^{i(k)}, p^{i(j)}) \quad \forall\, k = \overline{1,n_i},\ j = \overline{1,n_i}\\ (M_{il})_{kj} &= a_0(p^{i(k)}, p^{i(j)}) \quad \forall\, k = \overline{1,n_i},\ j = \overline{1,n_l}\end{aligned}$$

analogous for $M_{rr}, M_{ri}, M_{rl}, M_{ir}, M_{li}, M_{lr}$

We state the stiffness matrix $K := \begin{pmatrix} K_{ii} & K_{il} & K_{ir} \\ K_{li} & K_{ll} & K_{lr} \\ K_{ri} & K_{rl} & K_{rr} \end{pmatrix} \in \mathbb{R}_N^N$,

the mass matrix $M := \begin{pmatrix} M_{ii} & M_{il} & M_{ir} \\ M_{li} & M_{ll} & M_{lr} \\ M_{ri} & M_{rl} & M_{rr} \end{pmatrix} \in \mathbb{R}_N^N$ *and*

the displacement vector $\underline{u} := \begin{pmatrix} u_i \\ u_l \\ u_r \end{pmatrix} \in \mathbb{C}^N$ *with* $\begin{aligned} u_i &= \left(u^{i(j)}\right)_{j=\overline{1,n_i}} \\ u_l &= \left(u^{l(j)}\right)_{j=\overline{1,n_l}} \\ u_r &= \left(u^{r(j)}\right)_{j=\overline{1,n_r}} \end{aligned}$.

The flux vector is defined as $\underline{w} \in \mathbb{C}^N$ *with the components*

$$\underline{w}_i = \begin{cases} 0 & \text{for } i \in \{1, ..., n_i\} \\ \int_{\Gamma_L} \tilde{w}_l p^{l(i)}(x)\, ds =: w_{l,i} & \text{for } i \in \{n_i + 1, ..., n_i + n_l\} \\ \int_{\Gamma_R} \tilde{w}_l(. - p)\, p^{r(i)}(x)\, ds =: w_{r,i} & \text{for } i \in \{n_i + n_l + 1, ..., N\} \end{cases}.$$

Remark 4.4.6 *We have implicitly dropped the elements according to Dirichlet nodes since* $u_{d(.)} = 0,\ w_{d(.)} = 0$

Including the quasi-periodicity (4.42) in the Galerkin-system (4.40) we achieve

$$\begin{pmatrix} K_{ii} & K_{il} & K_{ir} \\ K_{li} & K_{ll} & K_{lr} \\ K_{ri} & K_{rl} & K_{rr} \end{pmatrix} \begin{pmatrix} u_i \\ u_l \\ \gamma u_l \end{pmatrix} - \omega^2 \begin{pmatrix} M_{ii} & M_{il} & M_{ir} \\ M_{li} & M_{ll} & M_{lr} \\ M_{ri} & M_{rl} & M_{rr} \end{pmatrix} \begin{pmatrix} u_i \\ u_l \\ \gamma u_l \end{pmatrix} - \begin{pmatrix} 0 \\ w_l \\ -\gamma w_l \end{pmatrix} = 0. \tag{4.43}$$

Remark 4.4.7 *Some properties of mass and stiffness matrix:*

1. *K,M are sparse matrices.*
2. *We assume that the mesh is large enough that left and right boundary have no common element. There is no direct coupling between left and right nodes, which implies that*
$$K_{lr} = K_{rl} = M_{lr} = M_{rl} = 0.$$
3. *K, M are symmetric positive definite matrices, i.e. the diagonal blocks $K_{ii}, K_{ll}, K_{rr}, M_{ii}, ...$ are symmetric, positive definite.*

4.4.3 Three solution approaches

We present three approaches for computing the dispersion context. They are developed by the author and therefore no references can be given for the following methods. In the first and third approach presented we assume given frequency and search the propagation constant, i.e. $\gamma(\omega)$ and in the second one the propagation constant is given and we ask for the context $\omega(\gamma)$. All three result in eigenvalue problems (of linear or quadratic form).

For given $\omega \in \mathbb{R}_0^+$ we define the system matrix $\overline{K}$ with the blocks

$$\overline{K}_{**} := K_{**} - \omega^2 M_{**} \qquad \text{for } * = i, l, r \tag{4.44}$$

Approach 1: Schur-Complement Method for given ω (SC-Method)
This approach is analogous to the method used in the 1D model. We assume that ω given satisfies $\omega^2 \notin \sigma(M^{-1}K)$, i.e. $\overline{K}$ regular. We split the system matrix in inner and boundary nodes

$$\overline{K}(\omega) = \overline{K} = \left(\begin{array}{c|cc} \overline{K}_{ii} & \overline{K}_{il} & \overline{K}_{ir} \\ \hline \overline{K}_{li} & \overline{K}_{ll} & \overline{K}_{lr} \\ \overline{K}_{ri} & \overline{K}_{rl} & \overline{K}_{rr} \end{array}\right) =: \begin{pmatrix} \overline{K}_{ii} & \overline{K}_{ib} \\ \overline{K}_{bi} & \overline{K}_{bb} \end{pmatrix},$$

compute the Schur-complement

$$S := (-K_{bi}K_{ii}^{-1}K_{ib} + K_{bb}) =: \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} = S^T \in \mathbb{R}^{2\,n_l}_{2\,n_l} \tag{4.45}$$

and get

$$\begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} u_l \\ \gamma u_l \end{pmatrix} = \begin{pmatrix} w_l \\ -\gamma\, w_l \end{pmatrix}.$$

Multiplying the first line with γ and adding first and second line elimenates w_l and we get a **quadratic eigenvalue problem** in γ:

$$\boxed{\gamma^2 S_{12} u_l + \gamma(S_{11} + S_{22})u_l + S_{21}u_l = 0.} \tag{4.46}$$

Conclusion:
The Schur-Complement Method results in a quadratic eigenvalue problem with real matrices of moderate size ($n_l \times n_l$) (compared to the original problem dimension $N = n_i + 2n_l$ with $n_i \gg n_l$). But it has the drawback that the computation of the Schur-complement requires the inversion of the "large" matrix K_{ii} for every given ω and destroys sparsity of matrices, moreover we cannot state special properties of the block matrices of S.
We have to look for solution methods of quadratic eigenvalue problems of the form:

$$\text{Search } x \in \mathbb{C}^n \text{ and } \lambda \in \mathbb{C} \text{ with } |\lambda| = 1: \quad (\lambda^2 A + \lambda B + A^T)x = 0 \quad \text{with } B = B^T \tag{4.47}$$

with A, B real dense matrices of quite moderate size.

Approach 2: Given propagation constant γ

We start with the Galerkin-system

$$K \begin{pmatrix} u_i \\ u_l \\ \gamma u_l \end{pmatrix} - \omega^2 M \begin{pmatrix} u_i \\ u_l \\ \gamma u_l \end{pmatrix} = \begin{pmatrix} 0 \\ w_l \\ -\gamma w_l \end{pmatrix} \tag{4.48}$$

and bear in mind that K, M are symmetric and positive definite matrices.
If the right side of the Galerkin-system (4.48) was zero, the problem would turn into a generalized eigenvalue problem.
This states the question after a matrix transformation which eliminates the right side while preserving symmetry and positive definiteness, i.e. we serach a transformation of the form $T^H K T - \omega^2 T^H M T$.

We can reformulate vectors to get a possible transformation matrix T via

$$(K - \omega^2 M) \underbrace{\begin{pmatrix} I_i & 0 \\ 0 & I_l \\ 0 & \gamma I_l \end{pmatrix}}_{:=T} \begin{pmatrix} u_i \\ u_l \end{pmatrix} = \begin{pmatrix} 0 \\ I_l \\ -\gamma \end{pmatrix} w_l.$$

Multiplying with $\tilde{T}^H := \begin{pmatrix} I_i & 0 & 0 \\ 0 & \gamma I_l & I_l \end{pmatrix}$ from the left eliminates the right side of the system, but destroys symmetry.

Considering the fact that $\gamma = e^{i\beta p}$ and hence $\gamma.\bar{\gamma} = 1$, we can expand $\tilde{T}^H$ to $\tilde{T}^H = \underbrace{\begin{pmatrix} I_i & 0 \\ 0 & \gamma I_l \end{pmatrix}}_{\text{regular}} T^H$, i.e. $T^H w = 0$.

We can transform the Galerkin system by multiplying with

$$T^H := \begin{pmatrix} I_i & 0 & 0 \\ 0 & I_l & \bar{\gamma} I_l \end{pmatrix} \tag{4.49}$$

from the left into a **generalized eigenvalue problem**

$$\boxed{T^H K T \tilde{u} = \omega^2 T^H M T \tilde{u}} \qquad \text{with } \tilde{u} := \begin{pmatrix} u_i \\ u_l \end{pmatrix}. \tag{4.50}$$

Remark 4.4.8 *Properties of the matrices $T^H KT, T^H MT$*

1. *The matrices are complex-valued through $\gamma \in \mathbb{C}$*
2. *The matrices are obviously hermitian, since K, M are hermitian (symmetric).*
3. *The positive definiteness is preserved:*
   $(T^H KTx, x) = (KTx, Tx) > 0 \; \forall x \neq 0$, since $(Kx, x) > 0 \; \forall x \neq 0$ and
   $(Tx = 0 \Leftrightarrow x = 0)$.
4. *The transformation preserves sparsity of the matrices.*

Conclusion:
For given $\gamma \in \mathbb{C}$ the method requires the solution of a generalized eigenvalue problem

$$\text{Search } \lambda \in \mathbb{R}_0^+ \text{ and } x \in \mathbb{C}^m : \quad Ax = \lambda Bx$$

with complex-valued, sparse, hermitian and positive definite matrices A, B of dimension $(m \times m)$, where $m = n_i + n_l$.

Approach 3: Inner-Node-Matrix Method for given ω (INM-Method)

In the Schur-Complement Approach we got a quadratic eigenvalue problem to compute γ by given frequency ω.
The second approach (for given γ) gives the idea for another method for given frequency avoiding the computation of the Schur-complement.

We start with the system matrix

$$\overline{K}(\omega) = \begin{pmatrix} \overline{K}_{ii} & \overline{K}_{il} + \gamma\overline{K}_{ir} \\ \overline{K}_{li} & \overline{K}_{ll} + \gamma\overline{K}_{lr} \\ \overline{K}_{ri} & \overline{K}_{rl} + \gamma\overline{K}_{rr} \end{pmatrix} \begin{pmatrix} u_i \\ u_l \end{pmatrix} = \begin{pmatrix} 0 \\ w_l \\ -\gamma w_l \end{pmatrix}.$$

Mutliplying with $\begin{pmatrix} I_i & 0 & 0 \\ 0 & \gamma I_l & I_l \end{pmatrix}$ from the left side eliminates the right side and we get

$$\begin{pmatrix} \overline{K}_{ii} & \overline{K}_{il} + \gamma\overline{K}_{ir} \\ \gamma\overline{K}_{li} + \overline{K}_{ri} & \gamma\overline{K}_{ll} + \gamma^2\overline{K}_{lr} + \overline{K}_{rl} + \gamma\overline{K}_{rr} \end{pmatrix} \begin{pmatrix} u_i \\ u_l \end{pmatrix} = \begin{pmatrix} 0 \\ \gamma w_l - \gamma w_l \end{pmatrix}. \tag{4.51}$$

Extracting γ leads to a quadratic eigenvalue problem

$$\left(\gamma^2 \begin{pmatrix} 0 & 0 \\ 0 & \overline{K}_{lr} \end{pmatrix} + \gamma \begin{pmatrix} 0 & \overline{K}_{ir} \\ \overline{K}_{li} & \overline{K}_{ll} + \overline{K}_{rr} \end{pmatrix} + \begin{pmatrix} \overline{K}_{ii} & \overline{K}_{il} \\ \overline{K}_{ri} & \overline{K}_{rl} \end{pmatrix} \right) \begin{pmatrix} u_i \\ u_l \end{pmatrix} = 0$$

under consideration of the special structure of $\overline{K}$ mentioned in Remark 4.4.7 the quadratic term vanishes.
We get a **generalized linear eigenvalue problem**

$$\boxed{\begin{pmatrix} \overline{K}_{ii} & \overline{K}_{il} \\ \overline{K}_{ir}^T & 0 \end{pmatrix} \begin{pmatrix} u_i \\ u_l \end{pmatrix} = \gamma \begin{pmatrix} 0 & -\overline{K}_{ir} \\ -\overline{K}_{il}^T & -(\overline{K}_{ll} + \overline{K}_{rr}) \end{pmatrix} \begin{pmatrix} u_i \\ u_l \end{pmatrix}.} \tag{4.52}$$

Conclusion: The Inner-Node-Matrix Approach results in a generalized eigenvalue problem

Search $x \in \mathbb{C}^m$ and $\lambda \in \mathbb{C}$ with $|\lambda| = 1$:

$$Ax = \lambda Bx \quad \text{of the form } A = \begin{pmatrix} M_1 & G \\ F^T & 0 \end{pmatrix},\ B = \begin{pmatrix} 0 & -F \\ -G^T & -M_2 \end{pmatrix}$$

The matrices A, B are real-valued, sparse and of dimension $(m \times m)$ with $m := n_i + n_l$.
If we assume that ω is given the way that $\overline{K} = K - \omega^2 M$ is regular, then the diagonal blocks M_1, M_2 are regualr and the matrix $A - B$ is regular and symmetric.

Remark 4.4.9

1. *The question arises if through dropping w_l out of the system by adding two blocks of equations this has probably an unwanted effect on the spectrum, i.e. one drops eigenvalues ?*
   Rewriting the system gives

$$\begin{pmatrix} \overline{K}_{ii} & \overline{K}_{il} & 0 \\ \overline{K}_{il}^T & \overline{K}_{ll} & I_l \\ \overline{K_{ri}}^T & 0 & 0 \end{pmatrix} \begin{pmatrix} u_i \\ u_l \\ w_l \end{pmatrix} = \gamma \begin{pmatrix} 0 & -\overline{K}_{ir} & 0 \\ 0 & 0 & 0 \\ 0 & -\overline{K}_{rr} & I_l \end{pmatrix} \begin{pmatrix} u_i \\ u_l \\ w_l \end{pmatrix}$$

   One can see that adding the last two line blocks eliminates N_l zero lines on the right side of the eigenvalue problem. In the chapter of eigenvalue theory we will see that these lines accord to infinite eigenvalues which we are not interested in. The spectrum of finite eigenvalues remains unchanged through this adding of equations. We get all interesting eigenvalues if we solve the Inner-Node-Matrix system.

2. Interpretation of the Inner-Node-Matrix Problem:
   We treat the question of what weak formulation leads directly to the Inner-Node-Matrix system:
   Setting $\tilde{w}_r = \tilde{w}_l(. - p)$ and choosing the searchspace V_p and the testspace $V_{p2} := V_0 \cap \{v \in V = H^1(\Omega_p) \,|\, \gamma v(x_1, x_2) = v(x_1 + p, x_2)\}$

Remark 4.4.10 *We have chosen for test and searchspace the whole space, claimed the periodicity condition for u explicitly. Then we introduced a variable w for the flux and treated it independent of u. We discretized the weak formulations and hoped that the achieved matrices can be transformed the way that the unknowns according to w will get eliminated and that we can reduce to a quadratic system. This was quite an intuitive approach, but we succeeded. But through transformations, reduction of variables and choosing the flux independent of u, do we still solve the original problem ?*
Now we give a mathematical accurate approach by a problem related choice of test and searchspace which consider the quasi-periodicity. This approach has the big advantage that the boundary integral, which we former come up by introducing the independent variable w, vanishes already in the weak formulation.

4.4.4 Stating quasi-periodic test and search space

We want that the quasi-periodicity is already considered in search and testspace and that the both spaces are isomporph.
Search and testspace have to fulfill the Dirichlet-condition, i.e. they have to be subspace of $V_0 := \{ v \in (H^1(\Omega_p)) \,|\, v = 0 \text{ on } \Gamma_D \}$.

The searchspace The solution has to satisfy the quasi-periodicity condition

$$u(x+p) = \gamma u(x) \quad \forall\, x \in \Gamma_L. \tag{4.53}$$

This holds if the searchspace is restricted to

$$V_p(\gamma) := \{ v \in V_0 \,|\, v(x+p) = \gamma v(x) \text{ for almost all } x \text{ on } \Gamma_L \} \subset V_0. \tag{4.54}$$

The quasi-periodicity condition for the flux follows from the quasi-periodicity of u.

The testspace The testspace should also represent the periodicity, which implies that test and searchspace are isomorph, i.e. let μ be an arbitrary complex scalar and define

$$V_p(\mu) := \{ v \in V_0 \,|\, v(x+p) = \mu v(x) \text{ for almost all } x \text{ on } \Gamma_L \} \qquad \text{with } \mu \in \mathbb{C} \text{ fixed .} \tag{4.55}$$

The weak formulation of the unit cell leads to

Search for a solution $u \in V_p(\gamma)$: $\quad \forall v \in V_p(\mu)$

$$\begin{aligned} 0 &= -\int_{\Omega_p} div(a\nabla u)v\, dx - \omega^2 \int_{\Omega_p} uv dx \\ &= \int_{\Omega_p} a(x)\nabla u(x)\nabla^T v(x)\, dx - \int_{\Gamma_L \cap \Gamma_R} u(x)v(x)\, ds - \omega^2 \int_{\Omega_p} u(x)v(x)\, dx. \end{aligned}$$

The remained boundary integral can be expressed as

$$\begin{aligned} \int_{\Gamma_L \cap \Gamma_R} u(x)v(x)\, ds &= \int_{\Gamma_L} u(x)v(x)\, ds + \int_{\Gamma_R} u(x)v(x)\, ds \\ &= \int_{\Gamma_L} \frac{\partial u}{\partial n}(x)v(x)\, ds + \int_{\Gamma_L} (\frac{\partial u}{\partial n(x+p)}(x+p))v(x+p)\, ds \\ &= \int_{\Gamma_L} u(x)v(x)(1-\gamma\cdot\mu)ds = (1-\gamma\cdot\mu)\int_{\Gamma_L} u(x)v(x)ds. \end{aligned}$$

Obviously, the boundary integral over the periodic bounds vanishes, if we choose

$$\mu := \frac{1}{\gamma}. \tag{4.56}$$

Weak formulation with quasi-periodic test and searchspace

Find $u \in V_p(\gamma)$:

$$\int_{\Omega_p} a(x)\nabla u(x)\nabla^T v(x)\,dx - \omega^2 \int_{\Omega_p} u(x)v(x)\,dx = 0 \quad \forall v \in V_p(\gamma^{-1}) \tag{4.57}$$

$$a_1(u,v) - \omega^2 a_0(u,v) = 0 \quad \forall v \in V_p(\gamma^{-1}) \tag{4.58}$$

Finite element discretization With shape functions $p^j(.)$ satisfying

$$\begin{aligned} p^j(x_i) &= \delta_{ij} \\ p^{l(j)}(x) &= p^{r(j)}(x+p) \qquad \forall x \text{ on } \Gamma_L \; \forall j \in \{1,..,n_l\} \end{aligned}$$

we choose the FE-subspaces of serach and testspace

$$V_{0h} := span\{\, p^i \,|\, i \in rg(i(.)) \cap rg(l(.))\,\} \tag{4.59}$$

$$V_{ph}(\gamma) := \{\, u_h \,|\, u_h = \sum_{j=1}^{n_i} u^{i(j)} p^{i(j)} + \sum_{j=1}^{n_l} u^{l(j)}(p^{l(j)} + \gamma p^{r(j)}),\; u^j \in \mathbb{C}\} \tag{4.60}$$

$$V_{ph}(\gamma^{-1}) := span\{\, p^{i(j)}\,\}_{j=\overline{1,n_i}} \cap span\{\, \gamma p^{l(j)} + p^{r(j)}\}_{j=\overline{1,n_l}}\}. \tag{4.61}$$

Choosing $v_h = p^{i(j)}$ for $j = \overline{1,n_i}$ and $v_h = \gamma p^l(j) + p^r(j)$ for $j = \overline{1,n_l}$ leads to $n_i + n_l$ equations for the $n_i + n_l$ components of $\underline{u} \in \mathbb{C}^{n_i+n_l}$. We get the Galerkin-system equation

$$\begin{pmatrix} K_{ii} & K_{il} + \gamma K_{ir} \\ \gamma K_{li} + K_{ri} & \gamma^2 K_{lr} + \gamma(K_{ll} + K_{rr}) + K_{rl} \end{pmatrix} \begin{pmatrix} u_i \\ u_l \end{pmatrix} \\ -\omega^2 \begin{pmatrix} M_{ii} & M_{il} + \gamma M_{ir} \\ \gamma M_{li} + M_{ri} & \gamma^2 M_{lr} + \gamma(M_{ll} + M_{rr}) + M_{rl} \end{pmatrix} \begin{pmatrix} u_i \\ u_l \end{pmatrix} = 0 \tag{4.62}$$

where K_{**}, M_{**} $(* = i,l,r)$ denote the blocks of stiffness and mass matrix defined in (4.43).

Note that $K_{lr} = K_{rl} = 0$.

Reformulation of the three solution approaches

Given propagation constant γ with $\gamma\bar{\gamma} = 1$

Setting $\begin{pmatrix} u_i \\ u_l \end{pmatrix} = \begin{pmatrix} I & 0 \\ 0 & \gamma \end{pmatrix} \begin{pmatrix} I & 0 \\ 0 & \bar{\gamma} \end{pmatrix} \begin{pmatrix} u_i \\ u_l \end{pmatrix}$ gives

$$\begin{pmatrix} K_{ii} & \bar{\gamma} K_{il} + K_{ir} \\ \gamma K_{li} + K_{ri} & (K_{ll} + K_{rr}) \end{pmatrix} \begin{pmatrix} u_i \\ \gamma u_l \end{pmatrix} \\ -\omega^2 \begin{pmatrix} M_{ii} & M_{il} + \gamma M_{ir} \\ \gamma M_{li} + M_{ri} & \gamma^2 M_{lr} + \gamma(M_{ll} + M_{rr}) + M_{rl} \end{pmatrix} \begin{pmatrix} u_i \\ u_l \end{pmatrix} = 0. \tag{4.63}$$

Since this transformation is regular for $\gamma \neq 0$, the transformed problem has the same spectrum. The former formulation is helpful since it provides the positive definiteness of the transformed system.

We see if we choose $\overline{K}_{**} = K_{**} + M_{**}$ and extract the blocks in γ to the right side, we get the generalized eigenvalue problem

$$\begin{pmatrix} \overline{K}_{ii} & \overline{K}_{il} \\ \overline{K}_{ri} & 0 \end{pmatrix} (u_i u_l) = \gamma \begin{pmatrix} 0 & -\overline{K}_{ir} \\ -\overline{K}_{li} & -\overline{K}_{ll} - \overline{K}_{rr} \end{pmatrix} (u_i u_l) \,. \tag{4.64}$$

This is the eigenvalue problem stated through the INM-Approach.

Concerning the SC-Method: If we take the Schur-complement in (4.64) or (4.63) via eliminating the first line block we get

$$-\gamma^2 \underbrace{\overline{K}_{li}\overline{K}_{ii}^{-1}\overline{K}_{ir}}_{S_{12}} - \gamma(\underbrace{\overline{K}_{li}\overline{K}_{ii}^{-1}\overline{K}_{il} + \overline{K}_{ri}\overline{K}_{ii}^{-1}\overline{K}_{ir} - \overline{K}_{ll} - \overline{K}_{rr}}_{=S_{11}+S_{22}}) - \underbrace{K_{ri}\overline{K}_{ii}^{-1}\overline{K}_{il}}_{=S_{21}} u_l = 0 \tag{4.65}$$

with S_{ij} Schur-complement block of (4.45). That means, we achieve the quadratic eigenvalue problem of the SC-Method.

