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An inverse scattering problem in metallic waveguides filled with bianisotropic material

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Abstract

This paper presents an analysis with the aim of characterizing an arbitrary linear, bianisotropic material inside a metallic waveguide. The result is that if the number of propagating modes are the same inside and outside the material under test, it is possible to determine the propagation constants of the modes inside the material by using scattering data from two samples with different lengths. Some information can also be obtained on the cross-sectional shape of the modes, but it remains an open question if this information can be used to characterize the material. The method is illustrated by numerical examples, determining the complex permittivity for lossy isotropic and anisotropic materials.

1 Introduction

In order to obtain a well controlled environment for making material measurements, it is common to do the measurements in a metallic cavity or waveguide. The geometrical constraints of the waveguide walls impose dispersive characteristics on the propagation, *i.e.*, the wavelength of the propagating wave depends on frequency in a nonlinear manner. In order to correctly interpret the measurements, it is necessary to provide a suitable characterization of the waves inside the waveguide. This is well known for isotropic materials [2,3,7,16], bi-isotropic (chiral) materials [5,13], and even anisotropic materials where an optical axis is along the waveguide axis [1,6,11,12], but for general bianisotropic media with arbitrary axes there are so far very few results available. In principle, an optimization approach as in [7,12] can be designed, where the material parameters are found by minimizing the distance between measured and simulated *S*-parameters. However, this method is typically plagued by non-uniqueness and similar numerical issues, and we seek a more direct method, providing physical insight to the problem.

We present in this paper a partial solution to an inverse scattering problem in a waveguide geometry. First, the direct problem is solved by defining modes in an arbitrary linear material. This solution helps us define an *N*-port model of the scattering problem, which is then utilized in the inverse problem. Most of the references mentioned so far only treats the single-mode case, but the formalism in this paper is ready for an arbitrary number of modes. However, in practical applications the single-mode case is usually preferable since it is difficult to measure higher order modes.

General results corresponding to the analysis presented in Section 4 of this paper can be found in [4, 17]. In these papers, the fundamental eigenvalue problem defining the modes in a bianisotropic material is defined and explored for general orthogonality properties, but it is not applied to a scattering problem. There is a scattering formalism for discontinuities in [17], but it is rather vague and there is also some confusion about propagating and evanescent modes in this paper. This is better accounted for in [4], but the formalism is only used to study the excitation of modes, not in a scattering problem. In [18, 19], a coupled-mode analysis is performed for bianisotropic waveguides, *i.e.*, the fields inside the material are expanded in terms of modes corresponding to an isotropic material. The scattering problem is not treated here either, but there are some graphs of dispersion relations in [18].

In this paper, we use an eigenvalue problem of the form used in [4, 17] to define modes propagating in a metallic waveguide filled with a bianisotropic material. The approach is related to similar spectral decompositions used in homogenization theory [14, 15], where the boundary conditions of the waveguide are replaced by periodic boundary conditions. Using these modes, we define an expansion of the electromagnetic field, which is then used in a mode-matching analysis of the scattering problem. In order to deduce the general properties of this formulation, the quasi-orthogonality results from [4, 17] are used heavily, and they are repeated in Section 4.

When dealing with bianisotropic materials, notation is often an issue. In this paper, we use a six-vector notation which substantially reduces the length of the paper [10]. This is introduced in Section 2. In Section 3 we illustrate what makes the isotropic case so simple, namely that it is possible to define an eigenvalue problem independent of both frequency and propagation constant. As is seen in Appendix A, where we derive the corresponding second order equations, this seems impossible for a general bianisotropic material. In Section 4 we define the general eigenproblem in terms of a first order differential equation. A particularly important result is the quasi-orthogonality (4.6), which is also derived in [4], and in a different formulation in [17]. The forward scattering problem is treated in Section 5, and the inverse scattering problem in Section 6. The resulting algorithm is tested in a numerical example for a non-magnetic, isotropic lossy dielectric medium in Section 7, and some conclusions are given in Section 8.

2 Notation

We consider time-harmonic waves in a waveguide of infinite extent in the z-direction, as in Figure 1. The electromagnetic fields then satisfy (time convention $e^{-i\omega t}$)

$$\nabla \times \boldsymbol{H} = -\mathrm{i}\omega \boldsymbol{D} = -\mathrm{i}\omega(\boldsymbol{\epsilon}\boldsymbol{E} + \boldsymbol{\xi}\boldsymbol{H})$$
(2.1)

$$\nabla \times \boldsymbol{E} = i\omega \boldsymbol{B} = i\omega(\boldsymbol{\mu}\boldsymbol{H} + \boldsymbol{\zeta}\boldsymbol{E})$$
(2.2)