Conclusion:
The reformulation of test and searchspace constitutes a mathematical accurate method with the result that INM-Method and SC-Method does not change, but are achieved without any transformation or at least only transformation to Schur-complement form, for the method in which we have given γ only by a similarity transformation from the right side.
Thus in the analogous to approach 2,3 the spectra of the formulated eigenvalue problems is equal to the spectra of solution of the Galerkin-system problem. The difference in the spectrum of SC-method and Inner-Node-Matrix Method will be discussed in the next but one chapter.

4.4.5 Include damping effects

There are many complex damping effects (depending on temperature, frequency, friction, material ...). Our aim is to consider two variants of damping in our model

1. **Material damping**
   This effect can be included to our model by adding a viscous damping term in the initial partial differential equation. It became naturalized (by engineers) to use a damping matrix which is proportional to the mass matrix or a combination of mass and stiffness matrix in the discretized matrix equation. This approximation is called *Rayleigh-damping*.

2. **Wave reflection at periodic perturbations**
   In each cell the incident wave gets reflected at the electrode with the result that at certain frequencies these reflected waves can interfere constructively and the amplitude of the propagating wave decreases with each cell. This attenuation occurs even independent of material damping.
   To be able to compute the dispersion relation also within the stopband we need to consider this attenuation effect in our model. Up to now we only considered the dispersion curves which belongs to undamped Bloch waves (through assuming $\alpha = 0$), i.e. the purely propagating modes.
   We are mainly interested in Bloch waves with α smallest in magnitude.

We model each damping effect on its own first.

Modeling attenuation evoked by reflection at electrodes

This effect is considered by quasi-periodic boundary conditions with non-zero attenuation in (4.37) of the classical formulation on the unit cell Ω_p.
We start with the classical formulation and consider

$$\gamma := e^{(\alpha+i\beta)p}$$

The variational formulations and discretizations (for general test-space and quasi-periodic test-spaces) are equal to the undamped problem, since we always treated γ as a general complex scalar.

Concerning the three solution methods In the Schur-Complement and Inner-Node-Matrix Method, where the frequency ω is given and we search for γ, we only have to redefine the desired solution sets in the stated eigenvalue-problems. We recall that we ware priorly interested in complex eigenvalues with norm 1.

Considering damping effects we are interested in eigenvalues with α smallest in magnitude

Approach 1: Schur-Complement Method
The method described for the undamped variant does not use the fact that the desired γ has norm 1. Therefore, only the set of desired eigenvalues has to be extended, the problem type stays the same. If we are mainly interested in propagation constants where attenuation is smallest in magnitude, we get the quadratic eigenvalue problem:

Search $u_l \in \mathbb{C}^m$ and $\gamma := e^{(\alpha+i\beta)p} \in \mathbb{C}$ with $|\alpha|$ small:

$$\gamma^2 S_{12} u_l + \gamma(S_{11} + S_{22}) u_l + S_{12}^T u_l = 0 \tag{4.66}$$

with $S := -\overline{K}_{ib}^T \overline{K}_{ii} \overline{K}_{ib} + \overline{K}_{bb} = S^T$.

Approach 3: Inner-Node-Matrix Method
The undamped version presented in the Inner-Node approach does not use the special form of γ. Therefore, only the set of desired eigenvalues extends (analogous to approach 1).
If we are interested in propagation constants with attenuation smallest in magnitude, the solution approach results in the general eigenvalue problem:

Search $\begin{pmatrix} u_i \\ u_l \end{pmatrix} \in \mathbb{C}^{(n_i+n_l)}$ and $\gamma := e^{(\alpha+i\beta)p} \in \mathbb{C}$ with $|\alpha|$ small

$$\begin{pmatrix} \overline{K}_{ii} & \overline{K}_{il} \\ \overline{K}_{ir}^T & 0 \end{pmatrix} \begin{pmatrix} u_i \\ u_l \end{pmatrix} = \gamma \begin{pmatrix} 0 & -\overline{K}_{ir} \\ -\overline{K}_{il}^T & -(\overline{K}_{ll} + \overline{K}_{rr}) \end{pmatrix} \begin{pmatrix} u_i \\ u_l \end{pmatrix} \tag{4.67}$$

with $\overline{K}_{**}$ real-valued and sparse and $\overline{K}_{ll}, \overline{K}_{rr}, \overline{K}_{ii}$ regular f.ü. (ω).

Approach 2: given propagation constant $\gamma := e^{(\alpha+i\beta)p}$
We have to adapt the transformation matrix $T(\gamma)$, since we used the fact $\gamma.\bar{\gamma} = 1$, in the undamped model.

With two distinct transformations from the left T_1 and the right T_2, we get the generalized eigenvalue problem

Search $\tilde{u} \in \mathbb{C}^{(n_i+n_l)}$ and $\omega^2 \in \mathbb{R}_0^+$:

$$T_1^H K T_2 \tilde{u} = \omega^2 T_1^H M T_2 \tilde{u} \tag{4.68}$$

with $T_1 = \begin{pmatrix} I_i & 0 \\ 0 & I_l \\ 0 & \bar{\gamma}^{-1} I_l \end{pmatrix}$, $T_2 = \begin{pmatrix} I_i & 0 \\ 0 & I_l \\ 0 & \gamma I_l \end{pmatrix}$ and $\tilde{u} = \begin{pmatrix} u_i \\ u_l \end{pmatrix}$.

We see that for the attenuated variant we loose complex-symmetry and positive definiteness of the matrices.

But the main drawback of computing ω depending on $\gamma := e^{(\alpha+i\beta)p}$ is that one has to provide a two dimensional array (α, β) to get the dispersion relation. But how should this array be chosen, especially in the case that one is interested in a special frequency domain. This method is suited to compute only pure propagating modes. If one is interested in damping effects this method is not recommended due to the complicated data preparation. Up to this it will not be analyzed anymore.

Modeling material damping

In elasticity friction depends on change of strains and on the velocity u_t. Material damping can be included to our model by adding a linear viscous damping term $c\frac{\partial u}{\partial t}$, where c is a differential operator in space, to the wave equation leading to

$$\mathrm{div}_x\left(a(x)\nabla_x u(x,t)\right) + c\frac{\partial u}{\partial t} = u_{tt}(x,t).$$

By the harmonic ansatz, we get

$$-div_x(a(x)\nabla u(x)) + i\omega c\, u(x) - \omega^2 u = 0.$$

Through a variant of Bloch's Theorem we get quasi-periodicity with attenuation, i.e.

$$\exists \alpha, \beta \in \mathbb{R}\, \forall x \in \Omega: \quad u(x) = u_p(x)e^{(\alpha+i\beta)x} \tag{4.69}$$

with $u_p(x)$ periodic function,i.e. $u_p(x) = u_p(x+p)\, \forall x \in \Omega$.
This is obviously equal to

$$\exists \alpha, \beta \in \mathbb{R}\, \forall x \in \Omega: u(x+p) = u(x)e^{(\alpha+i\beta)p}. \tag{4.70}$$

Therefore we can reduce the computation geometry to the unit cell with according boundary condition, i.e. set $\gamma := e^{(\alpha+i\beta)p}$.
It is commonly used to model the damping term in the discretized equation as a linear combination of stiffness and mass matrix as damping matrix. This is known as *Rayleigh-damping*.
We assume given positive damping coefficients c_K, c_M :

$$C := c_K K + c_M M. \tag{4.71}$$

Since K, M are symmetric and positive definite matrices, these facts are also implied on the damping matrix C.
This is equal to define the damping operator in the partial differential equation as

$$c\,\frac{\partial u}{\partial t}(.) := (c_M\, I + c_K a(.)\frac{\partial^2}{\partial x^2})\frac{\partial u}{\partial t}(.),$$

where c_M and c_K are material-depending constants.
Considering Rayleigh-damping the FE-Galerkin-system of equation (4.40) expands to

$$K\underline{u} + i\omega \underbrace{(c_K K + c_M M)}_{=C}\underline{u} - \omega^2 M\underline{u} - \underline{w} = 0. \tag{4.72}$$

Splitted in inner and periodical boundary nodes we get

$$\begin{pmatrix} K_{ii} & K_{il} & K_{ir} \\ K_{li} & K_{ll} & K_{lr} \\ K_{ri} & K_{rl} & K_{rr} \end{pmatrix} \begin{pmatrix} u_i \\ u_l \\ \gamma u_l \end{pmatrix} + i\omega \begin{pmatrix} C_{ii} & C_{il} & C_{ir} \\ C_{li} & C_{ll} & C_{lr} \\ C_{ri} & C_{rl} & C_{rr} \end{pmatrix} \begin{pmatrix} u_i \\ u_l \\ \gamma u_l \end{pmatrix} - \omega^2 \begin{pmatrix} M_{ii} & M_{il} & M_{ir} \\ M_{li} & M_{ll} & M_{lr} \\ M_{ri} & M_{rl} & M_{rr} \end{pmatrix} \begin{pmatrix} u_i \\ u_l \\ \gamma u_l \end{pmatrix} = \begin{pmatrix} 0 \\ w_l \\ -\gamma w_l \end{pmatrix}. \tag{4.73}$$

Material damping and the three solution methods
Approach 1 and 3: given frequency ω
For given ω we define the system matrix by

$$\overline{K}_{**}(\omega) = \overline{K}_{**} := K_{**} + i\omega C_{**} - \omega^2 M_{**} \quad \text{for } * = i, l, r \tag{4.74}$$

and have the following problem to solve

$$\underbrace{\begin{pmatrix} \overline{K}_{ii} & \overline{K}_{il} & \overline{K}_{ir} \\ \overline{K}_{li} & \overline{K}_{ll} & \overline{K}_{lr} \\ \overline{K}_{ri} & \overline{K}_{rl} & \overline{K}_{rr} \end{pmatrix}}_{=:\overline{K}} \begin{pmatrix} u_i \\ u_l \\ \gamma u_l \end{pmatrix} = \begin{pmatrix} 0 \\ w_l \\ -\gamma w_l \end{pmatrix}. \tag{4.75}$$

That means approach 1 and 3 are formally analogous to their variants for damping through reflection at the electrodes. With one difference that through considering material damping the system matrix $\overline{K}$ gets complex, but maintains (complex) symmetric (not hermitian!).

Approach 2 will not be treated for the reasons discussed in the paragraph of attenuation caused by periodic perturbations.

4.5 Mathematical modeling of periodical piezoelectric equations in periodical geometry

Now we want to apply the developed methods of the periodic wave equation on the piezoelectric problem.
We have to combine two problems, the piezoelectric system equations and the properties implied by the periodic geometry, this will be done the following way: We state the piezoelectric problem in classical and weak form on an infinite periodic geometry first. We formulate an abstract version of Bloch's theorem and restrict the problem to the unit cell. Then we introduce the properties of the Finite Element Method for "standard" piezoelectric problems, i.e. problems with Neumann and Dirichlet boundaries only. This stepwise construction leads us to an obvious adaptation of the methods introduced for the quasi-periodic wave equation in order to apply them to piezoelectric systems.

4.5.1 Piezoelectric equations, periodic geometry and Floquet-Bloch Theorem

To simulate the behavior of displacement vector function $u(.,.) \in C^{2,2}((\mathbb{R}^2, \mathbb{R}_0^+); \mathbb{R}^d)$ for $d = 2, 3$ and the scalar potential $\Phi(.,.) \in C^{2,0}((\mathbb{R}^2, R_0^+); \mathbb{R})$ we have to solve the piezoelectric system equations

$$\begin{aligned} \operatorname{div}_x(c^E Bu - e^T \nabla_x \Phi) &= \rho(x) \frac{\partial^2 u}{\partial t^2} && (4.76) \\ \operatorname{div}_x(eBu - \varepsilon^S \nabla_x \Phi) &= 0 && (4.77) \end{aligned}$$

with $Bu = S = \frac{1}{2}(\nabla_x^T u + \nabla_x u)$ and $\rho(x_1, x_2) = \rho(x_1 + p, x_2)$ on an infinite periodic cluster Ω shown in figure 4.5 and $\Omega_T := (\Omega, [0, T])$.
We assume all field distribution to be harmonic, i.e.

$$\begin{aligned} \hat{u}(x,t) &= e^{i\omega t} u(x) \in \mathbb{C}^d && \forall (x,t) \in \Omega_T, \\ \hat{\Phi}(x,t) &= e^{i\omega t} \Phi(x) \in \mathbb{C} && \forall (x,t) \in \Omega_T, \\ u(x,t) &= \Re\{\hat{u}(x,t)\} && \forall (x,t) \in \Omega_T, \\ \Phi(x,t) &= \Re\{\hat{\Phi}(x,t)\} && \forall (x,t) \in \Omega_T. \end{aligned}$$

For easier notation and the fact that derivatives after time become multiplications, we use the complex distribution and take the real part after computation. This is valid since all applied operations are linear.

We have already motivated problem setting (short-circuited electrodes)with boundary conditions and underlying geometry at the beginning of this section. Figure 4.5 shows once more the infinite geometry.

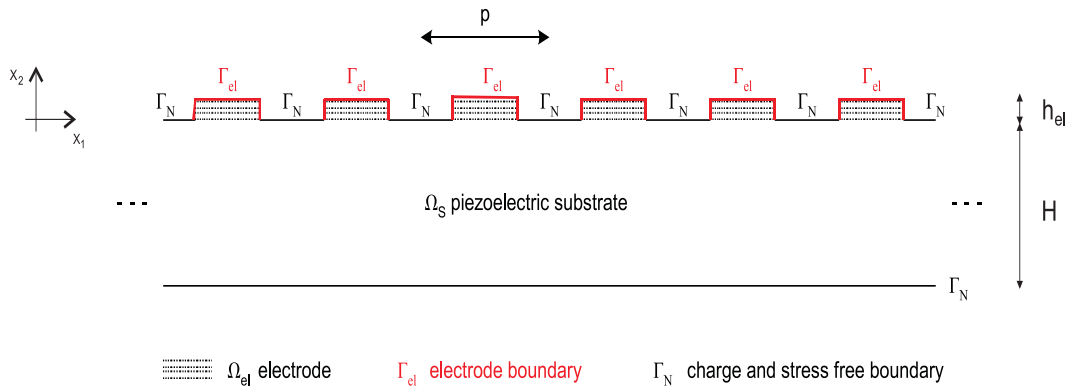

Figure 4.5: Infinite periodical cluster (Ω) of the piezoelectric model

We state the **classical formulation** of the piezoelectric model by

Searching for a $(u, \Phi) \in (C^2(\Omega, \mathbb{C}^d), C^2(\Omega, \mathbb{C}))$ which satisfies :

$$\begin{aligned} -\text{div}\,(c^E Bu + e^T \nabla\Phi) &= \rho\omega^2 u \\ -\text{div}\,(eBu - \varepsilon^S \nabla\Phi) &= 0 \end{aligned} \tag{4.78}$$

with the boundary conditions (let n denote the outer normal vector)

$$\begin{array}{llll} stress-free & T.n = 0 & \text{on } \Gamma := \partial\Omega, & \\ short-circuit & \Phi = 0 & \text{on } \Omega_{el} & \Rightarrow \Phi = 0 \text{ on } \Gamma_{el}, \\ charge-free & D.n = 0 & \text{on } \Gamma_N & . \end{array} \tag{4.79}$$

with domains and boundaries defined according to Figure 4.5 by

$\Omega_S := \mathbb{R} \times (-H, 0)$ (the domain of piezoelectric substrate),
$\Omega_{el} := \cup_{k\in\mathbb{Z}^*}(\frac{kp}{4}, \frac{3kp}{4})$ (the domain of electrodes),
$\Gamma_{int} = \overline{\Omega}_S \cap \overline{\Omega}_{el}$ (interface of piezoelectric substrate and electrodes),
$\Gamma := \partial\Omega$,
$\Gamma_{el} := \partial\Omega \cap \partial\Omega_{el}$ and
$\Gamma_N := \partial\Omega \setminus \Gamma_{el}$.

Again we try to apply Bloch's theorem in order to simplify the problem to the unit cell and to get an explicit dispersion relation. Now we formulate first the weak formulation.

Remark 4.5.1 *on interface condition between the two materials (substrate and electrodes): The interface conditions on the interface electrode-substrate are given by*

$$\begin{aligned} \lim_{x\in\Omega_{el}\to y} u(x) &= \lim_{x\in\Omega_S\to y} u(x) \quad \forall\, y\in\Gamma_{int}, \\ \lim_{x\in\Omega_{el}\to y} \Phi(x) &= \lim_{x\in\Omega_S\to y} \Phi(x) \quad \forall\, y\in\Gamma_{int}, \\ T.n_S &= -T.n_{el} \qquad\qquad on\ \Gamma_{int}, \\ D.n_S &= -D.n_{el}=0 \qquad\qquad on\ \Gamma_{int}. \end{aligned}$$

Stepwise construction of the weak formulation of piezoelectric equations

1. We multiply with testfunctions v and Ψ and integrate over Ω

$$\begin{aligned} -\int_\Omega v^T \operatorname{div}(T)\,dx \;-\; \omega^2 \int_\Omega v^T \rho\, u\, dx &= 0, \\ -\int_\Omega \Psi \operatorname{div}(D)\,dx &= 0. \end{aligned}$$

2. Integration by parts and consideration of the symmetry of T $((\nabla v)^T T = (Bv)^T T)$ leads to

$$\begin{aligned} \int_\Omega (Bv)^T : T\,dx \;-\; \int_{\partial\Omega} v^T T.n\,ds - \omega^2 \int_\Omega v^T \rho\, u\, dx &= 0, \\ \int_\Omega (\nabla\Psi)^T D\,dx \;-\; \int_{\partial\Omega} \Psi\, D.n\,ds &= 0. \end{aligned}$$

3. Under consideration of the boundary conditions we get

$$\begin{aligned} \int_\Omega (Bv)^T : T\,dx \;-\; \omega^2 \int_\Omega v^T \rho\, u\, dx &= 0, \\ \int_\Omega (\nabla\Psi)^T D\,dx \;-\; \int_{\Omega_{el}} \Psi\, D.n\,ds &= 0. \end{aligned}$$

4. Choosing the testspace

$$V_0 := \{\, (v,\Psi) \in (H^1(\Omega,\mathbb{C}^d), H^1(\Omega,\mathbb{C}) \mid \Psi = 0\ in\ \Omega_{el} \,\} \tag{4.80}$$

and taking the search space V_0, we finally get the **weak problem formulation** Find $(u,\Phi) \in V_0$ such that for all (v,Ψ) in V_0 :

$$\begin{aligned} \int_\Omega (Bv)^T : c^E\, Bu\; dx \;+\; \int_\Omega (Bv)^T : e^T (\nabla\Phi)\,dx \;-\; \omega^2 \int_\Omega v^T \rho\, u\, dx &= 0 \\ \int_\Omega (\nabla\Psi)^T e\, Bu\, dx \;-\; \int_\Omega (\nabla\Psi)^T \varepsilon^S \nabla\Phi\, dx &= 0. \end{aligned} \tag{4.81}$$

According to the periodic geometry, i.e. all coefficients are periodic, we restrict the calculation to the unit cell and achieve an explicit dispersion relation. We have to adopt Blochs method to the piezoelectric problem. This time we develop an abstract variant acting on the weak formulation of the problem.

Abstract version of Bloch's theorem:

Theorem 4.5.2
Let V_0 be the Hilbert space stated in (4.80).
We define the shift operator $T_p : V_0 \to V_0$ mapping $u(x_1, x_2)$ to $T_p u(x_1, x_2) := u(x_1 + p, x_2)$.
We assume, that the two bilinear forms $a,b : V \times V \to \mathbb{R}$ are symmetric and are invariant over T_p, i.e.

$$T_p(a(.,.)) = a(T_p(.), T_p(.)), \tag{4.82}$$
$$T_p(b(.,.)) = b(T_p(.), T_p(.)). \tag{4.83}$$

Then every eigenvector $u_k \in V_0$ corresponding to the eigenvalues λ_k of the weak generalized eigenvalue problem

$$a(u_k, v) = \lambda_k b(u_k, v) \quad \forall\, v \in V_0$$

can be fully described by quasi-periodic eigenfunctions $(\psi_j)_{j=1,\dots,m}$ satisfying

$$a(\psi_j, v) = \lambda_i b(\psi_j, v) \quad \forall\, v \in V_0 \tag{4.84}$$

of the form (in weak sense)

$$\exists\, \alpha_j, \beta_j \in \mathbb{R} : \quad T_p \psi_j = e^{(\alpha_j + i\beta_j)p} \psi_j. \tag{4.85}$$

m denotes the geometric multiplicity of λ_i.

Proof idea:
The proof is analogous to the already described version of Bloch's theorem.

Remark 4.5.3 *on Bloch's theorem*
Every eigenvector (u, Φ) in V_0 of the weak problem (4.81) can be decomposited in quasi-periodic eigenvectors

$$\begin{array}{rclcrcl} u(x_1,x_2) & = & \sum_{j=1}^{m(\omega)} c_{1,j}\psi_j & \text{with} & \psi_j(x_1+p,x_2) & = & e^{(\alpha_j+i\beta_j)p}\psi_j(x_1,x_2), \\ \Phi(x_1,x_2) & = & \sum_{j=1}^{m(\omega)} c_{2,j}\eta_j & \text{with} & \eta_j(x_1+p,x_2) & = & e^{(\alpha_j+i\beta_j)p}\eta_j(x_1,x_2) \end{array} \tag{4.86}$$

with (ψ, η) eigenvectors corresponding to ω and $m = m(\omega)$ denoting the geometric multiplicity of ω.

I.e. every solution (u, Φ) in V_0 of (4.81) is fully described by the solution of its Bloch waves on the unit cell.

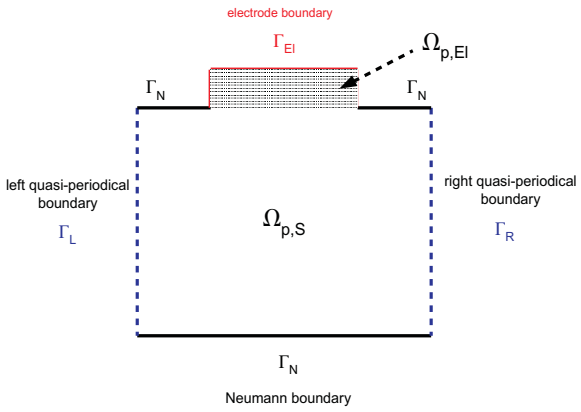

Figure 4.6: Restriction to the unit-cell for quasi-periodic solution

4.5.2 Restriction to the unit cell

We restrict the formulation (4.81) to the unit cell Ω_p according to Figure 4.6 and introduce the following notations $\Omega_{p,S} := (0,p)\times(-H,0)$, $\Omega_{p,el} := (\frac{p}{4},\frac{3p}{4})\times(0,h_{el})$, $\overline{\Omega}_p := \overline{\Omega}_{el,p}\cup\overline{\Omega}_{S,p}$, $\Gamma_l = \{0\}\times(-H,0)$, $\Gamma_r = \{p\}\times(-H,0)$ and the Neumann boundary Γ_N according to Figure 4.6.

Search for a $(u,\Phi) \in V_0 := \{(u,\Phi)\in(H^1(\Omega_p,\mathbb{C}^2),H^1(\Omega_p,\mathbb{C}))|\Phi = 0 \text{ on } \Omega_{el}\}$:

$$\begin{aligned}\int_{\Omega_p}(Bv)^T : T(u,\Phi)\,dx - \omega^2\int_{\Omega_p}u^T v\,dx &= \int_{\Gamma_L\cup\Gamma_R} v^T T(u,\Phi).n\,ds\\ \int_{\Omega_p}(\nabla\Psi)^T D(u,\Phi)\,dx &= \int_{\Gamma_L\cup\Gamma_R}\Psi D(u,\Phi).n\,ds \qquad (4.87)\end{aligned}$$

for all (v,Ψ) in V_0,

with the already implemented boundary conditions

$$\begin{aligned}T.n = 0 \quad &\text{on } \partial\Omega_p\\ D.n = 0 \quad &\text{on } \Gamma_N\\ \Phi = 0 \quad &\text{on } \Omega_{p,el}\end{aligned}$$

and the quasi-periodical boundary conditions which we have not considered yet and are achieved by differentiation

$$\begin{aligned}u_r &= \gamma u_l\\ T_r.n_r &= -\gamma\, T_l.n_l \qquad \text{with } \gamma := e^{(\alpha+i\beta)p}. \qquad (4.89)\\ D_r.n_r &= -\gamma\, D_l.n_l\end{aligned}$$

4.5.3 FE-discretization of the unit cell Ω_p

We choose a regular triangulation of the unit cell Ω_p with n nodes $(x^{(1)}, ..., x^{(n)})$ and $x^{(i)} = (x_1^{(i)}, x_2^{(i)})$ for all i. Then we split up the nodes into $n = n_i + n_e + n_l + n_r$ with n_e denoting the nodes corresponding to electrode, n_l, n_r according to the left and right boundary (quasi-periodical bounds) nodes and n_i denoting all remaining nodes, which we call inner nodes and which again also includes the Neumann nodes.
According to the partitiion we introduce the index mappings

$$l(.), r(.), i(.), e(.) : \{1, ..., n_*\} \rightarrow \{1, ..., n\}.$$

Furthermore, we assume that the left and right boundary nodes match, i.e. they satisfy

$$x_{r(i)} = x_{l(i)} + (0, p) \text{ for } i = \overline{1, n_l}.$$

FE-discretization of piezoelectric problems with Dirichlet and Neumann BCs
In order to get an idea of the properties of FE-matrices of piezoelectric problems, we first treat "standard" boundary problems, i.e. we assume only Neumann and Dirichlet boundary conditions. For this problems we state the piezoelectric Galerkin-system and analyze the matrix properties.
We choose Neumann conditions on right and left boundaries, i.e. we solve the weak problem (4.96) with the search and test space V_0.

We choose the FE-subspaces of $V = H^1(\Omega_p)^{d+1}$ and V_0 by

$$\begin{aligned}
V_h &:= span\{p^{(j)}, j = \overline{1, n} \,:\, p^{(j)} \text{ FE-base function acc. to node } x_j\}^{d+1} && \subset V \\
&= span\{p^{(j)} e_k, j = \overline{1, n} \,:\, p^{(j)} \text{ FE-base function for } x_j, k = \overline{1, d+1}\} && \\
V_{0h} &:= \{(u_h, \Phi_h) \mid \begin{array}{ll} u_h = \sum_{j=1}^{n} u^{(j)} p^{(j)} & \text{with } u^{(i)} \in \mathbb{C}^d \\ \Phi_h = \sum_{j=1,\, j \notin Rg(e(.))}^{n} \phi^{(j)} p^{(j)} & \text{with } \Phi^{(j)} \in \mathbb{C} \end{array} \} && \subset V_h
\end{aligned},$$

where e_k denotes the k-th unit vector in $\mathbb{R}^{d+1}$ and $Rg(f(.))$ denotes the range (image) of a function $f(.)$.

We approximate the solution of (4.96) by solving the discretized weak problem:
Search $(u_h, \Phi_h) = (\sum_i u^{(i)} p^{(i)}, \sum_i \Phi^{(i)} p^{(i)}) \in V_{0h}$ satisfying for all (v_h, Ψ_h) in V_{0h}:

$$\begin{aligned}
\int_{\Omega_p} (Bv_h)^T : T(u_h, \Phi_h)\, dx - \omega^2 \int_{\Omega_p} u_h^T v_h\, dx &= \int_{\Gamma_L \cup \Gamma_R} v_h^T T(u_h, \Phi_h).n\, ds \\
\int_{\Omega_p} (\nabla \Psi_h)^T D(u_h, \Phi_h)\, dx &= \int_{\Gamma_L \cup \Gamma_R} \Psi D(u_h, \Phi_h).n\, ds. \qquad (4.90)
\end{aligned}$$

The **Galerkin-FE-problem** denotes searching $\underline{u} \in \mathbb{C}^{d \cdot N_u}, \underline{\Phi} \in \mathbb{C}^{N_\Phi}$:

$$\boxed{\begin{pmatrix} K_{uu} & K_{u\Phi} \\ K_{\Phi u} & -K_{\Phi\Phi} \end{pmatrix} \begin{pmatrix} \underline{u} \\ \underline{\Phi} \end{pmatrix} - \omega^2 \begin{pmatrix} M_{uu} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \underline{u} \\ \underline{\Phi} \end{pmatrix} = 0.} \tag{4.91}$$

This $N := d \cdot N_u + N_\Phi$ equations are achieved through following notation:
$N_\Phi := n - n_e$ *and* $N_u := n$ *and* e_k *denoting the k-th unit vector of* $\mathbb{R}^d$ *for* $k = \overline{1,d}$

$\underline{u} := \begin{pmatrix} u^{(1)} \\ \vdots \\ u^{(N_u)} \end{pmatrix}$ *with* $u^{(j)} \in \mathbb{C}^d$ *by discretization* $u_h := \sum_i u^{(i)} p^{(i)}$

$\underline{\Phi} := \begin{pmatrix} \Phi^{(1)} \\ \vdots \\ \Phi^{(N_\Phi)} \end{pmatrix}$ *with* $\Phi^{(j)} \in \mathbb{C}$ *by discretization* $u_h := \sum_i \Phi^{(i)} p^{(i)}$.

Using a derivative tensor $B_h p^{(i)}$ *according to each shape function* $p^{(i)}$, *which is defined by* $u^{(i)} B_h p^{(i)}(x) = B(u^{(i)} p^{(i)}(x))$ *we state*

1. *the* **mechanical stiffness matrix** $K_{uu} \in \mathbb{R}^{d \cdot N_u}_{d \cdot N_u}$ *by blocks* $K^{(ij)}_{uu}$ *in* $\mathbb{R}^d_d$
   with $(K^{(ij)}_{uu})_{mk} = \int_{\Omega_p} ((B_h p^{(i)}) e_m)^T : c^E (B_h p^{(j)}) e_k dx$ *for* $m, k = 1, ..d$,

2. *the* **dielectric stiffness matrix** $K_{\Phi\Phi} \in \mathbb{R}^{N_\Phi}_{N_\Phi}$ *by* $(K_{\Phi,\Phi})_{ij} := \int_{\Omega_p} (\nabla p^{(i)})^T \varepsilon^S \nabla p^{(j)} dx$,

3. *the* **piezoelectric coupling matrices** $K_{u\Phi} = K^T_{\Phi u} \in \mathbb{R}^{N_u}_{N_\Phi}$ *by blocks* $K^{(ij)}_{u\Phi} \in \mathbb{R}^d$
   with $(K^{(ij)}_{u\Phi})_k := \int_{\Omega_p} (e_k (B_h p^{(j)})^T : e^T \nabla p^{(j)} dx$ *and*

4. *the* **mechanical mass matrix** $M_{uu} \in \mathbb{R}^{d \cdot N_u}_{d \cdot N_u}$ *by* $M_{uu,ij} := \int_{\Omega_p} p^{(i)} \rho p^{(j)} dx$.

Remark 4.5.4 on the piezoelectric FE-matrices

1. In practice the matrices are assembled elementwise and not nodewise as written above for easier notation.

2. The notation of the system matrices used in (4.91) is the common formulation of FE-discretisized piezoelectric problems.

3. The matrices have the following properties:
   $K_{\Phi\Phi} = K^T_{\Phi\Phi}, K_{uu} = K^T_{uu}$ are positive definite .
   $M_{uu} = M^T_{uu}$ is positive definite.
   $K_{u\Phi} = K^T_{\Phi u}$.

4. The not-null-elements of the mechanical stiffness matrix K_{uu} are of quantities $\approx 10^{10}$, while the not-null-elements of the dielectric stiffness matrix $K_{\Phi\Phi}$ are of quantities $\approx 10^{-10}$ due to the coefficient tensors.
   This requires scaling of eigenvalue problems and/or robust algorithms .

FE-discretization of piezoelectric problems with quasi-periodic boundary conditions To consider quasi-periodic boundary conditions we start again at the weak formulation of (4.96), but this time we incorporate the quasi-periodic boundary conditions (4.89) by stating quasi-periodic test and search spaces:

Search and test space have to fulfill the Dirichlet-condition, i.e. they have to be a subspace of $V_0 := \{ v \in (H^1(\Omega_p)) \,|\, v = 0 \text{ on } \Gamma_D \}$.

The search space The solution has to satisfy the quasi-periodicity condition (with $p = (p, 0)$)

$$u(x + p) = \gamma u(x) \, \forall x \in \Gamma_L. \tag{4.92}$$

This holds if the search space is restricted to

$$V_p(\gamma) := \{ (v, \psi) \in V_0 \,|\, v(x + p) = \gamma v(x),\ \psi(x + p) = \gamma \psi(x) \text{ a.e. on } \Gamma_L \} \subset V_0. \tag{4.93}$$

The quasi-periodicity condition for the flux follows from the quasi-periodicity of u.

The test space The test space should also represent the periodicity, which implies that test and search space are isomorph, i.e. let μ be an arbitrary complex scalar:

$$V_p(\mu) := \{ (v, \Psi) \in V_0 \,|\, v(x + p) = \mu v(x),\ \Psi(x + p) = \mu \Psi(x) \text{ a.e. on } \Gamma_L \}. \tag{4.94}$$

with $\mu \in \mathbb{C}$ arbitrary, but fixed.
Analogous to the model of the 2D wave equation the integral over the quasi-periodical boundary vanishes if one chooses

$$\mu := \frac{1}{\gamma}. \tag{4.95}$$

Weak formulation of piezoelectric problem with quasi-periodic boundary on unit cell Search for a $(u, \Phi) \in V_p(\gamma)$:

$$\begin{aligned} \int_{\Omega_p} (Bv)^T : T(u, \Phi) \, dx - \omega^2 \int_{\Omega_p} u^T v \, dx &= \int_{\Gamma_L \cup \Gamma_R} v^T T(u, \Phi).n \, ds \\ \int_{\Omega_p} (\nabla \Psi)^T D(u, \Phi) \, dx &= \int_{\Gamma_L \cup \Gamma_R} \Psi D(u, \Phi).n \, ds \end{aligned} \tag{4.96}$$

for all $(v, \Psi) \in V_p(\frac{1}{\gamma})$.

FE-discretization of quasi-periodic piezolectric problem With shape functions $p^j(.)$ satisfying

$$\begin{aligned} p^j(x_i) &= \delta_{ij} \\ p^{l(j)}(x) &= p^{r(j)}(x+p) \qquad \forall x \text{ on } \Gamma_L \; \forall j \in \{1,..,n_l\} \end{aligned}$$

we choose the FE-subspaces of search and testspace

$$V_{0h} := span\{\, p^i \,|\, i \in rg(i(.)) \cap rg(l(.)) \,\},$$

$$V_{ph}(\gamma) := \{\, (u_h, \Phi_h) \,| \begin{array}{rcll} u_h &=& \sum_{k=1}^{d} \sum_{j=1}^{n_i} u_k^{i(j)} p^{i(j)} e_k + & \\ &+& \sum_{k=1}^{d} \sum_{j=1}^{n_l} u_k^{l(j)} (p^{l(j)} + \gamma p^{r(j)}) e_k, & u_k^j \in \mathbb{C} \\ \Phi_h &=& \sum_{j=1}^{n_i} \Phi^{i(j)} p^{i(j)} + \sum_{j=1}^{n_l} \Phi^{l(j)} (p^{l(j)} + \gamma p^{r(j)}), & \Phi^j \in \mathbb{C} \end{array} \},$$

$$V_{ph}(\gamma^{-1}) := span\{\, p^i(j) \,\}_{j=\overline{1,n_i}} \cap span\{\, \gamma p^{l(j)} + p^{r(j)} \}_{j=\overline{1,n_l}}, \}^{d+1}.$$

Choosing $(v_h, \Psi_h) = p^{i(j)} e_k$ for $j = \overline{1, n_i}$ and $(v_h, \Psi_h) = (\gamma p^l(j) + p^r(j)) e_k$ for $j = \overline{1, n_l}$ for $k = \overline{1, d+1}$ leads to $N(n_i + n_l) \cdot (d+1)$ equations for the $(n_i + n_l) \cdot (d+1)$ components of $(\underline{u}, \underline{\Phi}) \in \mathbb{C}^{(n_i+n_l)\cdot(d+1)}$.

We get **Galerkin-system**:

$$\begin{pmatrix} K_{ii} & K_{il} + \gamma K_{ir} \\ \gamma K_{li} + K_{ri} & \gamma(K_{ll} + K_{rr}) \end{pmatrix} \begin{pmatrix} u_i \\ u_l \end{pmatrix} - \omega^2 \begin{pmatrix} M_{ii} & M_{il} + \gamma M_{ir} \\ \gamma M_{li} + M_{ri} & \gamma(M_{ll} + M_{rr}) \end{pmatrix} \begin{pmatrix} u_i \\ u_l \end{pmatrix} = 0, \tag{4.97}$$

where K_{st}, M_{st} $(s,t = i,l,r)$ are blocks of stiffness and mass matrix of the piezoelectric system according to inner, left and right boundary nodes. Note that $K_{lr} = K_{rl} = 0$.

By the following notation

$$\begin{aligned} K_{st} &:= \begin{pmatrix} K_{uu,st} & K_{u\Phi,st} \\ K_{\Phi u,st} & -K_{\Phi\Phi,st} \end{pmatrix} && \text{for } s,t \in \{i,l,r\} \\ M_{ss} &:= \begin{pmatrix} M_{uu,ss} & 0 \\ 0 & 0 \end{pmatrix} && \text{for } s \in \{i,l,r\} \\ y_s &:= \begin{pmatrix} u_s \\ \Phi_s \end{pmatrix} && \text{for } s \in \{i,l\} \end{aligned} \tag{4.98}$$

we can apply the solution approaches presented for the Helmholtz-type model directly to the coupled field problem.
But we introduce material damping first, i.e. we consider Raleigh damping in the piezoelectric system.

4.5.4 Rayleigh-damping for the piezoelectric FE-system

We want to consider Rayleigh-damping to the mechanical field, i.e. with given parameters c_K, c_M we define the damping matrix

$$C_{uu} := c_K M_{uu} + c_M K_{uu}. \tag{4.99}$$

The system (4.91) extends to the **damped piezoelctric FE-Galerkin system**
Search $\underline{u} \in \mathbb{C}^{d \cdot N_u}, \underline{\Phi} \in \mathbb{C}^{N_\Phi}$:

$$\begin{pmatrix} K_{uu} & K_{u\Phi} \\ K_{\Phi u} & -K_{\Phi\Phi} \end{pmatrix} \begin{pmatrix} \underline{u} \\ \underline{\Phi} \end{pmatrix} + i\omega \begin{pmatrix} C_{uu} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \underline{u} \\ \underline{\Phi} \end{pmatrix} - \omega^2 \begin{pmatrix} M_{uu} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \underline{u} \\ \underline{\Phi} \end{pmatrix} = \begin{pmatrix} w_u \\ w_\Phi \end{pmatrix} \tag{4.100}$$

and the damped analog of (4.101) to

$$\begin{pmatrix} K_{ii} & K_{il} + \gamma K_{ir} \\ \gamma K_{li} + K_{ri} & \gamma(K_{ll} + K_{rr}) \end{pmatrix} \begin{pmatrix} u_i \\ u_l \end{pmatrix} + i\omega \begin{pmatrix} C_{ii} & C_{il} + \gamma C_{ir} \\ \gamma C_{li} + C_{ri} & \gamma(C_{ll} + C_{rr}) \end{pmatrix} \begin{pmatrix} u_i \\ u_l \end{pmatrix} - \omega^2 \begin{pmatrix} M_{ii} & M_{il} + \gamma M_{ir} \\ \gamma M_{li} + M_{ri} & \gamma(M_{ll} + M_{rr}) \end{pmatrix} \begin{pmatrix} u_i \\ u_l \end{pmatrix} = 0 \tag{4.101}$$

the definition (4.98) is extended by

$$C_{ss} := \begin{pmatrix} C_{uu,ss} & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} c_K M_{uu,ss} + c_M K_{uu,ss} & 0 \\ 0 & 0 \end{pmatrix} \tag{4.102}$$

for $s \in \{i, l, r\}$.

4.5.5 Schur-Complement and Inner-Node-Matrix Method for piezoelectric problem

For already stated reasons we apply only approach 1 and 3 (given ω) to the problem.
For given ω we define the system matrices

$$\overline{K}_{st} := K_{st} - \omega^2 M_{st} \qquad s, t = i, l, r \tag{4.103}$$

$$\overline{K^C}_{st} := \overline{K}_{st} + i\omega C_{st} - \omega^2 M_{**} \qquad s, t = i, l, r \tag{4.104}$$

$\overline{K}$ is symmetric and real-valued and $\overline{K^C}$ is complex-valued and complex-symmetric.
We assume a given ω for which $\overline{K}$ and $\overline{K^C}$ is regular.

Due to the SC-Method we get a quadratic eigenvalue problem
(with $N_l := (d+1) \cdot n_l$)

$$\boxed{\text{Search } \gamma \in \mathbb{C}, y_l \neq 0 \in \mathbb{C}^{N_l} : \quad \gamma^2 S_{12} y_l + \gamma(S_{11} + S_{22}) y_l + S_{12}^T y_l = 0} \tag{4.105}$$

$$\begin{array}{lrll} \text{with} & S_{12} & := & -\overline{K}_{li}\overline{K}_{ii}^{-1}\overline{K}_{ri}^T \\ & S_{11} & := & -\overline{K}_{li}\overline{K}_{ii}^{-1}\overline{K}_{li}^T + \overline{K}_{ll} = S_{11}^T \qquad \in \mathbb{R}_{N_l}^{N_l} \text{ for undamped system (4.91)} \\ & S_{22} & := & -\overline{K}_{ri}\overline{K}_{ii}^{-1}\overline{K}_{ri}^T + \overline{K}_{rr} = S_{22}^T \\ & S_{12} & := & -\overline{K^C}_{li}\overline{K^C}_{ii}^{-1}\overline{K^C}_{ri}^T \\ & S_{11} & := & -\overline{K^C}_{li}\overline{K}_{ii}^{-1}\overline{K^C}_{li}^T + \overline{K^C}_{ll} = S_{11}^T \qquad \in \mathbb{C}_{N_l}^{N_l} \text{ for damped system (4.100)} \\ & S_{22} & := & -\overline{K^C}_{ri}\overline{K^C}_{ii}^{-1}\overline{K^C}_{ri}^T + \overline{K^C}_{rr} = S_{22}^T \end{array}$$

For the Inner-Node-Matrix Method we get a generalized linear eigenvalue problem
for the undamped system (4.91) we search $\gamma \in \mathbb{C}, \begin{pmatrix} y_i \\ y_l \end{pmatrix} \neq 0 \in C_{N_l+N_i}^{N_l+N_i}$:

$$\boxed{\begin{pmatrix} \overline{K}_{ii} & \overline{K}_{il} \\ \overline{K}_{ir}^T & 0 \end{pmatrix} \begin{pmatrix} y_i \\ y_l \end{pmatrix} = \gamma \begin{pmatrix} 0 & -\overline{K}_{ir} \\ -\overline{K}_{il}^T & -(\overline{K}_{ll} + \overline{K}_{rr}) \end{pmatrix} \begin{pmatrix} y_i \\ y_l \end{pmatrix}} \tag{4.106}$$

and for the damped system (4.100) we search $\gamma \in \mathbb{C}, \begin{pmatrix} y_i \\ y_l \end{pmatrix} \neq 0 \in C_{N_l+N_i}^{N_l+N_i}$:

$$\boxed{\begin{pmatrix} \overline{K^C}_{ii} & \overline{K^C}_{il} \\ \overline{K^C}_{ir}^T & 0 \end{pmatrix} \begin{pmatrix} y_i \\ y_l \end{pmatrix} = \gamma \begin{pmatrix} 0 & -\overline{K^C}_{ir} \\ -\overline{K^C}_{il}^T & -(\overline{K^C}_{ll} + \overline{K^C}_{rr}) \end{pmatrix} \begin{pmatrix} y_i \\ y_l \end{pmatrix}} \tag{4.107}$$

Remark 4.5.5 *If $Ay = \gamma By$ denote the linear eigenvalue problems (4.106) or respectively (4.107), the matrix $(A - B)$ is regular and (complex-)symmetric. This is valid through the assumption imposed on the choice of ω.*

Chapter 5

General theory and numerics of algebraic eigenvalue problems

We discuss three different types of eigenvalue problems: the standard, the generalized linear and the quadratic eigenvalue problem.
This chapter starts with defining these eigenvalue problems, followed by an introduction to the main ideas which underlie numerical solution methods. A short overview of the software packages needed is given.

A good overview and comparison of state-of-the-art eigenvalue solvers is given in [8],
In the following the superscript * denotes 'transposed' if real arithmetic is used and 'transposed complex conjugate' if complex arithmetic is used.

5.1 Definitions and types of eigenvalue problems

5.1.1 The standard eigenvalue problem

Let A be a $n \times n$ square matrix over $\mathbb{R}$ or $\mathbb{C}$. Searching scalars $\lambda \in \mathbb{C}$ and vectors $x \in \mathbb{C}^n$ satisfying

$$Ax = \lambda x \quad \textbf{(SEP)} \tag{5.1}$$

forms *the standard eigenvalue problem.*

An *eigenvalue* λ of a matrix A is defined as a complex root $p_A(\lambda) = 0$ of the characteristic polynomial of the matrix A

$$p_A(\lambda) := det(\lambda I - A). \tag{5.2}$$

Hence eigenvalues are complex numbers λ for which the matrix pencil $(\lambda I - A)$ becomes singular.

The set of all eigenvalues is called *the spectrum of a matrix* denoted by $\sigma(A)$:

$$\begin{aligned} \sigma(A) &:= \{\lambda \in \mathbb{C} \,|\, det(\lambda I - A) = 0\} \\ &= \{\lambda \in \mathbb{C} \,|\, (\lambda I - A) \text{ singular}\} \end{aligned} \tag{5.3}$$

Let λ be an eigenvalue of A. A non-zero vector $x \in \mathbb{C}^n$ satisfying

$$Ax = \lambda x \quad \text{with } \lambda \in \sigma(A)$$

is called *(right) eigenvector* corresponding to the eigenvalue λ of A. The pair (λ, x) is called a *(right) eigenpair* of A.
A non-zero vector $y \in \mathbb{C}^n$, which satisfies

$$y^* A = \lambda y^* \quad \text{with } \lambda \in \sigma(A),$$

is called a *left eigenvector* for the eigenvalue λ of A. The pair (λ, y) is called a *left eigenpair* of A.

If λ is an eigenvalue of A, then the *eigenspace* associated with λ is defined as the nullspace $\mathcal{N}(\lambda I - A)$.

The characteristic polynomial is of order n, hence counting multiplicities the polynomial has n complex roots , i.e. the matrix A has n eigenvalues $\lambda_i \in \mathbb{C}$. The *algebraic multiplicity* n_a of an eigenvalue λ_i is the multiplicity of λ_i as a root of the characteristic polynomial. The dimension of the corresponding eigenspace specifies the *geometric multiplicity* n_g. An eigenvalue is called *defective*, if the geometric multiplicity is lower than the algebraic one. Two obvious facts:

1. Eigenvectors of distinct eigenvalues are linearly independent.
2. $1 \leq n_g \leq n_a$

Some matrix properties imply a special structure to the spectrum, i.e.

matrix	spectrum	eigenvectors
A real	$\lambda_i \in \mathbb{R}$ or $\lambda_i \in \mathbb{C}$ in pairs : λ_i , $\bar{\lambda}_i$	$x_i \in \mathbb{R}^n$ $x_i, \bar{x}_i$
A real and $A = A^T$	$\lambda \in \mathbb{R}$	$x_i \in \mathbb{R}^n$
$A = A^*$	$\lambda_i \in \mathbb{R}$ or $\lambda_i \in \mathbb{C}$ in pairs : λ_i ,$\bar{\lambda}_i$	$x_i \in \mathbb{R}^n$ $x_i, \bar{x}_i$

with $Ax_i = \lambda_i x_i$.

This additional information is helpful in constructing fast and reliable solvers for matrices of special structure.

5.1.2 The generalized (linear) eigenvalue problem

Let A, B be $n \times n$ square matrices over $\mathbb{R}$ or $\mathbb{C}$.
Searching scalars $\lambda \in \mathbb{C}$ and vectors $x \in \mathbb{C}^n$ satisfying

$$Ax = \lambda Bx \quad \textbf{(LEP)} \tag{5.4}$$

states *the generalized (linear) eigenvalue problem.*

The polynomial

$$p_{(A,B)}(\lambda) := det(\lambda B - A) \tag{5.5}$$

is called the *characteristic polynomial* of the matrix pair (A, B).
In contrast to the standard problem the characteristic polynomial of a matrix pair (A, B) need not to be of order n since

$$det(\lambda B - A) = \lambda^n . det(B) + \ lower\ terms.$$

Therefore one has to introduce finite and infinite eigenvalues.

Finite eigenvalues denotes eigenvalues in the common sense as in the SEP. The roots $p_{(A,B)}(\lambda) = 0$ of the characteristic polynomial are called *finite eigenvalues* of the matrix pencil $(A - \lambda B)$.
Let λ be a finite eigenvalue of (A, B). A non-zero vector $x \in \mathbb{C}^n$ is called a *general (right) eigenvector* according to λ if it solves

$$Ax = \lambda Bx.$$

The pair (λ, x) is a *(right) finite eigenpair.*
A non-zero vector $y \in \mathbb{C}^n$ is called a *general left eigenvector* according to λ, if it solves

$$y^* A = \lambda y^* B.$$

The pair (λ, y) is a *left finite eigenpair.*

If the degree d of the characteristic polynomial is lower than n, there are $(n - d)$ *infinite eigenvalues* per definition.
Through reformulation of the eigenvalue problem one can achieve a more accurate definition for infinite eigenvalues. Replacing the eigenvalue λ by the complex pair (α, β) with $\lambda = \frac{\alpha}{\beta}$ and $|\alpha|^2 + |\beta|^2 = 1$ leads to

$$\beta Ax = \alpha Bx, \tag{5.6}$$

which is equivalent to $Ax = \lambda Bx$ in the case of finite eigenvalues. We identify infinite eigenvalues with the pair $(1, 0)$ and *right / left eigenvectors* associated with an infinite eigenvalue as vectors $x, y \in \mathbb{C}^n$ satisfying

$$Bx = 0 \quad \text{or} \quad y^*B = 0 \quad \text{respectively.} \tag{5.7}$$

Connection between standard and generalized eigenvalue problems:
The standard problem is a special case of the generalized one by setting $B = I$.
If B is regular, the generalized eigenvalue problem $Ax = \lambda Bx$ can be transformed to standard form $B^{-1}Ax = \lambda x$. By similarity transformation we will show later that the generalized and the corresponding standard problem have the same spectrum.

5.1.3 The quadratic eigenvalue problem

The *nonlinear eigenvalue problem* of order k is defined as searching scalars $\lambda \in \mathbb{C}$ and vectors $x \in \mathbb{C}^n$, which satisfy

$$\lambda^k C_k x + \lambda^{k-1} C_{k-1} x + ... + \lambda C_1 x + C_0 x = 0, \tag{5.8}$$

with $C_l \in C_n^n$ for $l = 0, ..., k$.
The matrix polynomial $P_k(\lambda) := \lambda^k C_k + ... + \lambda C_1 + C_0$ is called λ-*matrix* of order k.

In this thesis we treat quadratic eigenvalue problems, i.e. λ-matrices of order 2.
The *characteristic polynomial of a quadratic pencil* is defined by

$$p_{P_2}(\lambda) := det(P_2(\lambda)) = det(\lambda^2 C_2 + \lambda C_1 + C_0) \tag{5.9}$$

Eigenvalues should be again defined as the roots of the characteristic polynomial, but since the number of roots depends on the regularity of the leading matrix C_2, we have to distinguish finite and infinite eigenvalues. Here a main difference to linear problems is implied by the fact that the characteristic polynomial of P_2 can have up to $2n$ complex roots.

Finite eigenvalues of the quadratic matrix pencil P_2 are defined as the roots of the characteristic polynomial $p_{P_2}(\lambda) = det(P_2(\lambda)) = 0$.
A *(right) eigenvector* according to a finite eigenvalue λ is a non-zero vector $x \in \mathbb{C}^n$ solving the matrix equation

$$P_2(\lambda)x = 0 \quad \text{with } \lambda \in \sigma(P_2) := \{\lambda_i \,|\, p_{P_2}(\lambda_i) = 0\}. \tag{5.10}$$

Analogously *left eigenvectors* are non-zero solutions $y \in C^n$ of

$$y^* P_2(\lambda) = 0 \quad \text{with } \lambda \in \sigma(P_2). \tag{5.11}$$

The pairs $(\lambda, x), (\lambda, y)$ are finite right/left *eigenpairs*.

If there are d finite eigenvalues, then there are $2n - d$ *infinite eigenvalues* by definition. To get an accurate definition of infinite eigenvalues and the corresponding eigenvectors, the problem has to be again reformulated. Replacing λ by the pair (α, β) with $\lambda = \frac{\alpha}{\beta}$ and normalized by $|\alpha|^2 + |\beta|^2 = 1$ one gets

$$\alpha^2 C_2 x + \alpha \beta C_1 x + \beta^2 C_0 x = 0. \tag{5.12}$$

By this the pair $(1, 0)$ stands for *infinite eigenvalues* of P_2 and the quotient $\lambda = \frac{\alpha}{\beta}$ with $|\beta| > 0$ denotes finite eigenvalues of P_2.
This implies defining *right/left eigenvectors associated to infinite eigenvalues* as non-zero vectors $x, y \in \mathbb{C}^n$ solving

$$C_2 x = 0, \quad \text{or } y^* C_2 = 0 \text{ respectively.} \tag{5.13}$$

Since there are $2n$ eigenvalues (finite and infinite), in general the eigenvectors cannot form an independent set in $\mathbb{C}^n$. With the effect that two distinct eigenvalues may have the same eigenvector.

Some matrix properties imply special structure of the spectrum of QEPs:
For $P_2(\lambda_i) = C_2 \lambda_i^2 + C_1 \lambda_i + C_0 = 0$ we get

matrices	spectrum	eigenvectors
P_2 regular	$2n$ finite eigenvalues	
P_2 real	$\lambda_i \in \mathbb{R}$ or complex conjugate pairs $(\lambda_i, \bar{\lambda}_i)$	x_i real $(\lambda_i, x_i) \Rightarrow (\bar{\lambda}_i, \bar{x}_i)$

5.2 Numerics of eigenvalue problems

There is a wide range of numerical solution methods for eigenvalue problems. A large part of methods assume hermitian and positive definite matrices. Since it turns out that the matrices of the problems modeled in Chapter 4 do not fulfill these assumptions, we concentrate on algorithms which work with non-hermitian general matrices. Moreover one always has to bear in mind that the matrices can be singular.

To get a first impression of a given eigenvalue problem it is sense- and useful to compute the whole spectrum. In problems derived from assembling the piezoelectric equations the system matrices are very ill-conditioned. The non-zero coefficients of the mechanical stiffness matrix K_{uu} are of the order 10^{10} whereas the non-zero coefficients of the block modeling the electric potential $K_{\Phi\Phi}$ are of the order 10^{-10} (see also Appendix A). To

get first reliable results and reference values we look for well-understood, robust and reliable methods. This leads us to direct methods and especially to the QR/QZ-algorithm [8].

Analogous to linear equation solvers we apply iterative methods to eigenvalue problems to get faster algorithms. These methods have the advantage that they need fewer factorizations, do not destroy sparsity of the matrices and, e.g. in case of Jacobi-Davidson method, the linear equations arising can be solved approximately. There are two main advantages of iterative methods. First, some iterative methods suffice only with matrix-vector products, i.e. the explicit knowledge of the system matrices is not necessary. Secondly, it is possible to specify a (small) part of the spectrum which one is interested in. Only the eigenpairs with specified properties, e.g. largest/smallest real/imaginary part, largest/smallest magnitude or eigenvalues next to a given complex target γ, are computed.

We introduce the Arnoldi method [35], [11] for solving standard and generalized linear problems iteratively. Concerning quadratic problems we present a linearization method to generalized problems and the nonlinear expansion of Jacobi-Davidson algorithm.

The theory of these methods (QR-QZ,Arnoldi, Jacobi-Davidson) is first described in detail for solving standard problems, which is technically less complicated. Then the main ideas get expanded to the generalized and nonlinear case.
Understanding the theory underlying and motivation of the algorithms leads to an idea of constructing problem dependent structure preserving methods.

We start with some helpful tools often used in solving eigenvalue problems.

5.2.1 Some facilities - transformations, factorizations and decompositions

Before applying an eigenvalue routine it is often advisable to transform the system to a simpler problem or to a problem with higher convergence rate.
After solving the transformed problem, the back transformation of the spectrum and of the corresponding eigenvectors should be easy to perform.

Similarity transformation At first we are looking for transformations which have no effect on the spectrum of the matrix pencil

$$P_l(\lambda) := \begin{cases} \lambda^2 C_2 + \lambda C_1 + C_0 & l = 2 \quad \text{corresponding to QEP} \\ \lambda B - A & l = 1 \quad \text{corresponding to LEP and SEP}(B = I) \end{cases} ,$$

where C_i, A, B are general $n \times n$ matrices over $\mathbb{C}$.
The corresponding characteristic polynomial is $det(P_l(\lambda))$. The spectrum (set of finite eigenvalues) is denoted by $\sigma(P_l)$.

Theorem 5.2.1 *Similarity transformations*
If U, V are regular $(n \times n)$ matrices, then

$$\sigma(P_l) = \sigma(U^* P_l V). \tag{5.14}$$

$$(\lambda_i, y_i) \text{ solves } \quad U^* P_l(\lambda_i) V y_i = 0. \quad \Leftrightarrow \quad (\lambda_i, x_i := V y_i) \text{ solves } \quad P_l(\lambda_i) x_i = 0 \tag{5.15}$$

The last equivalence holds for infinite eigenvalues $\lambda_i = \infty$.

Proof: Every eigenvalue λ_i of P_l is a root of the characteristic polynomial of $U^* P_l V$:

$$0 = det(U^* P_l(\lambda_i) V) = \underbrace{det(U^*)}_{\neq 0} \cdot det(P_l(\lambda_i)) \underbrace{det(V)}_{\neq 0} \quad \Leftrightarrow \quad det(P_l(\lambda)) = 0 \quad \Rightarrow \quad (5.14).$$

For finite eigenvectors equivalence (5.15) is obvious by regularity of U, V.
For $\lambda_i = \infty$: for l=1 since U, V regular

$$U^* B V y = 0 \quad \Leftrightarrow \quad U^{-*} U^* B V y_i = B V y_i = B x_i = 0 \quad \text{with } x_i = V y_i$$

$for\ l = 2:$ analogous.

□

If the matrices U, V are unitary ($U^* U = I$ and $V^* V = I$) we call these transformations *unitary similarity transformations*. For real matrices replace unitary by orthogonal.

There are some eigenvalue problems of special structure which are easier to solve than general ones (e.g. system matrices of diagonal, tridiagonal, triangular or Hessenberg form). It is often useful to transform the given problem first to some reduced form, if possible, and then solving the simpler problem.
If this is done by similarity transformations the spectrum does not change and the back transformations of eigenvectors are easy to perform (one matrix-vector multiplication $V y_i$).

For instance, if a given matrix A has n independent eigenvectors, one can find a unitary (orthogonal) matrix Q which *diagonalizes* A, i.e.

$$A = Q D Q^*$$

with D diagonal matrix. Normalized eigenvectors are given by the columns of Q. The corresponding eigenvalues are the diagonal elements of D.

Spectral transformation In many cases it makes sense to transform the spectrum as well. We will see that iterative methods have fast convergence to dominant eigenvalues, i.e. eigenvalues of largest magnitude which are separated from the rest of the spectrum. If one is interested in eigenvalues near to a given complex target γ of generalized linear problems, we can accelerate the convergence rate by solving a transformed eigenvalue problem where the desired eigenvalues lie at the end of the spectrum.

At first we create an eigenvalue problem in which the desired eigenvalues are close to zero by the *shift*

$$(A - \gamma B)x = (\lambda_i - \gamma)Bx. \tag{5.16}$$

Via inverting the problem the searched eigenvalues get dominant

$$Bx = \frac{1}{\lambda_i - \gamma}(A - \gamma B)x. \tag{5.17}$$

Theorem 5.2.2 *Spectral transformation*
Starting from the generalized eigenvalue problem

$$Ax_i = \lambda_i Bx_i$$

the spectral transformation with shift μ *denotes the transformed LEP*

$$Bx_i = \mu_i(A - \gamma B)x_i.$$

The transformation and the according back-transformation of the spectrum satisfy

$$\begin{aligned} \sigma(B, A - \gamma B) &= \{ \frac{1}{\lambda_i - \gamma} \mid \lambda_i \in \sigma(A, B) \}, \\ \sigma(A, B) &= \{ \frac{1}{\mu_i} + \gamma \mid \mu_i \in \sigma(B, A - \gamma B) \}. \end{aligned}$$

$$(\mu_i, x_i) \text{ solves } Bx_i = \mu_i(A - \gamma B)x \quad \Leftrightarrow \quad (\lambda_i, x_i) := (\gamma + \frac{1}{\mu_i}, x_i) \text{ solves } Ax_i = \lambda_i Bx_i$$

or respectively

$$(\lambda_i, x_i) \text{ solves } Ax_i = \lambda_i Bx_i \quad \Leftrightarrow \quad (\frac{1}{\lambda_i - \gamma}, x_i) \text{ solves } x = (A - \gamma B)^{-1}Bx$$

The eigenvectors maintain unchanged through these spectral transformations.

If $(A-\gamma B)$ is a regular pencil, one can construct a standard eigenvalue problem out of the spectral transformation. Similarity transformation leads to

$$(A-\gamma B)^{-1}Bx_i \;=\; \frac{1}{\lambda_i-\gamma}\,x_i \tag{5.18}$$

or

$$B(A-\gamma B)^{-1}y_i \;=\; \frac{1}{\lambda_i-\gamma}\,y_i \tag{5.19}$$

respectively. In problem (5.18) the eigenvectors are unchanged, for (5.19) one has to apply $x_i = (A-\gamma B)^{-1}y_i$ for back-transforming.

Methods using spectral transformation and (5.18) or (5.19) carry the supplement *shift-and-invert (SI).*

Spectral transformations and SI-methods are used to

- shift interior eigenvalues to the end of the spectrum,
- transform generalized linear to standard problems in case that B is singular and if there is a complex number γ for which the pencil $(A-\gamma B)$ is regular.

Schur decomposition One can compute the eigenvalues of a general matrix by transforming the matrix to (quasi-)triangular form (see Remark 5.2.5 for the definition of quasi-tringalur matrices). The eigenvalues are given by the diagonal entries. If the eigenvectors are required, they can be computed by solving a triangular system and then back transforming it according to the original problem.

Definition 5.2.3 *Schur decomposition*
A unitary (orthogonal) similar transformation of a square matrix A to Schur form *is defined by the decomposition*

$$A = QTQ^* \tag{5.20}$$

with Q unitary (orthogonal) and T upper triangular (quasi-triangular) in complex (real) arithmetic.
The columns of Q are called Schur vectors.

Computing eigenvalues and eigenvectors see generalized case ($B = I$).

Definition 5.2.4 *Generalized Schur decomposition*
A unitary (orthogonal) similarity transformation of a matrix pencil $(A-\lambda B)$ *to* generalized Schur form *is done by the decomposition*

$$A - \lambda B = Q(T_A - \lambda T_B)Z^* \tag{5.21}$$

with Q, Z *unitary (orthogonal) matrices and* T_A, T_B *triangular (quasi-triangular).*
The columns of Q, Z *are called* generalized Schur vectors .

The eigenvalues of a triangular pencil are easy to get and since the transformation was similar the spectrum does not change through this transformation, we get

$$\sigma(A, B) = \sigma(T_A, T_B) = \{\frac{T_{A,ii}}{T_{B,ii}} | i = 1, ...n\}. \tag{5.22}$$

Eigenvectors to finite eigenvalues can be achieved by solving a triangular system $(T_A - \lambda_i T_B)y_i = 0 \rightarrow y_i$ or for infinite eigenvalues by computing the nullspace of a triangular system $T_B y_i = 0$ and by applying the back transformation to the original problem afterwards by $x_i = Z y_i$.

Remark 5.2.5 *to* T_A, T_B *(quasi-)triangular:*
If real arithmetic is used and complex eigenvalues appear, it is impossible to transform the matrices to triangular form. One has to admit (2×2) *diagonal blocks. Each block* D_i *represents a complex conjugate pair of eigenvalues* $\lambda_i, \bar{\lambda}_i$ *by satisfying* $\sigma(D_i) = \{\lambda_i, \bar{\lambda}_i\}$.
Triangular matrices with (2×2) *blocks on the diagonal are called* quasi-triangular.

5.2.2 The QR/QZ- algorithm - a direct method

The QR-method is a direct method (terminates in finite steps if exact arithmetic is provided) for solving a standard eigenvalue problem $Ax = \lambda x$. It is used

- for dense matrices of moderate size,
- for solving lower dimensional subproblems which occur in iterative subspace projection methods.

This method is numerically very reliable and the whole spectrum of the problem is computed.

The algorithm is based on computing the Schur factorization of A in the following steps:

1. *QR-factoriziation*
   Every square matrix A can be factorized into

   $$A = QR \tag{5.23}$$

   with Q unitary and R upper triangular.
   One has to remark that the QR-factorization of a Hessenberg matrix is much faster than the factorization of a general matrix.

2. The *QR-transformation* is defined by

   $$\begin{aligned} A &= QR \\ \tilde{A} &= RQ. \end{aligned} \tag{5.24}$$

   This performs a unitary similarity transformation of the original matrix, since $Q^*AQ = Q^*QRQ = RQ = \tilde{A}$.
   If A is Hessenberg, one can prove that the QR-transformation of A maintains Hessenberg form. Iterative application of QR-streps results in the convergence of $\tilde{A}$ to (quasi-)triangular form. In complex arithmetic the subdiagonal elements (in real arithmetic the subdiagonal elements corresponding to real eigenvalues) converge against zero.
   This means, through iteration $\tilde{A}$ converges against the Schur factorization of A.

3. Improvements to the QR-factorization:
   To achieve a better convergence rate (subdiagonal entries $\rightarrow 0$) a spectral transformation according to the actually iterated Hessenberg matrix is applied in each QR-step. This variant of QR-iteration is called *implicitly-shifted QR-transformation.*

4. The primal Hessenberg form in item 1 can be achieved through Givens rotation, Householder transformation or modified Gram-Schmidt methods ($\rightarrow$ Arnoldi procedure).

Remark 5.2.6 *If A is hermitian, the Hessenberg forms reduce to tridiagonal forms.*

The computational costs of the QR-method including reduction to Hessenberg form, implicite shifts and some other improvements are $\mathcal{O}(n^3)$ floating point operations ($\approx 10n^3$ if only eigenvalues are desired and $\approx 25n^3$ for computing eigenpairs). The memory

requirement is $\mathcal{O}(n^2)$.

The *QZ-algorithm* denotes the expansion of QR-method to generalized linear eigenvalue problems. Technically the algorithm becomes more complicated, but the main idea of reducing the matrix to generalized Schur form is similar:
At first A, B are reduced simultaneously by unitary similarity transformation the way A becomes Hessenberg and B upper triangular. In the next step QZ-iteration is applied to force A to get upper triangular as well while keeping B in form.
Applied with implicit shifts the existence of infinite eigenvalues poses no problems.
Computing eigenvalues requires approximately $30n^3$ floating point operations plus $16n^3$ for eigenvectors.

5.2.3 Iterative methods

The power method
The easiest iterative method for solving standard eigenvalue problems is the power method. We use it to motivate Krylov methods. The power method is a single vector iteration (only one eigenvector is computed). In case of convergence the method results in the eigenpair corresponding to the eigenvalue of largest magnitude.

Algorithm 5.2.7 *The power method*
Given start vector v;
for $k = 1, 2, 3...$
$v = \frac{v}{\|v\|}$;
$w = Av$;
$\theta = w^* v$;
if $(\|w - \theta v\| \leq \epsilon_M |\theta|)$ *break;*
$w = v$;
end for;

The functioning and properties of the power method can already be seen under assuming that A has n independent eigenvectors x_i with corresponding eigenvalues λ_i satisfying $|\lambda_1| > |\lambda_2| \geq |\lambda_3| ... \geq |\lambda_n|$:
Then the starting vector v_0 can be expanded as $v_0 = \sum_{i=1}^{n} \mu_i x_i$ (assume that $\mu_1 \neq 0$).

In the k-th step of the algorithm one gets (neglecting the normalization of w)

$$\begin{aligned} v_{k+1} &= A^k v_0 = \sum_i \mu_i A^k x_i = \sum_i \mu_i \lambda_i^k x_i \\ &= \lambda_1^k \left(\mu_1 x_1 + \sum_{i=2}^{n} \mu_i \underbrace{(\frac{\lambda_i}{\lambda_1})^k}_{\to 0} x_i\right) \\ &\to \lambda_1^k \mu_1 x_1 \text{ for } k \to \infty. \end{aligned}$$

If the starting vector has a part in the direction of the dominant eigenvector x_1, the power method converges to the eigenvector corresponding to the eigenvalue of largest magnitude. The rate of convergence depends on the ratio $|\frac{\lambda_1}{\lambda_2}|$. If this ratio is close to one, the convergence can get very slow.

The power method computes only one eigenvector, to achieve more eigenvectors one can deflate already converged eigenvectors. If we orthogonalize the starting vector v_0 against v_1 ($\mu_1 = 0$), the method will converge to the second largest eigenvector (if v is not orthogonal to v_2).

The main idea of iterative projection methods

The idea behind subspace projection method is to project the given eigenvalue problem onto lower dimensional subspaces. One achieves a smaller sized subproblem, solves this with much lower requirements and view the computed eigenvalues as approximations to the original problem.
The big question will be, how to choose the subspace on which we project the original problem.

There are two different projection techniques : *orthogonal* and *oblique* projection methods. We describe the functioning by means of the standard problem (SEP):

1. *Orthogonal projection onto a given subspace $\mathcal{K}$ of dimension $m \leq n$:*
   We want to project the problem of computing the eigenpairs of

   $$Ax = \lambda x \quad \text{with } x \in \mathbb{C}^n \text{ and } \lambda \in \mathbb{C} \tag{5.25}$$

   onto the subspace $\mathcal{K}$. That means we search an approximate eigenpair $(\tilde{\lambda}, \tilde{x})$ with $\tilde{\lambda} \in \mathbb{C}$ and $\tilde{x} \in \mathcal{K}$ which solves the problem with respect to the subspace $\mathcal{K}$. In more detail, the residual of $A\tilde{x} - \tilde{\lambda}\tilde{x}$ is zero with respect to the subspace in the sense that the residual is orthogonal to $\mathcal{K}$.
   This is imposed by the Galerkin condition

   $$v^*(A\tilde{x} - \tilde{\lambda}\tilde{x}) = 0 \quad \forall v \in \mathcal{K}, \tag{5.26}$$

in matrix notation this is equivalent to

$$(V^*AV - \tilde{\lambda}I)y = 0, \tag{5.27}$$

where $V \in C^{n\times m}$ unitary is the matrix representation of an orthonormal base of $\mathcal{K}$ and $\tilde{x}$ of (5.26) is forced to lie in the subspace $\mathcal{K}$ by choosing $\tilde{x} := Vy$.
The projected eigenvalue problem

$$V^*AVy = \tilde{\lambda}y \tag{5.28}$$

is of dimension $(m \times m)$ and its eigenvalues are viewed as approximations corresponding to the subspace $\mathcal{K}$ of the original eigenproblem (5.25).

This leads to the base procedure of orthogonal projection methods:

(a) Compute an orthonormal m-dimensional base V_m of the subspace $\mathcal{K}$.

(b) Compute the projection matrix : $V_m^*AV_m$

(c) Solve the projected eigenvalue problem: $V_m^*AV_my = \theta y$

The approximate eigenpair $(\theta, s) := (\theta, V_my)$ is called a *Ritz pair*, θ a *Ritz value* and s a *Ritz vector* corresponding to the subspace $\mathcal{K}$.

2. *Oblique projection technique on two given subspaces $\mathcal{K}$ and $\mathcal{L}$:*
The main difference to orthogonal projection methods is that we choose different test ($\mathcal{L}$) and search ($\mathcal{K}$) spaces. The approximate eigenvectors should lie in $\mathcal{K}$, but the corresponding residual should be orthogonal to the subspace $\mathcal{L}$.

We search a $\tilde{x}$ in $\mathcal{K}$ satisfying the *Petrov-Galerkin condition*

$$w^*(A - \lambda I)\tilde{x} = 0 \quad \forall\, w \in \mathcal{L}. \tag{5.29}$$

Assuming that matrix representations W of a base of $\mathcal{L}$ and V of a base of $\mathcal{K}$ are chosen *bi-orthogonal* $W^*V = I$, this yields in the projected eigenvalue problem

$$W^*AVy = \theta y.$$

We will only use orthogonal projection methods which are numerically more reliable than oblique methods.

Krylov methods - The Arnoldi method

The idea of orthogonal projection methods bases on the projection of the eigenvalue problem to a smaller dimensioned subspace. But how should one choose this subspace ?

The power method gives the motivation for Krylov methods. There we have built the sequence $v, Av, A^2v, ..., A^kv$ and discovered that it converges in direction of the eigenvector corresponding to the eigenvalue of largest magnitude. In general, it also contains information of eigenvector directions corresponding to eigenvalues near the dominant one. The power method only utilizes the last two vectors in each iteration step and without deflation techniques it delivers only one eigenvector.
Now we want to exploit more information of the iterated vector sequence and compute more than one eigenvector.
We choose our subspace

$$\mathcal{K}^m(A, v) := span\{v, Av, A^2v, ..., A^{m-1}v\}. \tag{5.30}$$

This subspace is called a *Krylov subspace of A of order m* and methods projecting on Krylov subspaces are termed *Krylov methods.*

Arnoldi method for SEP

The basic algorithm - computing an Arnoldi factorization

Constructing an orthonormal base of the Krylov subspace via the modified Gram-Schmidt method leads to the *Arnoldi procedure.*

Algorithm 5.2.8 (Arnoldi procedure)
Create an orthonormal base of $\mathcal{K}^m(A, v)$

$v_1 = \frac{v}{\|v\|}$
for $j = 1, 2, ..., m-1$
  $w = Av_j$
  for $i = 1, 2, ..., j$
    $h_{i,j} = w^* v_i$
    $w = w - h_{i,j} v_i$
  end
  $h_{j+1,j} = \|w\|_2$
  if $(h_{j+1,j} \approx 0)$ *break*
  $v_{j+1} = \frac{w}{h_{j+1,j}}$
end;

Formulating the Arnoldi procedure in matrix notation by setting

$$\begin{array}{lll} V_j & := & [v_1, v_2, ...v_j] \quad \text{a matrix with orthonormal columns} \\ (H_{m,m+1})_{i,j} & := & \begin{cases} h_{i,j} & \text{for } i \leq j+1 \\ 0 & \text{otherwise} \end{cases} \quad \text{is } (m \times m+1) \text{ upper Hessenberg} \\ H_{m,m} & & \text{denotes the submatrix formed of the first } (m \times m) \text{ block of : } H_{m,m+1} \end{array}$$

leads to

$$\begin{aligned} AV_m &= V_{m+1}H_{m,m+1} \\ &= V_m H_{m,m} + h_{m+1,m} v_{m+1} e_m^T. \end{aligned} \tag{5.31}$$

Furthermore we see

$$\begin{aligned} V_m^* A V_m &= V_m^* V_m H_{m,m} + h_{m+1,m} V_m^* v_{m+1} e_m^T \\ &= H_{m,m}. \end{aligned} \tag{5.32}$$

We achieved a projected eigenvalue problem of Hessenberg form.
We call a unitary transformation of A satisfying (5.31) and (5.32) a *m-step Arnoldi factorization* of A.

Remark 5.2.9 *If A is hermitian, (analogous the QR-algorithm) the Hessenberg matrix is a tridiagonal matrix and the associated variant of the Arnoldi method is called* Lanzcos method.

Eigenvalue approximations
The projected Hessenberg problem of size $(m \times m)$ is solved directly by the QR-algortihm and we get m eigenvalues.

If (θ, y) is an eigenpair of the projected problem:

$$H_{m,m} y = \theta y\,, \tag{5.33}$$

we get an approximate eigenpair for $Ax - \lambda x = 0$ due to

$$\begin{aligned} H_{m,m} y - \theta y &= 0 \\ V_m^* A V_m y - \theta y &= 0 \\ V_m^* (A V_m y - \theta V_m y) &= 0 \\ V_m^* (As - \theta s) &= 0 \quad \text{with } s := V_m y. \end{aligned}$$

Employing the eigenpair approximation to the original problem leads to a residual which is orthogonal to the projected subspace.
(θ, s) is a Ritz pair, θ a Ritz-value and s a Ritz-vector corresponding to the subspace $\mathcal{K}^m(A, v)$.
The norm of the residual leads to the *Ritz estimate*

$$\begin{aligned} \|As - \theta s\| &= \|AV_m y - \theta V_m y\| = \|H_{m,m} V_m y + h_{m+1,m} v_{m+1} e_m^T y_m - \theta V_m y\| \\ &= \|V_m (H_{m,m} y - \theta y + h_{m,m+1} v_{m+1} y_m\| \\ &= |h_{m+1,m}|\, |y_m|. \end{aligned}$$

If there is a breakdown in the Arnoldi procedure ($h_{j+1,j} = 0, v_{j+1} = 0$), the Ritz-values are exact eigenvalues, i.e.

$$\sigma(H_{jj}) \subset \sigma(A). \tag{5.34}$$

One has to mention that a small residual does in general not imply a small error for the eigenvalue/eigenvector approximation, but it can be used to construct stopping criteria.

Improvements - Restarting an Arnoldi method
In the above presented form of the algorithm one has to increase m as long as one gets all interested eigenvalues and the projected Hessenberg problem is solved by QR-algorithm. For large problems this can be very expensive in computation and storage requirement. We have to apply some improvements in order to keep m small while computing all eigenvalues of interest.
Another big problem is the fact that the required orthogonality of the computed Krylov base can hardly be hold in finite precision arithmetic if m becomes large.

In the analysis of the power method we have seen that the choice of the starting vector completely determines the approximate eigensolutions. How should we choose the new starting vector in order to take up as much desired information as possible from the actual Krylov space?
One obvious method of restarting is to compute an m-step Arnoldi factorization and the corresponding approximate eigenvalues. Then the spectrum is splitted in two disjoint sets: the set of good-fitting (k) and the set of unwanted ($p = m - k$) Ritz-values. The new starting vector can be chosen as a linear combination of eigenvectors according to the k wanted Ritz-values. This is one variant of *explicit restarting*.
We try to stick the information of a m-dimensional subspace into one vector. Coming up with this problem leads to the implicitly restarted Arnoldi method.

Implicitly Restarted Arnoldi Method - IRAM This technique combines the implicitly shifted QR-iteration and the m-step Arnoldi-factorization. Interesting eigenvalue information of an m-step Arnoldi factorization is extracted and compressed to a smaller (fixed-sized) k-step factorization.

Algorithm 5.2.10 *Computing an updated partial Arnoldi-factorization*
Assume an already computed $(m = k+p)$-Arnoldi factorization of $A : AV_m = V_m H + f_m e_m^T$.

1. *Extract Ritz-values from the Hessenberg matrix H and choose k wanted Ritz-values.*

2. *Apply p shifted QR-iterations of the form $(H - \mu_j I) = QR$:*

$$\begin{aligned} (A - \mu_j I)V - V(H - \mu I) &= f_m e_m^T \\ A\underbrace{(VQ)}_{V^+} - \underbrace{(VQ)}_{V^+}\underbrace{(RQ + \mu_i I)}_{H^+} &= f_m e_m^T Q. \end{aligned}$$

   After p steps the first k columns of the transformed m-step Arnoldi factorization turns out to be a k-step Arnoldi-factorization including the information according to the k chosen best-fitting Ritz-values

$$AV_k^+ = V_k^+ H_k^+ + f_k^+ e_k^T. \tag{5.35}$$

3. *Use the updated truncated Arnoldi factoization (5.35) as starting point and apply again p Arnoldi-steps to get a m-step Arnoldi factorization and go to step 1.*

Some computational aspects of IRAM Let $m = k + p$ denote the dimension of the Arnoldi-factorization of the Implicite Restarted Arnoldi Method. Moreover, k is the number of wanted eigenvalues and p the number of applied implicite QR-shift in each iteration step.

- If we choose k of moderate size, orthogonality of the base V_k can be preserved according to working precision also in finite arithmetic. No spurious eigenvalues can be produced by the lack of orthogonality.

- The storage requirement of the restarted version is of fixed size, i.e. $2nk + \mathcal{O}(k^2)$.

- On the computational cost of IRAM:
  We suffice with presenting the total cost of one iteration step of IRAM here, a specification in more detail and itemization in each step of the algorithm can be found in [8] p. 185. We define γ such that γn is the cost of a matrix-vector product Av with the system matrix A of dimension $n \times n$.

  The total cost of one IRAM iteration is

$$\gamma pn - 2[(5k - 2)p + 2p^2]n + 2k^2 n + \mathcal{O}((k + p)^3).$$

- On the stopping criterion (used also in ARPACK): A Ritz pair $(\theta, x) = (\theta, V_k y)$ is assumed to be converged if θ is in the set of wanted eigenvalues and

$$\underbrace{\|f_k\||e_k^* y|}_{\text{Ritz estimate}} \leq max(\|H_k\|\epsilon_M, tol \cdot |\theta|).$$

Moreover, the computed Ritz-pair (θ, x) is an exact eigenpair of a matrix $A+E$ near A, i.e.

$$(A+E)x = \theta x \quad \text{with } E = -(e_k^T s) f_k x^H,$$

where ϵ_M is the machine precision and the bound $tol \cdot |\theta|$ implies that $\|E\| \leq tol \cdot \|A\|$. For more specification we refer to [8] and [23].

Approximating interior eigenvalues Since the subspace chosen in the Arnoldi method is motivated by the power method one can imagine that the algorithm has fast convergence if we search dominant eigenvalues. One way to compute interior eigenvalues is to apply a spectral transformation of the problem. Interior eigenvalues can be computed by transforming the problem by matching spectral transformation before applying the Arnoldi algorithm. This method has the disadvantage that in each step a system $(A-\gamma I)^{-1}$ has to be solved.
There are some variants of the Arnoldi method which can handle the problem of approximating interior eigenvalues without explicit spectral transformations ($\leftarrow$ harmonic Ritz values). But for this approach the convergence can get very slow.

Krylov methods for generalized eigenvalue problems

Their are three ways of solving

$$Ax - \lambda Bx = 0$$

by Krylov methods:

- Transformation to a standard problem via Shift-and-Invert (SI)

  $$((A-\gamma B)^{-1}B - \mu I)x = 0.$$

  This is recommended if one is interested in interior eigenvalues, i.e. eigenvalues near the shift γ. This technique has the drawback that in each iteration $(A-\gamma B)^{-1}$ has to be solved. One gets good convergence rates to the interested eigenvalues by spectral transformation.

- M-Arnoldi method
  This method is implemented in the ARPACK software package, but has the restriction that the matrix B has to be hermitian and positive semi-definite. It works with B-inner-products, i.e. products of the form $(x,x)_B = (Bx,x)$. Since in our problem B is not positive definite this variant is only mentioned for completeness.

- Rational Krylov algorithm
  In an SI-Arnoldi method the shift is fixed. If one wants to vary it, one would have to reject the already computed subspace and start with a new one. This way one would

lose the whole information sticking in the old subspace. The rational Krylov method is a generalization of the SI-Arnoldi method which compensates this problem. One can vary the shifts and is able to achieve fast convergence of Ritz values according to a union around the chosen shifts.
The main idea is that we start with a SI-Arnoldi for a chosen shift μ_1, compute an orthonormal base V_k with

$$(A - \mu_1)^{-1} B V_k = V_{k+1} H_{k+1,k}$$

and evaluate the eigenvalues of $H_{k+1,k}$. After a few steps the Ritz-values according near the shift μ_1 are well approximated.
We choose a new shift μ_2. Then we have to transform the matrix V_{k+1} the way one can interpret the achieved matrix W_{k+1} (which span the same subspace $span(W_{k+1}) = span(V_{k+1})$) as orthogonal base for a SI-Arnoldi subspace for the shift μ_2. One can perform this transformation by applying a QR-decomposition, solving a triangular system and transforming matrices of size $(k+1)$.
For more detail see [8].

Jacobi-Davidson method for SEP

The Arnoldi method is an effective method for computing interior eigenvalues near a specified shift, if one uses shift-and-invert methods. With the drawback that one has to solve the system $(A - \gamma I)x = b$ accurately and efficiently. The Jacobi-Davidson algorithm provides a technique which manages with approximate (but still reasonable) solutions of the system. Hence precondition methods can be applied.
The Jacobi-Davidson method is an orthogonal projection method, but in contrast to the Arnoldi algorithm the projected matrix is of no special reduced structure. Hence solving the projected eigenvalue problem becomes more expensive.

Expansion of search space:
Assume that we have already computed the subspace base V_k of the k-th step. Then the projected eigenvalue problem is given through

$$V_k^* A V_k y = \theta y$$

and we can compute a desired Ritz-pair $(\theta_k, s := V_k y)$ belonging to V_k.
Now the question is how to expand the base V_k by the information given above?

The residual of the original problem

$$r := As - \theta_k s \tag{5.36}$$

provides information about the quality of the actual k-step eigenvalue approximation. The idea is to expand V_k by a correction $\Delta s \perp s$ of the Ritz-vector s the way the residual of the corrected vector $s + \Delta s$ vanishes according to the subspace orthogonal to s, i.e.

$$(I - ss^*)(A - \theta_k I)(\Delta s + s) = 0. \tag{5.37}$$

One can see that $r \in s^\perp := \{t : t^T x = 0\}$ through $(I - ss^*)(A - \theta_k)s = r - s\underbrace{s^*As}_{\theta_k} - \theta_k s\underbrace{s^*s}_{I} =$ r and therefore

$$(I - ss^*)(A - \theta_k I)\Delta s = -r \tag{5.38}$$

is valid.
In a final step one has to assure that Δs is orthogonal to s in (5.38). After forcing Δs into $s^\perp$ by replacing it with $(I - ss^*)\Delta s \in s^\perp$ we achieve the *Jacobi-Davidson correction equation* according to the residual r and the k-th Ritz-pair (θ_k, s), i.e.

$$(I - ss^*)(A - \theta_k I)(I - ss^*)\Delta s = -r. \tag{5.39}$$

This approach is motivated by the following decomposition of A

$$A = (I - ss^*)A(I - ss^*) + Ass^* + ss^*A - \theta_k ss^* \quad \text{with } \theta_k = s^*As.$$

If $\theta_k = \lambda$ is an exact eigenvalue, the correction equation (if solved accurately) gives the orthogonal complement of s to the exact eigenvector, i.e.

$$(A - \lambda I)(s + \Delta s) = 0$$

holds.

Algorithm 5.2.11 *Jacobi-Davidson for SEP $Ax = \lambda x$*

Projected matrix: $M_k := V_k^* A V_k$

Start settings:
$v_1 = \frac{v}{\|v\|}$; $M_1 = v_1^* A v_1$;
$\theta_1 = m_{11}$; $s = v_1$; $r = As - \theta_1 s$;

Iteration:

for $i = 1, 2, ..., m-1$

Solve Jacobi-Davidson correction equation (approximately)

$$(I - ss^*)(A - \theta_k I)(I - ss^*)\Delta s = -r$$

Orthogonalize via Gram-Schmidt procedure Δs *against* $V_k \rightarrow v_{k+1}$

Expand V_k *:* $V_{k+1} = [V_k, v_{k+1}]$

Expand M_k *:* $M_{k+1} = \begin{pmatrix} M_k & V_k^* A v_{k+1} \\ v_{k+1}^* A V_k & v_{k+1}^* A v_{k+1} \end{pmatrix}$

Solve projected eigenvalue problem $M_k y = \theta y$

Choose one fitting Ritz-vector θ_{k+1} *plus Ritz-vector* $s = V_{k+1} y$

Compute new residual: $r_{k+1} = As - \theta_{k+1} s$

Convergence test via residual

Restart:

$v_1 = s$;

Start again with iteration;

In the presented form the Jacobi-Davidson algorithm results in one desired eigenvector. If more eigenvectors are searched, one has to apply deflation techniques. After a satisfying approximation of the first Ritz-pair, one continues in a subspace spanned by the remaining eigenvectors. Deflation and restart techniques are used in e.g. Jacobi-Davidson-QR-algorithms.

5.2.4 Solving quadratic eigenvalue problems

In most application of quadratic eigenvalue problem the matrices are assumed to be hermitian and positive-definite. Here we deal only with methods which do not exploit special properties of matrices.
Let C_0, C_1, C_2 be general matrices in $\mathbb{C}^{n \times n}$ with the restriction that they do not have a common nullspace, i.e. we assume the quadratic pencil to be regular.

The main solution approaches :

- Transformation of the quadratic pencil to linear form
- Projection methods which project the QEP on a lower-dimensional quadratic problem and solve the lower-dimensioned problem by e.g. linearization-methods
- Newton methods (not treated here)

Transformation to linear form

We transform the quadratic problem

$$\lambda^2 C_2 x + \lambda C_1 x + C_0 x = 0 \tag{5.40}$$

by introducing a new variable

$$y := \lambda x. \tag{5.41}$$

The QEP (5.40) becomes explicitly linear in λ:

$$\begin{array}{lrcl} \text{(a)} & \lambda C_2 y + C_1 y + C_0 x & = & 0 \\ \text{(b)} & \lambda C_2 y + \lambda C_1 x + C_0 x & = & 0 \end{array}$$

Together with (5.41) we get two possible linear eigenvalue problems:

$$\begin{pmatrix} 0 & I \\ -C_0 & -C_1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \lambda \begin{pmatrix} I & 0 \\ 0 & C_2 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}, \tag{5.42}$$

$$\begin{pmatrix} 0 & I \\ -C_0 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \lambda \begin{pmatrix} I & 0 \\ C_1 & C_2 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}. \tag{5.43}$$

Without loss of generality we continue with approach (a). If A, B denote the system matrices in (5.42), we get a linear eigenvalue problem

$$Az = \lambda Bz \quad \text{with} \quad z = \begin{pmatrix} x \\ \lambda x \end{pmatrix}. \tag{5.44}$$

It remains to show the equivalence of the spectra of QEP and linearized form, i.e.

$$det(A - \lambda B) = det(\lambda^2 C_2 x + \lambda C_1 x + C_0 x), \tag{5.45}$$

which follows from the factorization

$$A - \lambda B = \underbrace{\begin{pmatrix} 0 & I \\ -I & -\lambda C_1 - C_0 \end{pmatrix}}_{det(.)=1} \begin{pmatrix} \lambda^2 C_2 x + \lambda C_1 x + C_0 x & 0 \\ 0 & I \end{pmatrix} \underbrace{\begin{pmatrix} I & 0 \\ -\lambda I & I \end{pmatrix}}_{det(.)=1}.$$

Remark 5.2.12 *The problem (5.44) is only explicitly linear, implicitly it is still quadratic. Treating the problem numerically as linear problem without respecting the spectral structure of the eigenvector z (as we do), can lead to a supplementary error.*

Algorithm 5.2.13 *Solve QEP by linearization via QZ-algorithm:*
Build linearization matrices (A, B) *referring to (5.42) or (5.43)*
Compute generalized Schur form of (A, B)*:*
$T_A = W^* A Z$, $T_B = W^* B Z$
for $j = 1, ..2n$
$\lambda_i = \frac{(T_A)_{ii}}{(T_B)_{ii}}$
Solve $(T_A - \lambda_i T_B)y = 0; z = Zy$
$z_1 := \frac{z(1:n)}{\|z(1:n)\|}$
$z_2 := \frac{z(n+1:2n)}{\|z(n+1:2n\|}$
$r_1 = \lambda_i^2 C_2 z_1 + \lambda_i C_1 z_1 + C_0 z_1$
$r_2 = \lambda_i^2 C_2 z_2 + \lambda_i C_1 z_2 + C_0 z_2$
Choose z_j *with minimal* r_j *as eigenvector* x_i *corresponding to* λ_i
end for

Solving linearized problem via iterative methods:
We assume a subspace method which can manage only with matrix*vector products Av, Bv and the system matrices need not be given explicitly. The products can be pieced efficiently together by the products corresponding to the smaller sized quadratic system matrices under exploiting the special structure of A, B.
If we want to use a SEP-solver routine or if we are interested in interior eigenvalues and want to utilize SI-methods, we have to provide $B^{-1}Av$ or $(A - \mu B)^{-1}Bv$. An efficient algorithm can be derived from factorization

$$B^{-1}A = \begin{pmatrix} 0 & I \\ -C_2^{-1}C_0 & -C_2^{-1}C_1 \end{pmatrix}, \tag{5.46}$$

$$(A - \mu B)^{-1}B = \begin{pmatrix} I & 0 \\ \mu I & I \end{pmatrix} \begin{pmatrix} (\mu^2 C_2 + \mu C_1 + C_0)^{-1} & 0 \\ 0 & I \end{pmatrix} \begin{pmatrix} -C_1 - \mu C_2 & -C_2 \\ I & 0 \end{pmatrix} \tag{5.47}$$

Instead of solving systems of dimension $(2n \times 2n)$ via exploiting the special structure the solution of $(n \times n)$ systems will be sufficient (e.g. sparse LU-factorization).

Algorithm 5.2.14 *Compute k eigenvalues of QEP by linearization via subspace projection*
Provide efficient matrix-multiplication and shift-and-invert-routines
Compute k desired eigenvalues via subspace method: (λ_i, z_i)
for $i = 1, ...k$
$z_1 := \frac{z(1:n)}{\|z(1:n)\|}$
$z_2 := \frac{z(n+1:2n)}{\|z(n+1:2n\|}$

$r_1 = \lambda_j^2 C_2 z_1 + \lambda_j C_1 z_1 + C_0 z_1)$
$r_2 = \lambda_j^2 C_2 z_2 + \lambda_j C_1 z_2 + C_0 z_2$
Choose z_j *with minimal* r_j *as eigenvector* x_i *corresponding to* λ_i
end for

The big advantage of linearization is the fact that, it can be solved with already introduced solvers for LEPs, but it has two main drawbacks. First the corresponding linear problem is double the dimension ($2n \times 2n$) and second in finite arithmetic the special form of the eigenvectors $z = (x, \lambda x)^T$ is not automatically implied. The information about the special structure is lost.
If this structure is respected in the algorithm, this leads to structure preserving methods. In these methods the projection subspace has to be expanded the way the special structure of the original problem will be implied on the projected problem. Moreover the projected problem has to be solved under respecting the structure as well. For detailed information see [11].

Jacobi-Davidson for quadratic problems

Jacobi-Davidson methods are used to avoid the disadvantage of lineraization (doubling the dimension, not respecting structure of eigenvector). It acts directly on the QEP, the subspace is expanded by corrections of the iterated Ritz-vectors analogously to the Jacobi-Davidson correction equation for SEPs. The correction equation can be again solved approximately.

Expansion of subspace - eigenvector correction:
Assume a given subspace V_k with already computed and chosen Ritz-pair $(\theta, u := V_k y)$ corresponding to the k-th step projected problem, i.e.

$$V_k P_2(\theta) V_k y = 0. \tag{5.48}$$

Analogous to the SEP version of Jacobi-Davidson we want to expand the subspace by improving the Ritz-vector s with respect to the residual $r := P_2(\theta)s$.
Assume $(\Delta\theta, \Delta s)$ is the exact orthogonal correction of (θ, s) to the according eigenpair solution

$$P_2(\theta + \Delta\theta)(s + \Delta s) = 0 \qquad \text{with } s \perp \Delta s. \tag{5.49}$$

Taking only first order terms of (5.49) into account

$$P_2(\theta + \Delta\theta)(s + \Delta s) = P_2(\theta)s + P_2(\theta)\Delta s + \Delta\theta \underbrace{(2 * \theta C_2 + \theta C_1)}_{P_2'(\theta)} s + \mathcal{O}(\Delta\theta\Delta s + \Delta\theta^2) \tag{5.50}$$

leads to

$$-r = P_2(\theta)\Delta s + \Delta\theta P_2'(\theta)s \qquad \text{with } \Delta s \perp s. \tag{5.51}$$

To expand the subspace we only need a correction Δs of the Ritz-vector s, therefore we are not interested in the term corresponding to the correction $\Delta\theta$. We can drop this term by testing equation (5.51) in a space orthogonal to $\Delta\theta P_2'(\theta)s$ but invariant for $-r = -P_2(\theta)s$ and $P_2(\theta)\Delta s$. This holds for testing with the space according to $(I - P_2'(\theta)ss^*)$ (since $s^*P_2(\theta)s = 0$):

$$-r = (I - P_2'(\theta)ss^*)P_2(\theta)\Delta s \qquad \text{with } \Delta s \perp s. \tag{5.52}$$

Then we restrict the search space in (5.52) in order to fulfill the orthogonality constraint implicitly. We constitute the *generalized Jacobi-Davidson correction equation* by

$$-r = (I - P_2'(\theta)ss^*)(P_2(\theta))(I - ss^*)\Delta s. \tag{5.53}$$

We get an expansion v_{k+1} by orthonormalizing the update Δs , i.e. (approximate) solution of the correction equation (5.53), against the columns of V_k.

Algorithm 5.2.15 *Jacobi-Davidson method for QEP* $P_2(\lambda)x = 0$

Projected matrices: $M_i^k := V_k^* C_i V_k$

Start settings:

Choose a $(n \times m)$ *orthonormal matrix* V

for $i = 1, ..3$ *compute* $M_i = V^* C_i V$

Iteration:

for $k = m, ..., m_{max} - 1$

Compute eigenpairs (θ, y) *of* $(\theta^2 M_2 + \theta M_1 + M_0)y = 0$

Choose a desired Ritz-pair $(\theta, u = Vy)$ *with* $\|y\| = 1$

Compute residural $r = P_2(\theta)u$

if $(\|r\|_2 < \epsilon)$ $\lambda = \theta; x = u;$ *STOP*

Solve Jacobi-Davidson correction equation (approximately) $\Delta u \perp u$

$$\left(I - P_2'(\theta)uu^*\right) P_2(\theta) \left(I - uu^*\right) \Delta u = -r$$

Orthogonalize via Gram-Schmidt Δu *against* $V \to v_{k+1}$ *with* $\|v_{k+1}\| = 1$

for i = 1,2,3 $M_i^{k+1} = \begin{pmatrix} M_i^k & V^* C_i v_{k+1} \\ v_{k+1}^* C_i V & v_{k+1}^* C_i v_{k+1} \end{pmatrix}$

Expand $V_{k+1} = [V_k, v_{k+1}]$

end for;

Settings for restart

Choose best m Ritz-pairs (θ_i, u_i) *from last step*

Orthonormalize $\{u_1, ..., u_m\} \to V_m$

Compute $M_i = V_i^* C_i V_i$ *for* $i = 1, 2, 3$

Restart;

We have presented the main ideas and theoretical background of the wide range of algorithms for solving standard, general linear and quadratic non-hermitian eigenvalue problems. The direct QZ-solver states a robust and reliable solving routine, but since it is direct, it requires direct factorization and destroys any sparsity of the system matrices.
The Arnoldi method with implicit restarts was presented in more detail, because it is implemented in ARPACK, a software package we use for solving the inner-node matrix problem. The method can handle sparse matrices and need no explicit knowledge of the system-matrices, if matrix-vector products are supplied.
The Jacobi-Davidson method was introduced, since it provides a method for solving quadratic eigenvalue problems without linearization.

5.3 Available software packages

There are some open source solver routines for solving non-hermitian linear eigenvalue problems. We introduce two of them: LAPACK which provides the direct QR/QZ-solver and ARPACK which is the implemented version of the implicitly restarted Arnoldi method. We briefly sketch the solvable problem types and the input paramters one has to supply for solving non-hermitian eigenvalue problems with each package.

5.3.1 The Linear Algebra Package LAPACK/LAPACK++

LAPACK provides dense matrix classes (complex and real), direct linear system solvers (factorizations) and direct solvers for linear (generalized and standard) eigenvalue problems via QR-QZ-algorithm optional in complex and real arithmecy.
LAPACK++ is the C++-extension of the Fortran90-kernel of LAPACK and provides object-oriented matrix classes and interfaces for symmetric solvers.

For the solution of non-hermitian generalized linear eigenvalue problems LAPACK [2] provides the routines DGGEV() for real and ZGGEV() for complex problems. The routines solve non-hermitian problems of the form $Ax = \lambda Bx$, where A, B are square, by the QZ-algorithm. Since the solver can handle multiple and infinite eigenvalues, there are no special restrictions on A, B. The whole spectrum and on demand all left and/or right eigenvectors are computed.
In order to apply the xGGEV()-routine, one only has to provide

- the problem dimensions and
- the matrices A, B in dense LAPACK-matrix-class form.

In addition to the QZ-solver LAPACK provides balancing and scaling routines xGGBAK and xGGBAK, which optionally preprocess the matrices A, B. In the balancing routine the

matrix pencil gets permuted in order to achieve that A, B are as nearly upper triangular as possible. The scaling routine provides a similarity transformation to get that the rows and columns of the matrices are as close in norm to 1 as possible. These tools can improve the speed and accuracy of the later applied QZ-algorithm. The transformations do not change the spectrum, but a back-transformation of the computed eigenvectors is required.
Since in piezoelectric problems the magnitude of elastic and electric stiffness matrix entries differ in a wide range, scaling routines are essential to get accurate results for this problem class. The problem of scaling eigenvalue problems will be discussed in Chapter 6 in more detail.

5.3.2 Arnoldi Package (ARPACK/ARPACK++)

The Arnoldi package provides the Implicit Restarted Arnoldi method sketched in algorithm 5.2.10. The theory of the underlying method is described in the users' guide for ARPACK [23]. In the users' guide of ARPACK++ [13] a detailed description of the implementational aspects are given.
ARPACK++ is the object-orientated extansion of ARPACK and has the same functionality.
The routines are separated into three problem classes : real symmetric , real non-symmetric and complex non-hermitian problems. Within these three classes are one differs between generalized and standard eigenvalue problems. In the following we will concentrate on the complex solver classes.

Remark 5.3.1 *on generalized eigenvalue problems solvable by the Arnoldi package*
Since ARPACK implements the M-Arnoldi method (described in subsection 5.2.3) for solving generalized problems, eigenvalue problems of the form $Ax = \lambda Bx$ can only be solved under the assumption that B is hermitian positive-definite, while the matrix A is of arbitrary form.

The main advantage of Arnoldi-methods is that the matrices have not to be given in explicit form, i.e. supplying the matrix-vector product is sufficient. The Arnoldi-Packages provides solving-classes which requires only user-defined matrix-vector-products (ArCompStdEig, ArCompGenEig).
There are two modes for each problem class concerning the part of the spectrum we want to compute:

In the regular mode one is interested in *nev* eigenvalues of largest/smallest magnitude or real/imaginary part. The user-supplied matrix-object classes have to provide the problem dimension and for the standard problem the product $OPx = Ax \rightarrow y$ and for the generalized problem $OPx = B^{-1}Ax \rightarrow y$ and $Bx \rightarrow z$.

In the shift and invert mode we want to compute nev eigenvalues closest to a complex shift σ. The user-supplied matrix-object classes have to provide the problem dimension and for standard problems the spectral shift operation $OPx = (A - \sigma I)^{-1}$ and for generalized problems $OPx = (A - \sigma B)^{-1} \rightarrow y$ and $Bx \rightarrow z$.

The required input parameters in the constructor of ArCompStdEig and ArCompGenEig are

- the dimension of the problem n
- the number of wanted eigenvalues nev
- one (in case of standard problem) or two (in case of generalized problem) matrix objects with the above described matrix-products according to the selected mode (OPx, Bx)
- (optional) the relative accuracy *tol* of Ritz values for the stopping criterion. By default it is set to machine precision. If convergence takes place, the computed eigenvalues λ fulfill
$$|\lambda - \lambda^*| < tol\,|\lambda|$$
where λ^* is the exact eigenvalue of A which is closest to λ.
- (optional) the dimension of the computed Arnildi-base $ncv = nev + p$. By default the parameter is set to $2 \cdot nev$, which is a good choice due to experience [8].
- (optional) a starting vector for the Arnoldi-process, by default a random vector is used.

Chapter 6

Application of Eigenvalue Theory

Now we combine the previous two chapters, i.e. we analyze and solve the problems stated in Chapter 4 with the theory and solvers provided in Chapter 5.
We have seen that special properties of the matrix pencil imply special properties of the spectrum. Thus we analyze the spectrum of the stated problems first and reflect how these properties can be used in computation. Then we check how open-source eigenvalue solvers can be applied to the posed problem-types. At the end of this chapter we deal with the problem of scaling eigenvalue problems, which is necessary for getting reasonable results in the case of piezoelectric problems.

We want to solve one of the following eigenvalue problems:

- *The Inner-Node-Matrix Method* leads to a larger sized, but linear eigenvalue problem
  Find $u = (u_i, u_l)^T \in \mathbb{C}^{N_i+N_l}$ and $\gamma \in \mathbb{C}$ solving

$$\boxed{\begin{pmatrix} \overline{K}_{ii} & \overline{K}_{il} \\ \overline{K}_{ir}^T & 0 \end{pmatrix} \begin{pmatrix} u_i \\ u_l \end{pmatrix} = \gamma \begin{pmatrix} 0 & -\overline{K}_{ir} \\ -\overline{K}_{il}^T & -(\overline{K}_{ll} + \overline{K}_{rr}) \end{pmatrix} \begin{pmatrix} u_i \\ u_l \end{pmatrix}.} \tag{6.1}$$

  All matrices are complex and K_{ll}, K_{rr}, K_{ii} are complex-symmetric.

- *The SC-method* leads to the quadratic problem

$$\boxed{\text{Search } \gamma \in \mathbb{C}, y_l \neq 0 \in \mathbb{C}^{N_l}: \quad \gamma^2 S_{12} y_l + \gamma(S_{11} + S_{22}) y_l + S_{12}^T y_l = 0,} \tag{6.2}$$

  where N_l is of moderate size with two variants of given problems, i.e. explicitly given dense matrices S_{ij} of moderate size, which were derived by inverting a matrix K_{ii} or secondly the matrices are implicitly given only by matrix-vector products, for which we need K_{ii}^{-1}. The matrices are complex and S_{11}, S_{22} are complex symmetric.

Remark 6.0.2 *The eigenvalue problems presented above are parameter-dependent, i.e. they have to be solved in each frequency step ω, since $\overline{K} = \overline{K}(\omega)$ and $S_{**} = S_{**}(\omega)$.*
In both problems we are interested in a few eigenvalues γ near the unit circle, i.e. $|\gamma| \approx 1$.

6.1 Spectral properties

6.1.1 The spectral connection between the alternative methods

We analyze the connection between the two methods. Since the methods describe the same problem, one has to check if the two alternatives lead to the same result, i.e. if they have the same spectrum or at least if the interesting eigenvalues occur in both problems and if these eigenvalues are equal and can be separated in the solution.
In the subsection on periodic search and test-spaces we have seen that the quadratic problem (6.2) arises from the linear problems (6.1) by forming the Schur-complement. It is obvious that the SC-problem has $2 \cdot N_l$ eigenvalues, since the matrices are of dimension $(N_l \times N_l)$ and the problem is quadratic, but that the Inner-Node-Matrix Problem has $N_i + N_l$ eigenvalues. Which eigenvalues do we drop in forming the Schur-complement ? Which effect is implied on the spectrum of a matrix by forming the Schur-complement ?
In order to determine the transformation of the spectrum we have to state and examine the SC-method as transformation of the INM-Problem. Applying the multiplication

$$\begin{pmatrix} I & 0 \\ (\overline{K}_{ir}^T + \gamma \overline{K}_{il}^T)\overline{K}_{ii}^{-1} & I \end{pmatrix} . \quad (6.1)$$

from the left to the Inner-Node-Matrix Problem leads to

$$\begin{pmatrix} \overline{K}_{ii} & \overline{K}_{il} + \gamma \overline{K}_{ir} \\ 0 & \gamma^2 S_{12} + \gamma(S_{11} + S_{22}) + S_{12}^T \end{pmatrix} \begin{pmatrix} u_i \\ u_l \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} . \quad (6.3)$$

The transformation matrix is regular and well-defined for all γ finite, i.e. the transformation is similiar. Therefore, if σ^* denotes the set of finite eigenvalues, $\sigma^*_{(6.1)} = \sigma^*_{(6.3)}$ holds. Through the decoupling of the lines according to u_i and u_l in (6.3), it is valid that

$$(\gamma, u_l) \text{ finite eigenpair of (6.2)} \Leftrightarrow (\gamma, \begin{pmatrix} -\overline{K}_{ii}^{-1}(\overline{K}_{il} + \gamma \overline{K}_{ir})u_l \\ u_l \end{pmatrix}) \text{ finite eigenpair of (6.3).}$$

Therefore the finite spectra of the INM and the SC Problem are equal, i.e.

$$\sigma^*_{(6.1)} = \sigma^*_{(6.2)} .$$

6.1.2 On symplectic-type pencils

Analyzing the symmetries of the matrix blocks in the INM-Problem and the special property that the quadratic problem is nearly of equal form as the according inverted quadratic eigenvalue problem one can state some helpful results on the form of the spectrum.

Special structure of the quadratic eigenvalue problem

Theorem 6.1.1

1. *If (γ, x_l) is a right eigenpair of*
$$\gamma^2 S_{12} x_l + \gamma(S_{11} + S_{22}) x_l + S_{12}^T x_l = 0 \tag{6.4}$$
then $(\frac{1}{\bar{\gamma}}, \bar{x})$ is a left eigenpair ($\bar{x}$ denotes the complex conjugate vector).

2. *For real-valued matrices (undamped system: $C = 0$) complex eigenvalues occur in quadruples*
$$\gamma \in \sigma_S \Rightarrow \frac{1}{\gamma}, \bar{\gamma}, \frac{1}{\bar{\gamma}} \in \sigma_S \tag{6.5}$$

Proof:

1. *Statement is valid due to symmetry of the matrices ($(S_{11} + S_{22}) = (S_{11} + S_{22})^T$):*
Let (γ, x) be a right eigenpair.
We view the left eigenvalue problem and transpose it
$$\begin{aligned} \mu^2 y^* S_{12} + \mu y^*(S_{11} + S_{22}) + y^* S_{12}^T &= 0 \quad |^T \\ \mu^2 S_{12}^T \bar{y} + \mu(S_{11} + S_{22})\bar{y} + S_{12}\bar{y} &= 0 \quad | \tfrac{1}{\mu^2}. \\ S_{12}^T \bar{y} + \tfrac{1}{\mu}(S_{11} + S_{22})\bar{y} + \tfrac{1}{\mu^2} S_{12}\bar{y} &= 0, \end{aligned}$$
i.e. $(\frac{1}{\mu}, \bar{y})$ is a right eigenpair.
For all $(\gamma = 0, x)$ right eigenpairs: $x \in \mathcal{N}(S_{12}) \Rightarrow \bar{x}^* S_{12}^T = x^T S_{12} = 0$, i.e. infinite left eigenpair $(\infty, \bar{x})$. Analogous for $\gamma = \infty$.

2. *Complex eigenvalue of real valued matrices come in complex conjugate pairs.*

Special structure of the linear eigenvalue problem

The analogous result can be stated for the linear INM-Problem. Let $(\gamma, \begin{pmatrix} x \\ y \end{pmatrix})$ be a finite non-zero right eigenpair of

$$\begin{pmatrix} M_1 & G \\ F^T & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \gamma \begin{pmatrix} 0 & -F \\ -G^T & -M_2 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \Rightarrow \begin{aligned} M_1 x &= -(G + \gamma F) y \\ (F^T + \gamma G^T) x &= -\gamma M_2 y \end{aligned} \tag{6.6}$$

If the problem acts related to the SC-method we can determine parameters $\alpha_1, \alpha_2 \in \mathbb{C}$ in such a way that $(\frac{1}{\gamma}, \begin{pmatrix} \alpha_1 \bar{x} \\ \alpha_2 \bar{y} \end{pmatrix})$ solves the left eigenvalue problem. Transposing the left eigenvalue problem we get

$$\begin{pmatrix} M_1 & F \\ G^T & 0 \end{pmatrix} \begin{pmatrix} \alpha_1 x \\ \alpha_2 y \end{pmatrix} = \frac{1}{\gamma} \begin{pmatrix} 0 & -G \\ -F^T & -M_2 \end{pmatrix} \begin{pmatrix} \alpha_1 x \\ \alpha_2 y \end{pmatrix} \tag{6.7}$$

then we express in form of (6.6)

$$\begin{aligned} \alpha_1 M_1 x &= -\tfrac{1}{\gamma}\, \alpha_2\, (G + \gamma F) y \\ \tfrac{1}{\gamma}\, \alpha_1\, (F^T + \gamma G^T) x &= -\tfrac{1}{\gamma^2}\, \alpha_2 (\gamma M_2) y \end{aligned}$$

Comparison of coefficients gives: $\gamma\, \alpha_1 = \alpha_2$

With setting $\alpha_1 = 1$ we state

Theorem 6.1.2

1. *To each* **finite non-zero** *right eigenpair* $(\gamma, \begin{pmatrix} x_i \\ x_l \end{pmatrix})$ *of the Inner-Node-Matrix eigenvalue problem (6.6)* $(\frac{1}{\gamma}, \begin{pmatrix} \bar{x}_i \\ \gamma \bar{x}_l \end{pmatrix}$ *is a left eigenpair,i.e.* $\gamma \in \sigma \Leftrightarrow \frac{1}{\gamma} \in \sigma$.

2. *For real-valued systems (undamped* $C = 0$*) complex eigenvalues of (6.6) occur in quadruples:*

$$\gamma \in \sigma_S \Rightarrow \ \frac{1}{\gamma}, \bar{\gamma}, \frac{1}{\bar{\gamma}} \in \sigma_S \tag{6.8}$$

Remark 6.1.3 *on structure preserving methods and symplectic matrices*
The presented spectral properties can be used for structure preserving methods.
The structure of the Inner-Node-Matrix system reminds on symplectic matrices, i.e. a matrix pencil $A - \lambda B$ *is called* symplectic *, if*

$$AJ^T = BJ^T \qquad \text{with } J = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix} \tag{6.9}$$

Structure preserving methods for symplectic matrices are introduced in Mehrmann [11].

The result that if γ is a finite eigenvalue, its reciprocal is one as well, can only be used in form of structure preserving methods in iterative methods which work with left and right eigenspaces, i.e. two-sided Lanczos methods. By using only methods which work with right eigenspaces, e.g. Krylov methods only use right eigenvectors in the construction of the projection subspaces, we will not take the full advantage out of this spectral result.

6.2 Solving the SC quadratic eigenvalue problem

Since we intend to use the Implicit Restarted Arnoldi solver and the QZ-Solver provided by ARPACK or respectively LAPACK, we can only solve linear eigenvalue problems. To apply these solvers on the SC-problem, one has to linearize the problem the way presented in (5.42) first and then call the solving routines with the linearized matrices.

6.2.1 Linearization of the SC-quadratic eigenvalue problem

Linearization of problem (6.4) leads to a LEP with the same spectrum

$$\begin{pmatrix} 0 & I \\ S_{12}^T & S_{11}+S_{22} \end{pmatrix} \begin{pmatrix} x \\ z \end{pmatrix} = \gamma \begin{pmatrix} I & 0 \\ 0 & -S_{12} \end{pmatrix} \begin{pmatrix} x \\ z \end{pmatrix} \text{ with } z = \gamma x, \qquad (6.10)$$

$$\text{abbreviated by} \quad L_A y = \gamma L_B y.$$

The generalized linear eigenvalue problem is a dense problem of "moderate" size $(2 \cdot n_l \times 2 \cdot n_l)$ with dense system matrices. We are interested in eigenvalues with $|\gamma|$ near 1.

Remark 6.2.1 *on the regualrity of the linearized matrices L_A, L_B*
The matrix S_{12} denotes the subdiagonal block of the Schur-complement of problem (6.1), therefore we can not state its regularity. Since we can not give any assertions on the regularity of L_A and L_B. shift-and-invert methods as well as a transformation to standard problem of the GEP 6.10 is not well-defined.

Solving the linearized SC-problem with the direct QZ-solver In section (5.3.1) we described the functioning and input parameters of the LAPACK routine xGGEV(), which provides the QZ-algorithm for real non-hermitian eigenvalue problems.
For using xGGEV() one has to provide the problem dimension and the linearized system matrices L_A, L_B in the dense matrix class of LAPACK.
Solving the linearized SC-problem via the LAPACK-QZ-solver include the following main steps:
Under the assumption of already assembled stiffness, mass and damping matrices K, M, C one has to perform

- the computation $\overline{K} = K + i\omega C - \omega^2 M$,
- the separation/mapping of $\overline{K}$ in block matrices according to inner, left and right nodes,
- the computation of Schur-complement blocks via LU-factorization of $\overline{K}_{ii}$
  $\rightarrow S_{12}, S_{11}, S_{22}$,

- the linearization matrices L_A, L_B of (6.10)
- a call of LAPACK xGGEV() with L_A, L_B

in each frequency step.

Algorithm 6.2.2 (QZ-Schur-PBCSolver) *We assume ready-assembled stiffness and mass matrices K, M, where rows and columns according to Dirichlet nodes are already dropped.*

Provide matrices according to inner,left and right nodes $\rightarrow K_{st}, M_{st}$ *for* $s,t = i,l,r$;

for all ω do

1. if(damping) *for* $s,t = i,l,r$ $\quad \overline{K}_{st} = \begin{pmatrix} K_{st} - \omega^2 M_{st} & -\omega(\tilde{\alpha} K_{st} + \tilde{\beta} M_{st}) \\ \omega(\tilde{\alpha} K_{st} + \tilde{\beta} M_{st}) & K_{st} - \omega^2 M_{st} \end{pmatrix}$;
   else *for* $s,t = i,l,r$ $\quad \overline{K}_{st} = K_{st} - \omega^2 M_{st}$;
2. LU-factorization of $\overline{K}_{ii}$, i.e. $\overline{K}_{ii} = LU$
3. Compute SC-blocks via back-substitution in LU, i.e.

$$\begin{aligned} LU\, T_{ir} &= \overline{K}_{ir}; && \rightarrow T_{ir} \\ S_{12} &= \overline{K}_{li} T_{ir}; \\ S_{22} &= \overline{K}_{ri} T_{ir} + \overline{K}_{rr}; \\ LU\, T_{il} &= \overline{K}_{il} && \rightarrow T_{il}; \\ S_{11} &= \overline{K}_{li} T_{il} + \overline{K}_{ll}; \end{aligned}$$

4. Build LAPACK-dense matrices L_A, L_B according to (6.10);
5. xGGEV$(2 \cdot N_l, 2 \cdot N_l, L_A, L_B, evals, evecs)$;
6. Compute $\alpha_j = |evals(j)|, \beta_j = arg(evals(j)) \qquad (j = 1, ..., 2 \cdot N_l)$;
   Choose n_{ev} pairs (α_j, β_j) with smallest $|\alpha_j|$;

Remark 6.2.3 *The Rayleigh-damping coefficients $\tilde{\alpha}, \tilde{\beta}$ can be chosen frequency-dependent, i.e. $\tilde{\alpha}(\omega), \tilde{\beta}(\omega)$.*

The main costs of Algorithm 6.2.2 consist in the computation of the LU-factorization for each ω and in the solution of the dense, but moderate-sized $(2 \cdot N_l \times 2 \cdot N_l)$ eigenvalue problem for each ω.

Solving the SC-problem with the Arnodli-package? Not possible. Due to Remark 6.2.1 the linearized problem (6.10) cannot be solved by the Arnoldi package. Nor does it fulfill the criteria of the generalized solver (L_B is not hermitian positive definite) neither can we state a well-defined similar standard eigenvalue problem.

6.3 Solving the Inner-Node-Matrix eigenproblem

On infinite and zero eigenvalues

Through reflections on the rank and nullspaces of the system matrices we want to get an idea of the number of interesting eigenvalues in the system. Therefore we compute the number of eigenvalue we are never interested in, i.e. zero and infinite eigenvalues, since this is equivalent with $|\alpha| = \infty$.

Infinite right eigenvectors $(x, y)^T$ lie in the nullspace of $B := \begin{pmatrix} 0 & -\overline{K}_{ir} \\ -\overline{K}_{li} & -\overline{K}_{ll} - \overline{K}_{rr} \end{pmatrix}$, since $N_i + N_l = rk[B] + dim(\mathcal{N})(B)$ we compute the rank of B (rk[B]). By the regularity of $K_{ll} + K_{rr}$ we get $rk[B] \leq N_l + \underbrace{rk[K_{il}]}_{:=m_l \leq N_l} \leq 2N_l$ and hence

$$dim(\mathcal{N}(B)) = N_i - m_l \geq N_i - N_l$$

The dimension of the nullspace of $A := \begin{pmatrix} \overline{K}_{ii} & \overline{K}_{il} \\ -\overline{K}_{ri} & 0 \end{pmatrix}$ gives the number of zero eigenvalues. Through $rk[A] \leq N_i + \underbrace{rk[K_{ri}]}_{:=m_r \leq N_l} \leq N_i + N_l$ there are $N_l - m_r \geq 0$ zero eigenvalues.

The main result is that the INM-Problem has at least $N_i - N_l$ infinite eigenvalues, i.e. we are interested in at most $2 \cdot N_l$ eigenvalues of the $N_i + N_l$ eigenvalues of the linear problem.

6.3.1 Spectral transformation

Setting up the problem we mentioned the fact that $A-B$ is complex symmetric and regular. In order to achieve a more regular problem, the first part of a spectral transformation results in

$$\begin{pmatrix} \overline{K}_{ii} & \overline{K}_{il} + \overline{K}_{ir} \\ \overline{K}_{ir}^T + \overline{K}_{il}^T & \overline{K}_{ll} + \overline{K}_{rr} \end{pmatrix} \begin{pmatrix} u_i \\ u_l \end{pmatrix} = (\gamma - 1) \begin{pmatrix} 0 & -\overline{K}_{ir} \\ -\overline{K}_{il}^T & -(\overline{K}_{ll} + \overline{K}_{rr}) \end{pmatrix} \begin{pmatrix} u_i \\ u_l \end{pmatrix} \quad (6.11)$$

General spectral transformations are used to shift the interesting part of the spectrum to the end of the spectrum which can be faster approximated by the most numerical methods. We have applied the shift to get a regular symmetric matrix on right side. Therefore we can treat the generalized problem as a standard one (without explicitly computing $(A-B)^{-1}B$).

$$\begin{pmatrix} 0 & -\overline{K}_{ir} \\ -\overline{K}_{il}^T & -(\overline{K}_{ll}+\overline{K}_{rr}) \end{pmatrix} \begin{pmatrix} y_i \\ y_l \end{pmatrix} = \lambda \begin{pmatrix} \overline{K}_{ii} & \overline{K}_{il}+\overline{K}_{ir} \\ \overline{K}_{ir}^T+\overline{K}_{il}^T & \overline{K}_{ll}+\overline{K}_{rr} \end{pmatrix} \begin{pmatrix} y_i \\ y_l \end{pmatrix} \tag{6.12}$$

with $\lambda = 1/(\gamma - 1)$

Remark 6.3.1 *on the spectrum of (6.12)*

1. *The transformed INM-Problem (6.12) has only finite eigenvalues, which seperate into $2 \cdot N_l$ non-zero ones and $N_i - N_l$ zeros.*

2. *The "symplectic" property of the spectrum transforms to*

$$\lambda \in \sigma^*_{(6.12)} \Leftrightarrow -\lambda - 1 \in \sigma^*_{(6.12)}.$$

3. *The part of the spectrum we are interested in, i.e. $|\gamma|$ near 1, distributes unclustered over $\mathbb{C} \setminus \{0\}$.*

4. *The infinite eigenvalues of (6.1) are shifted to 0.*

Extracting the interesting part of the spectrum There is no obvious clustering of the transformed spectrum according to the distance of $\gamma = \frac{1}{\lambda} + 1$ from the unit circle. But we know that the interesting eigenvalues satisfy $\lambda \neq 0$ and that there are only $2 \cdot N_l$ eigenvalues for which this holds. Therefore, one way to extract the interesting part is to compute the $2 \cdot N_l$ eigenvalues of largest magnitude and separate the interesting ones out of the computed set. Since in practical problems $N_l \ll N_i$ the possibility to reduce the computation on only $2 \cdot N_l$ instead of $N_i + N_l$ eigenvalues is of big numerical advantage in the use of iterative methods.

Remark 6.3.2 *Applying the shift has the disadvantage that the desired part of the spectrum, which is characterized in the original problem by the values near the unit-circle, get spread over the whole complex domain excluding zero. But first computing eigenvalues of largest magnitude is of much faster convergence than computing small one (harmonic Ritz values) and secondly we will see that this transformation is necessary in order to use the Arnoldi-package.*

Solving the Inner-Node-Matrix Problem with a direct QZ-solver The LAPACK-QZ-solver can be directly applied to the original INM-Problem (6.1) after conversion to dense LAPACK matrices, the following steps:
Under the assumption of already assembled stiffness,mass and damping matrices K, M, C one has to perform

- the computation $\overline{K} = K + i\omega C - \omega^2 M$,
- separation/mapping of $\overline{K}$ in block matrices according to inner, left and right nodes,
- building up the matrices A, B (in LAPACK-DENSE matrix type) according to INM-Problem (6.1),
- a call of LAPACK xGGEV() with A, B

in each frequency step.

Algorithm 6.3.3 (QZ-LEP-PBCSolver) *We assume ready-assembled stiffness and mass matrices K, M, where rows and columns according to Dirichlet nodes are already dropped.*

Provide matrices according to inner,left and right nodes $\rightarrow K_{st}, M_{st}$ *for* $s, t = i, l, r$;

for all ω do

1. if(damping) *for* $s, t = i, l, r$ $\quad \overline{K}_{st} = \begin{pmatrix} K_{st} - \omega^2 M_{st} & -\omega(\tilde{\alpha} K_{st} + \tilde{\beta} M_{st}) \\ \omega(\tilde{\alpha} K_{st} + \tilde{\beta} M_{st}) & K_{st} - \omega^2 M_{st} \end{pmatrix}$;
   else *for* $s, t = i, l, r$ $\quad \overline{K}_{st} = K_{st} - \omega^2 M_{st}$;
2. Build LAPACK-DENSE matrices A, B according to (6.1);
3. xGGEV$(N_l + N_i, N_l + N_i, A, B, evals, evecs)$;
4. Compute $\alpha_j = \ln(|evals(j)|), \beta_j = arg(evals(j)) \qquad (j = 1, ..., N_i + N_l)$;
   Choose n_{ev} pairs (α_j, β_j) with smallest $|\alpha_j|$;

Solving the Inner-Node-Matrix Problem with IRAM Neither the inner node problem (6.1) nor the problem (6.12) have a hermitian, positive matrix B, therefore the generalized Arnoldi solver cannot be applied. But the problem (6.12) can be transformed into a standard eigenvalue problem

$$(A - B)^{-1} B x = \lambda x$$

where we are searching for the $2 \cdot N_l$ eigenvalues of largest magnitude.

The main advantages of using an Arnoldi solver that we only search for $n_{ev} = 2 \cdot N_l$ eigenvalues of the $(N_i + N_l \times N_i + N_l)$ eigenvalue problem and that one suffices with matrix-vector product OPx of the transformed system. Therefore we have to provide a matrix-object class including the OPx operation $(A-B)^{-1}Bx$.
Under the assumption of already assembled stiffness, mass and damping matrices K, M, C one has to perform

- the computation $\overline{K} = K + i\omega C - \omega^2 M$,
- separation/mapping of $\overline{K}$ in block matrices according to inner, left and right nodes,
- set up sparse factorization of $(A-B) = LL^T$, define sparse multiplication with B by multiplications of blocks $\overline{K}_{st}$,
- a call of ArnoldiPackage with OPx.

in each frequency step.

Algorithm 6.3.4 (Arnoldi-LEP-PBCSolver) *We assume ready-assembled stiffness and mass matrices K, M, where rows and columns according to Dirichlet nodes are already dropped.*

Provide matrices according to inner, left and right nodes $\rightarrow K_{st}, M_{st}$ $for\ s,t = i,l,r$;

for all ω do

1. if(damping) $for\ s,t = i,l,r$ $\overline{K}_{st} = \begin{pmatrix} K_{st} - \omega^2 M_{st} & -\omega(\tilde{\alpha}K_{st} + \tilde{\beta}M_{st}) \\ \omega(\tilde{\alpha}K_{st} + \tilde{\beta}M_{st}) & K_{st} - \omega^2 M_{st} \end{pmatrix}$;
   else $for\ s,t = i,l,r$ $\overline{K}_{st} = K_{st} - \omega^2 M_{st}$;
2. Provide class for sparse OPx.MultMv$(x) = (LL^T)^{-1}Bx$,
   i.e. sparse Cholesky-factorization
   $$LL^T = A - B$$
3. ArnoldiPackage$(N_l + N_i, OPx, n_{ev} = 2 \cdot N_l, evals, evecs)$;
4. Compute $\alpha_j = \ln(|1 + \frac{1}{evals(j)}|), \beta_j = arg(\frac{1}{evals(j)})$ $\quad (j = 1, ..., 2 \cdot N_l)$;
   Choose n_{ev} pairs (α_j, β_j) with smallest $|\alpha_j|$;

For each frequency one has to provide once a sparse-Cholesky factorization of the complex-symmetric matrix $(A-B)^{-1}$. For each matrix-mulitplication in the Arnoldi solver one has to perform

- a sparse matrix-vector product $y = Bx \rightarrow y$,
- solving $LL^T w = y \rightarrow w$, i.e. forward-backward substitution.

6.4 Scaling of eigenvalue problems

Solving piezoelectric problems according to Algorithms 6.2.2 - 6.3.4 leads to convergence, but gives irrational results. We explain this problems on standard eigenvalue problems. There is a roundoff-error around $\epsilon_M \|A\|$ with ϵ_M denoting the machine precision, if one solves a standard eigenvalue problem $Ax = \lambda x$. The system matrix due to piezoelectric problems is very ill-conditioned and therefore converged eigenvalues can be senseless. Through scaling methods one wants to reduce the norm of A by a similarity transformation DAD^{-1}.

Matrix Balancing used in QZ-algorithm presented for standard problems

There are two steps in matrix balancing, i.e. permutation and scaling [2].

1. **Permutation** has the effect that A is transformed by a similarity transformation to block upper triangular form in order to achieve that later algorithm have faster convergence. P is permutation matrix.

$$\tilde{A} = PAP^T = \begin{pmatrix} \tilde{A}_{11} & \tilde{A}_{12} & \tilde{A}_{13} \\ 0 & \tilde{A}_{22} & \tilde{A}_{23} \\ 0 & 0 & \tilde{A}_{33} \end{pmatrix}$$

   The block $\tilde{A}_{11}, \tilde{A}_{33}$ are upper triangular, while A_{22} has general form, i.e. the matrix is in Schur-form "outside" the block A_{22}. One has to mention that often no according permutation can be found.

   Permuting results in faster convergence of later QR-iterations.

2. Scaling is the main trick for solving piezoelectric problems, applied before an eigenvalue routine it improves the accuracy achieved afterwards. We want to apply similarity transformations in such a way that the matrix A is balanced the way that the norms of rows and columns are equal in magnitude.

$$\tilde{\tilde{A}} = D\tilde{A}D^{-1} \text{ with } D = \begin{pmatrix} I & 0 & 0 \\ 0 & D_{22}^{-1} & 0 \\ 0 & 0 & I \end{pmatrix}.$$

Since in the balancing routine only similarity transformation are used, the spectrum does not change, i.e. $\sigma(A) = \sigma(\tilde{A}) = \sigma(\tilde{\tilde{A}})$, but it has to bear in mind that the eigenvectors need to be back-transformed, therefore one has to store the transforming matrices. This method of balancing is used in the QZ-algorithm and is provided in LAPACK by the xGEBAL() routine.

For scaling generalized eigenvalue problems one provides two regular matrices D_1, D_2 the way that D_1AD_2, D_1BD_2 have row and column norms near 1. Then we solve the similar eigenvalue problem

$$D_1AD_2x = \gamma D_1BD_2x.$$

6.4.1 Scaling of piezoelectric problems

A piezoelectric problem based scaling can be applied in order to achieve reasonable reasonable results in the Arnoldi method as well. The elements of the stiffness blocks of the piezoelectric problem are of following magnitude

$$\begin{aligned} \overline{K}_{uu} &\approx \mathcal{O}(10^{10}) \\ \overline{K}_{\Phi\Phi} &\approx \mathcal{O}(10^{-10}) \\ \overline{K}_{u\Phi} &\approx \mathcal{O}(1). \end{aligned}$$

Therefore with the scaling matrix $D = \begin{pmatrix} 10^{-5}I_{N_u} & 0 \\ 0 & 10^{5}I_{N_\Phi} \end{pmatrix}$ the transformed matrix satisfies

$$\tilde{K} = DKD = \begin{pmatrix} 10^{-10}\overline{K}_{uu} & \overline{K}_{u\Phi} \\ \overline{K}_{\Phi u} & 10^{10}\overline{K}_{\Phi\Phi} \end{pmatrix} \tag{6.13}$$

Applying this scaling on the inner, left and right blocks of K, implies that the transformed generalized eigenvalue problem according to (6.12) is much better scaled, i.e. all elements are of order $\mathcal{O}(1)$.

Trick: Scaling of material data Since the block matrices of the stiffness matrix depend linearly on the material data, the following scaling of the material tensors and mass density (notation according to Chapter 2)

$$\tilde{c}^E = 10^{-10}c^E, \quad \tilde{\varepsilon}^S = 10^{10}\varepsilon^S, \quad \tilde{e} = e, \quad \tilde{\rho} = 10^{-10}\rho \tag{6.14}$$

is equal to the transformation (6.13). One only has to ensure that the material data also enter linearly into the boundary conditions. This holds for the boundary conditions presented in Chapter 4, i.e. for Dirichlet, Neumann and periodic boundaries.

Conclusion: If the scaling of material data according to (6.14) is applied during assembling of stiffness and mass matrices, the presented Algorithms 6.2.2 - 6.3.4 lead in general to more accurate results.

Chapter 7

Numerical Results

In this chapter we present results of simulations of the dispersion context of SAW-filter-type structures. We start with simulating the influence of periodic pertubations on the solution of a pure mechanical model problem. Therefore the elastic strain problem is solved first on a non-perturbed infinite strip and then for a periodically perturbed strip. In this numerical experiment the effect of periodic perturbation on the dispersion context can be seen very well.
The piezoelectric problem is solved for TV- and GSM-filter related periodic structures. Finally,we give some concluding remarks on the quality of the developed mathematical model according to the gained results.

Before presenting the numerical results we give some remarks on the implmentation, the presentation of the results:

On the implementation The FE-matrix assembling is done by the Finite Element Package FEPP [33] developed at the University of Linz.
Three different dispersion context solvers, developed within this thesis, are implemented and compared to each other in this chapter:

- Solving the Schur-complement problem via linearization and under application of the direct Lapack-QZ solver, i.e. Algorithm 6.2.2
- Solving the Inner-node problem with the direct Lapack-QZ solver, i.e. Algorithm 6.3.3.
- Solving the Inner-node problem with the iterative Arnoldi-package and with $n_{ev} = 2 \cdot N_l$ eigenvalues to compute, i.e. Algorithm 6.3.4.

We set the number of computed Arnoldi vectors to $2 \cdot n_{ev}$ and the accuracy for the stopping criterion of the Arnoldi solver to working precision. This setting implies that Arnoldi and

direct QZ-solver achieve equal accuracy. Therefore we can compare the solvers to each other by the calculation times required.

On the presentation of simulated dispersion diagrams One gains the propagation constants (α, β) out of the computed eigenvalues γ through the context $\gamma = e^{(\alpha+i\beta)p}$.
Since $e^{(\alpha+i\beta)p} = e^{(\alpha+i(\beta+\frac{2\cdot k\pi}{p}))p}$ for all $k \in \mathbb{Z}$, β can not be uniquely calculated. In general one defines β in $(-\pi, \pi]$.
In general we present the dispersion curves by the functional context $(\alpha \cdot p, \beta \cdot p, f)$ for given frequencies $f = \frac{\omega}{2\pi}$ and $\beta \in (-\pi, \pi]$.
SAW-designers are mainly interested in the dispersion context near stop-bands regions, which as already mentioned in Chapter 2 is characterized by propagation constants of the form $(\alpha, \beta = \frac{\pi}{p})$ and propagating modes of the form $(0, \beta)$. Therefore for presenting zooms in the stop-band region β is continued to the region $[0, \frac{2\pi}{p})$.

7.1 The effect of periodic perturbations on a pure mechanical problem

We want to present the influence of periodic perturbations on the dispersion context of the elastic plane strain problem. We compare diagrams with and without periodic perturbations, which is modeled by a periodical arrangement of Dirichlet (Γ_D) and Neumann (Γ_N) boundaries.

Under the assumption of time-harmonic excitation, i.e. we assume $u(x,t) = u(x) \cdot e^{i\omega t} \in \mathbb{C}^2$ we state the strong formulation of elastic plane strain problem on the infinite strip Ω_S by: Find $u = (u_1, u_2) : \Omega_S \to \mathbb{C}^2$ satisfying

$$\begin{aligned} -divT &= \omega^2 \rho\, u \quad \text{in } \Omega_S \qquad \text{with } T = c\, Su \ \text{ (Hook's law)} \\ u &= 0 \qquad \text{on } \Gamma_D \\ T \cdot n &= 0 \qquad \text{on } \Gamma_N \end{aligned} \tag{7.1}$$

with $S = \begin{pmatrix} \frac{\partial u_1}{\partial x_1} & \frac{1}{2}(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1}) \\ \frac{1}{2}(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1}) & \frac{\partial u_2}{\partial x_2} \end{pmatrix}$ and $c = c^E$ the elastic stiffness tensor of the used substrate material.

We calculate the dispersion context for the geometries shown in Figure 7.1 and 7.1.

Figure 7.1: Underlying geometry without periodic perturbations

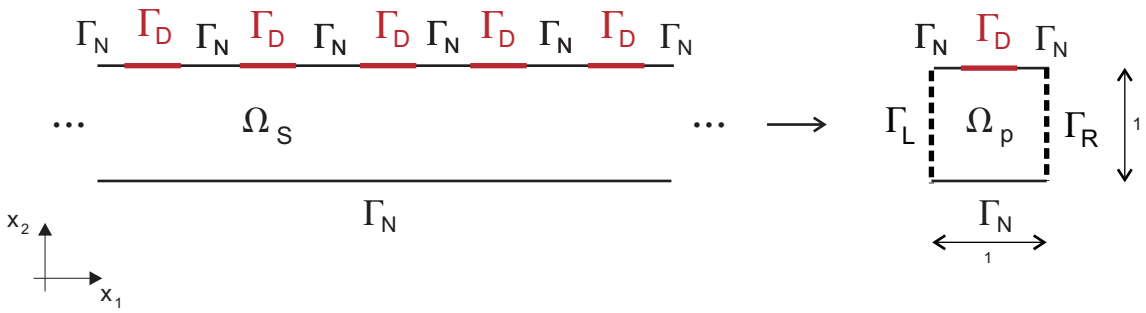

Figure 7.2: Underlying geometry with periodic perturbations

Restricted to the corresponding unit-cell the stated model problem 7.2 turns into

$$\begin{aligned} -divT &= \omega^2 \rho u && \text{in } \Omega_p \qquad \text{with } T = c\,Su \text{ (Hook's law)} \\ u &= 0 && \text{on } \Gamma_D \\ T \cdot n &= 0 && \text{on } \Gamma_N \\ u(x_1, x_2) &= u(x_1 + p, x_2) && \text{for } (x_1, x_2) \in \Gamma_L \end{aligned} \tag{7.2}$$

In the following presented results, red points correspond to propagation constants of the form $(\alpha \cdot p, \pi)$, i.e. the reflected waves interfere constructively, green points correspond to propagation constants of the form $(0, \beta \cdot p)$, i.e. pure propagating modes and blue points to (α, β), i.e. the remaining calculated complex propagation constants.

Effect of periodic perturbations: 3D and 2D representation

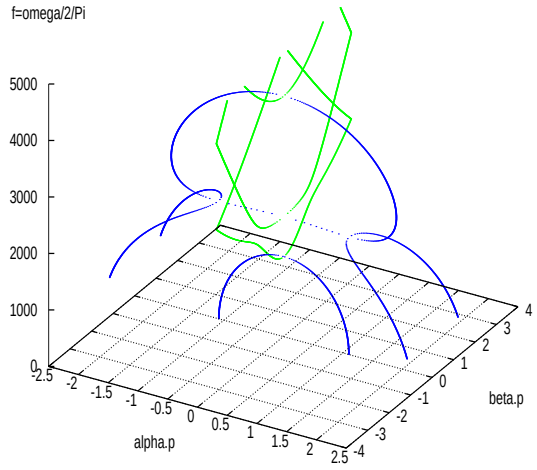

Figure 7.3: Elastic plane strain without periodic perturbation

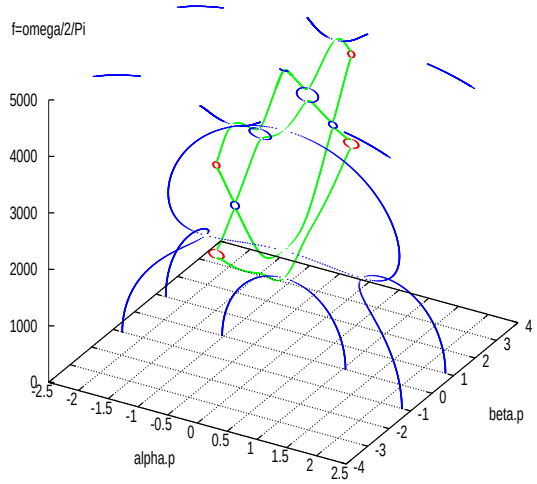

Figure 7.4: Elastic plane strain with periodic perturbation

The red rings in Figure 7.4 represent the stop-bands, while in the non-perturbed analog the pure-propagating modes are continuous.

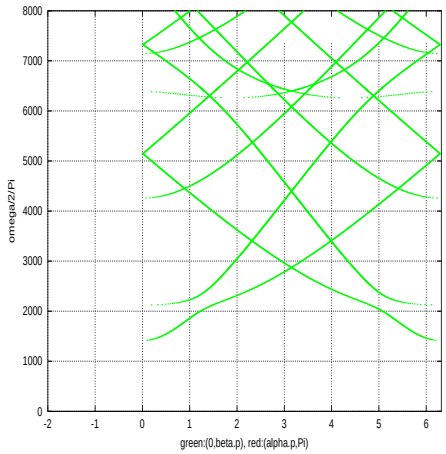

Figure 7.5: Elastic plane strain on non-perturbed geometry

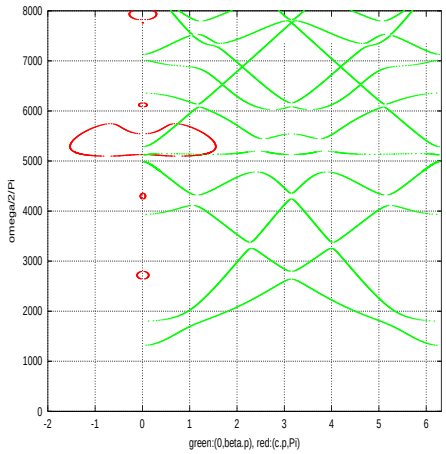

Figure 7.6: Elastic plane strain on periodic geometry

7.2 Simulation of piezoelectric problems

In Chapter 2 we presented two piezoelectric models:

- *Model with 3 degrees of freedom (dofs) per node :* u_1, u_2, Φ
  We assume no displacement in the x_3-direction and displacement and potential are not depending on the x_3-coordinate, i.e. $u(x_1, x_2, t) \in \mathbb{R}^2$ and $\Phi(x_1, x_2, t) \in \mathbb{R}$.
  This problem is simulated with the real-life data of a TV-filter.

- *Model with 4 degrees of freedom per node :* u_1, u_2, u_3, Φ
  Due to the anisotropy of the material wave components in the x_3-direction can occur in practical applications. The deviation of the ideal case is considered by allowing constant behavior of the fields in x_3-direction:

  $$\begin{array}{rcll} \frac{\partial u_i}{\partial x_3} & = & 0 & \text{for } u = (u_1, u_2, u_3)^T \in \mathbb{R}^3 \\ \frac{\partial \Phi}{\partial x_3} & = & 0 & \end{array} .$$

  The diagram of dispersion for this problem type is simulated with the data of a GSM-filter.

In both models we simulate short-circuited electrodes, i.e. we set the potential to zero on the electrodes Ω_{El}.

The center frequency of the stop-band

The frequency, in which a periodically arranged electrodes yields in maximal reflection, i.e. the reflected waves interfere constructively, satisfies

$$f_c = \frac{v}{2p}. \tag{7.3}$$

v denotes the propagation velocity of a surface wave in the material. SAWs have the property that their velocity v is much slower than electromagnetic waves. The frequency f_c is supposed to approximate the center of the stop-band in the dispersion context.
The propagation of Rayleigh-waves in anisotropic materials depend on the crystal class and the orientation ("Euler Angles") with respect to the propagation direction. Therefore the velocity of surface waves depends on the used material, its crystal class and the direction of propagation. Since we want only to get an idea in which frequency domain the stop-band can be suspected, we suffice with approximative values for the velocity v of Rayleigh waves. For exact values due to crystal classes and orientation see Auld [5].

	v
Lithium Niobate $LiNbO_3$	$3300 \leq v \leq 3900 m/s$
Lithium Tantalate $LiTaO_3$	$3100 \leq v \leq 3300 m/s$
Silicon Si	$\approx 4900 m/s$

On the underlying mathematical model and plate modes

Through using Dirichlet or Neumann conditions on the bottom of the used geometry we simulated a piezoelectric strip with finite depth. This means that we model a plate and there are plate modes as well as surface waves in the results. These plate modes can be filtered out, by computing the energy in the whole domain and compare it to the energy on the half domain. If the energy is concentrated near the surface, we have a surface wave. This method is used in the doctor thesis of M.Hofer [14]. The problem is only mentioned for completeness reasons and will not be further treated within this thesis.

Piezoelectric problems

Dispersion context of TV-filter-like structure: $d = 2$
We simulate the piezoelectric problem with 3 degrees of freedom ($u \in \mathbb{C}^2, \Phi \in \mathbb{C}$) under the usage of Lithium Niobate ($LiNbO_3$) for piezoelectric substrate and aluminium for electrodes. The used material data are listed in Appendix A.

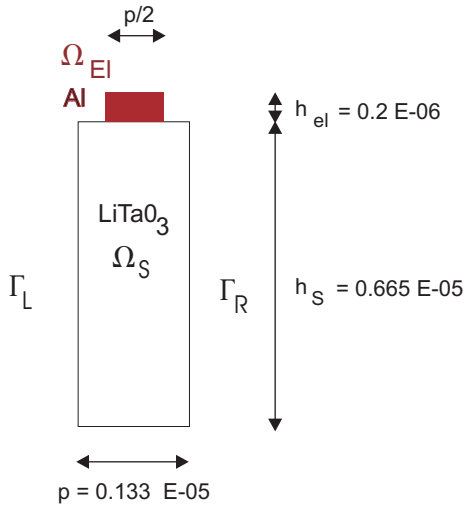

Figure 7.7: Unit cell of simulated TV filter problem

With the geometry data of the unit-cell presented Figure 7.7 one can estimate a center frequency near

$$3.3\ 10^7\text{Hz} \leq f_0 \leq 3.9\ 10^7\text{Hz}.$$

We simulate the piezoelectric problem (4.96) for $d = 2$ and S, E according to (4.3)-(4.4) on the unit cell presented in Figure 7.7.

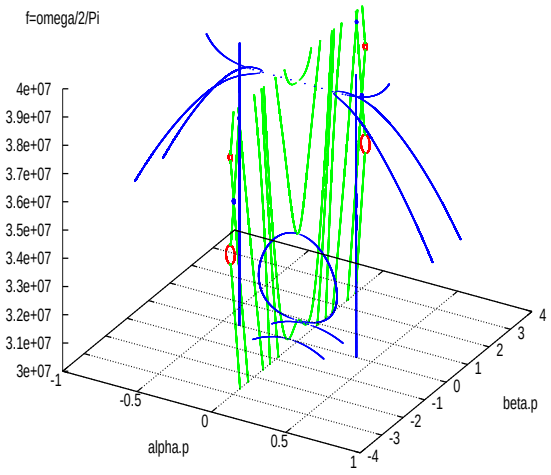

Figure 7.8: Dispersion context for TV-filter structure (short-circuited electrodes)

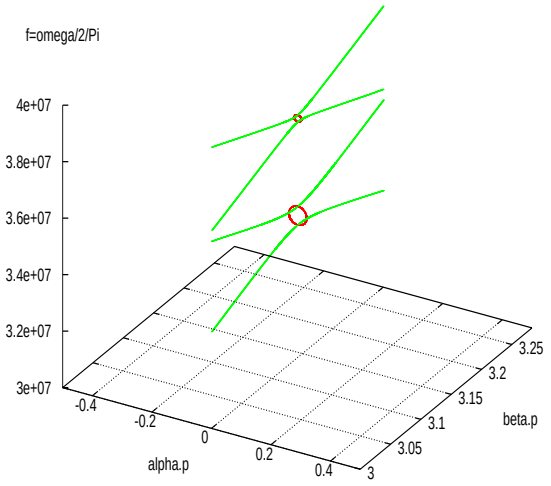

Figure 7.9: Short-circuited TV-filter-structure: zoom in stopband region (β periodically continued)

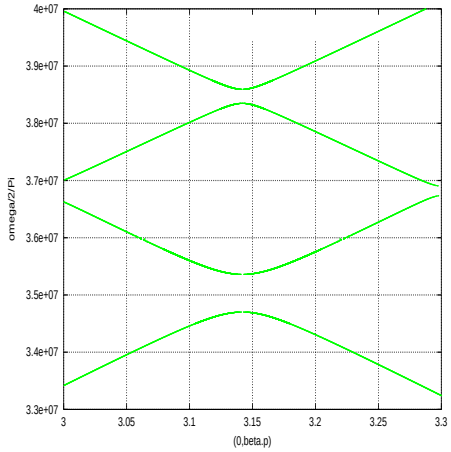

Figure 7.10: TV-filter-structure: 2D-plot of pure propagating modes in stop-band region

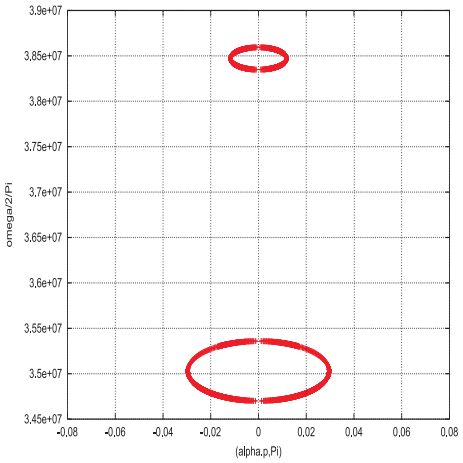

Figure 7.11: TV-filter-structure: 2D plot of stop-bands

Dispersion context of GSM-filter-like structure: $d = 3$ For simulating the piezoelectric problem with 4 degrees of freedom (u_1, u_2, u_3, Φ) in each node we use the following unit cell of a GSM-filter-related periodic structure shown in Figure 7.12

- Material for piezoelectric substrate: Lithium Tantalate $LiTaO_3$
- Material for electrodes: Aluminium Al

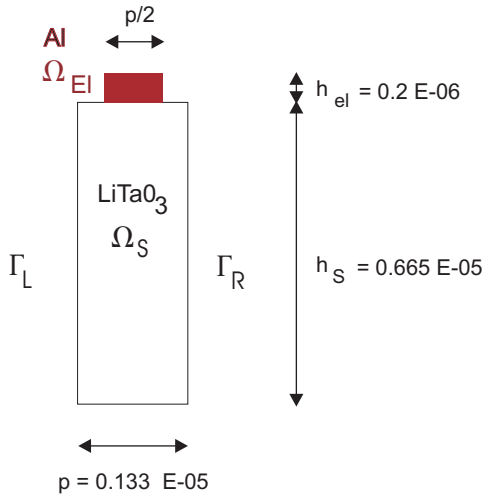

Figure 7.12: Unit cell for simulating $LiTa0_3$ GSM-filter-structure $(d = 3)$

We use a mesh of rectangles, with 36 nodes ($\cdot$ 4 degrees of freedom) on each periodic bound and $N_i = 4 \cdot n_i = 1386$ degrees of freedom of inner nodes and a unit cell of the form shown in Figure 7.12.
With these settings we get the dispersion context (3D) shown in Figure 7.2. A zoom to the stop-band is given in Figure 7.2. For a better presentation of the stop-band region, the calculated propagation constants are periodically continued, i.e. $\beta \in [0, \frac{2\pi}{p}]$.

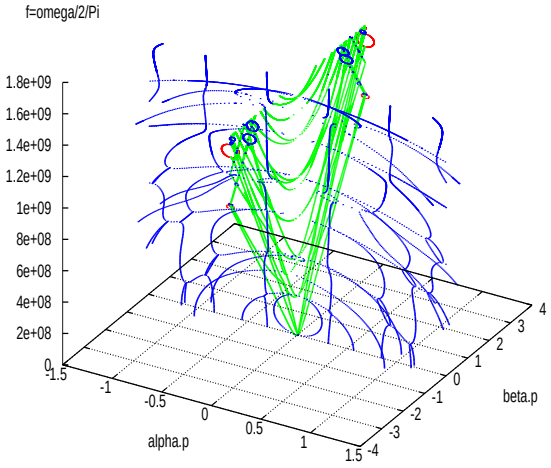

Figure 7.13: Dispersion context for $LiTaO_3$ GSM-filter structure (short-circuited)

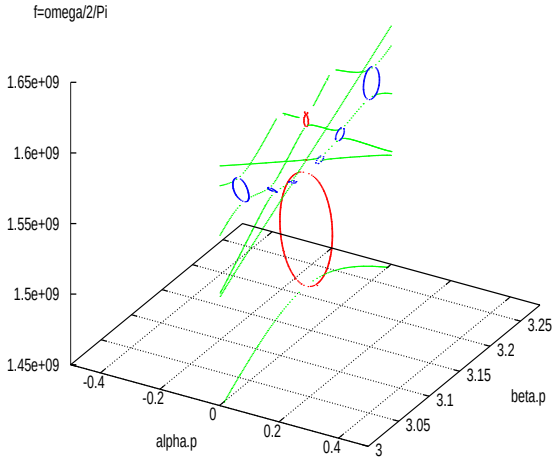

Figure 7.14: $LiTaO_3$ GSM Filter: zoom in stop band region (β periodically continued)

7.2.1 Comparison of three algorithms

Now we want to compare the three implemented algorithms, developed in Chapter 6 and itemized once more at the beginning of this chapter. The parameters were set the way the different solvers yield the same accuracy, therefore one can analyze their quality by comparing the computational times required fo solving the dispersion context for one frequency step $f = \frac{\omega}{2\pi}$ for the presented GSM-filter-type problem.

Since the used FE-software package FEPP does not provide a sparse matrix class for complex matrices, the presented algorithms are tested using dense matrices, i.e. the problem dimension is bounded and the main computational costs are governed by dense matrix operatations. But even using dense matrices, we get reasonable and satisfying results. The solvers can be analyzed and compared. In the following tabulars the computational costs of each step in the various solver is listed. One sees that the main costs bases on the dense matrix multiplication, but with these results one can predetermine the behaviour of the solvers under the usage of sparse matrices.

One frequency step: No Damping, GSM 4 dofs

Complex non-hermitian IRAM	in sec	in sec (Arnoldi)	
Time for creating and solving EP (omega)	847		
Time for ArSolve (omega)	807		
Time for Cholesky-factorization	100		
Time for Arnoldi loop (without creating problem)	670		
Time for Op.x		632	
Time for reorthognolaziation		14	
Time for solving Hessenberg subeigenproblem	6		
Time for getting QR-shifts	0.002		
Total number of update iterations			1
Total number of OPx operation			261
Total number of reorthogonalization steps			260
Total number of restarts			0

QZ-Schur-PBC-Solver	in sec
Time for creating and solving EP (omega)	326
Time for LU-inversion (SchurComplement)	256
Time for calculate Schur-Matices	58
Time for solving QEP	9

QZ-LinerEP-Solver	in sec
Time for creating and solving LEP (omega)	1952
Time for solving LEP via QZ	1943

One frequency step: Rayleigh-Damping, GSM-structure 4 dofs

Complex non-hermitian IRAM	in sec	in sec (Arnoldi)	
Time for creating and solving EP (omega)	800		
Time for Cholesky-factorization	99		
Time for Arnoldi loop (without creating problem)	622		
Time for Op.x		632	
Time for reorthognolaziation		14	
Time for solving Hessenberg subeigenproblem		6	
Time for getting QR-shifts		0.0002	
Total number of update iterations			1
Total number of OPx operation			261
Total number of reorthogonalization steps			259
Total number of restarts			0

QZ-Schur-PBC-Solver	in sec
Time for creating and solving EP (omega)	3300
Time for LU-inversion (SchurComplement)	2500
Time for calculate Schur-Matices	474
Time for solving QEP	65

QZ-LinerEP-Solver	in hours
Time for creating and solving LEP (omega)	9 h

Looking at the computation times of the various steps we can expect an immense acceleration by the usage of sparse factorizations, sparse matrices and sparse matrix-operations. The comparison of computational requirments show that the SC-QZ-solver and the INM-Arnoldi-solver are suited also for bigger problems.

Rayleigh-damping and absorbing boundary conditions

The problem of Rayleigh-damping is not of big practical need for these problem types, since the used piezoelectric substrates are nearly lossless. Moreover, if one wants to achieve reasonable results, one has to be aware of frequency dependent Rayleigh-damping parameters, which are very tricky to state. The main cause for posing the problem of Rayleigh-damping in the problem formulation of this thesis is that Rayleigh-damping problem leads to complex problems as the consideration of absorbing boundary conditions (ABC) do. These boundary conditions provide a possibility for modeling bulk wave radiation shown in the dispersion diagram in Chapter 2. ABCs are not considered in the models used within this thesis, but an expansion of the implemented solvers to these methods should be possible. Absorbing boundary conditions of first and second order are modeled in [14].

Chapter 8

Conclustions and Further Remarks

Within this thesis the full machinary of mathematical problem solving was presented. We started with the physical problem formulation. We stated a step-by-step mathematical modeling using Floquet-Bloch theory for modeling periodic structures, coupled field theory due to the piezoelectric effect and complex problems due to damping effect (or absorbing boundary conditions). Three solution approaches, i.e. "Gamma-Given-Method" for pure-propagating modes, SC-Method and INM-Method, were developed and analyzed. The methods were developed within this thesis and therefore no references can be given. A comprehensive theory for algebraic eigenvalue problems were given and applied for constructing algorithms for solving the SC- and the INM-method with an ansatz to structure preserving methods. Three different solvers were implemented and compared. Within numerical experiments the influence of periodic perturbations on dispersion diagrams were presented.

The work can directly be continued in the following directions:

- improve presented solvers by using sparse matrix operations

and with more mathematical work

- absorbing boundary conditions of arbitrary order
- or introducing infinite elements in the discretization in order to model bulk wave radiation.

Appendix A

Material data used in simulation

We state the coefficients of practical matirials used in simulation of GSM-filter. The data are cited out of [18].
The coefficient tensors are described in the form according to

$$\begin{array}{rcl} T & = & c^E S \; - \; e^T E \\ D & = & eS \; + \; \varepsilon^S E \end{array} \quad \text{with } T = \begin{bmatrix} T_{xx} \\ T_{yy} \\ T_{zz} \\ T_{yz} \\ T_{xz} \\ T_{xy} \end{bmatrix}, \; S = \begin{bmatrix} S_{xx} \\ S_{yy} \\ S_{zz} \\ 2 \cdot S_{yz} \\ 2 \cdot S_{xz} \\ 2 \cdot S_{xy} \end{bmatrix}.$$

Piezoelectric materials used for piezoelectric substrate

LithiumNiobate $(LiNbO_3)$
Mechanical stiffness tensor

$$c^E = \begin{pmatrix} 22.7965 & 6.519 & 6.519 & 0 & 0 & 0 \\ 6.519 & 19.8432 & 5.4775 & 0 & -0.7884 & 0 \\ 6.519 & 5.4775 & 19.8432 & 0 & 0.7884 & 0 \\ 0 & 0 & 0 & 7.18285 & 0 & -0.7884 \\ 0 & -0.7884 & 0.7884 & 0 & 5.9645 & 0 \\ 0 & 0 & 0 & -0.7884 & 0 & 5.9645 \end{pmatrix} . 10^{10} \text{ Newton}/m^2$$

Piezoelectric coupling tensor

$$e = \begin{pmatrix} -1.7847 & -0.3062 & -0.3062 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2.4365 & 0 & -3.7159 \\ 0 & -2.4365 & 2.4365 & 0 & -3.7159 & 0 \end{pmatrix}$$

Dielectric permittivity tensor

$$\varepsilon^S = \begin{pmatrix} 2.364245 & 0 & 0 \\ 0 & 4.106988 & 0 \\ 0 & 0 & 4.106988 \end{pmatrix} . 10^{-10}\ As/Vm$$

Density of material $\rho = 4628 kg/m^3$

Lithium Tantanate, 0 deg cut $(LiTaO_3)$
Mechanical stiffness tensor

$$c^E = \begin{pmatrix} 23.28 & 4.65 & 8.36 & -1.05 & 0 & 0 \\ 4.65 & 23.28 & 8.36 & 1.05 & 0 & 0 \\ 8.36 & 8.36 & 27.59 & 0 & 0 & 0 \\ -1.05 & 1.05 & 0 & 9.49 & 0 & 0 \\ 0 & 0 & 0 & 0 & 9.49 & -1.05 \\ 0 & 0 & 0 & 0 & -1.05 & 9.315 \end{pmatrix} . 10^{10}\ N/m^2$$

Piezoelectric coupling tensor

$$e = \begin{pmatrix} 0 & 0 & 0 & 0 & 2.64 & -1.86 \\ -1.86 & 1.86 & 0 & 2.64 & 0 & 0 \\ -0.22 & -0.22 & 1.71 & 0 & 0 & 0 \end{pmatrix}$$

Dielectric permittivity tensor

$$\varepsilon^S = \begin{pmatrix} 3.621286 & 0 & 0 \\ 0 & 3.621286 & 0 \\ 0 & 0 & 3.76295 \end{pmatrix} . 10^{-10}\ As/Vm$$

Density of material $\rho = 7454 kg/m^3$

Non-Piezoelectric material used for electrodes

Aluminium (Al)
Mechanical stiffness tensor

$$c^E = \begin{pmatrix} 10.78 & 5.493 & 5.493 & 0 & 0 & 0 \\ 5.493 & 10.7800 & 5.493 & 0 & 0 & 0 \\ 5.493 & 5.493 & 10.78 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2.645 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2.645 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2.645 \end{pmatrix} . 10^{10}\ N/m^2$$

Piezoelectric coupling tensor (non-piezoelectric material)

$$e = e^T = 0$$

Dielectric permittivity tensor

$$\varepsilon^S = \begin{pmatrix} 0.0885 & 0 & 0 \\ 0 & 0.0885 & 0 \\ 0 & 0 & 0.0885 \end{pmatrix} As/Vm$$

Density of material $\rho = 2700 kg/m^3$

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Eidesstattliche Erklärung

Ich, Sabine Zaglmayr, erkläre an Eides statt, dass ich die vorliegende Diplomarbeit selbstständig und ohne fremde Hilfe verfasst, andere als die angegebenen Quellen und Hilfsmittel nicht benutzt bzw. die wörtlich oder sinngemäss entnommenen Stellen als solche kenntlich gemacht habe.

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