for $(x, y) \in \Omega$ and z arbitrary, with the boundary conditions $\hat{\boldsymbol{n}} \times \boldsymbol{E} = \boldsymbol{0}$ and $\hat{\boldsymbol{n}} \times \boldsymbol{H} = \boldsymbol{J}_{\mathrm{S}}$, where $\boldsymbol{J}_{\mathrm{S}}$ is the surface current. The surface current is usually unknown, and the boundary condition $\hat{\boldsymbol{n}} \times \boldsymbol{H} = \boldsymbol{J}_{\mathrm{S}}$ should be considered as a means of determining $\boldsymbol{J}_{\mathrm{S}}$, not as a restrictive condition on \boldsymbol{H} . The PEC condition $\hat{\boldsymbol{n}} \times \boldsymbol{E} = \boldsymbol{0}$ is sufficient to calculate the fields. To shorten the notation, we introduce the fields

$$\mathbf{e} = \begin{pmatrix} \mathbf{E} \\ \mathbf{H} \end{pmatrix}, \quad \mathbf{d} = \begin{pmatrix} \mathbf{D} \\ \mathbf{B} \end{pmatrix} = \begin{pmatrix} \boldsymbol{\epsilon} & \boldsymbol{\xi} \\ \boldsymbol{\zeta} & \boldsymbol{\mu} \end{pmatrix} \begin{pmatrix} \mathbf{E} \\ \mathbf{H} \end{pmatrix} = \mathsf{M}\mathbf{e}$$
(2.3)

and the operator

$$\nabla \times \mathsf{Je} = \begin{pmatrix} \mathbf{0} & -\nabla \times \mathbf{I} \\ \nabla \times \mathbf{I} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{E} \\ \mathbf{H} \end{pmatrix}$$
(2.4)



Figure 1: Geometry of the waveguide. The "complex" material may be anisotropic, bianisotropic, lossy, etc, but has to be linear.

Maxwell's equations with boundary conditions can then be written

$$\nabla \times \mathsf{Je} = \mathrm{i}\omega\mathsf{Me}, \quad (x,y) \in \Omega; \qquad \hat{n} \times \mathsf{Je} = \begin{pmatrix} -\mathbf{J}_{\mathrm{S}} \\ \mathbf{0} \end{pmatrix}, \quad (x,y) \in \partial\Omega$$
(2.5)

In the typical case when the material parameters do not depend on z, it is natural to introduce the Fourier transform pair

$$\hat{\mathbf{e}}(x,y,\beta) = \int_{-\infty}^{\infty} e^{-i\beta z} \mathbf{e}(x,y,z) \,dz$$
(2.6)

$$\mathbf{e}(x,y,z) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}\beta z} \hat{\mathbf{e}}(x,y,\beta) \,\mathrm{d}\beta$$
(2.7)

Maxwell's equations are then (where $\nabla_{\perp} = \hat{x}\partial_x + \hat{y}\partial_y$)

$$(\nabla_{\perp} + i\beta\hat{\boldsymbol{z}}) \times J\hat{\boldsymbol{e}} = i\omega M\hat{\boldsymbol{e}}, \quad (x,y) \in \Omega; \qquad \hat{\boldsymbol{n}} \times J\hat{\boldsymbol{e}} = \begin{pmatrix} -\widehat{\boldsymbol{J}}_{S} \\ \boldsymbol{0} \end{pmatrix}, \quad (x,y) \in \partial\Omega \quad (2.8)$$

If M is a hermitian symmetric positive definite matrix, *i.e.*, $M^{H} = M$ and $e_{0}^{H}Me_{0} \geq \theta |e_{0}|^{2}$ for some positive constant θ and all six-vectors e_{0} , this is a well posed eigenvalue problem for a self-adjoint operator for each fixed β , ω being the eigenvalue. A detailed account in the homogenization setting, where the PEC boundary condition is replaced by periodic boundary conditions, can be found in [15].

Should M not be hermitian symmetric, a similar analysis of the well-posedness can be made using a singular value decomposition. Though, we shall assume that

(2.8) defines suitable modes even in the nonhermitian case, where the typical effect is that properties such as orthogonality disappear [4].

3 Isotropic materials

The equation (2.8) defines the eigenvalue ω as a function of the parameter β . To illustrate how this problem corresponds to the classical approach to isotropic waveguides, we now digress a bit to treat this special case.

The first order system (2.8) can be written as a second order system,

$$(\nabla_{\perp} + i\beta\hat{\boldsymbol{z}}) \times \mathsf{J}\mathsf{M}^{-1}(\nabla_{\perp} + i\beta\hat{\boldsymbol{z}}) \times \mathsf{J}\hat{\mathsf{e}} = -\omega^{2}\mathsf{M}\hat{\mathsf{e}}$$
(3.1)

We now assume the material matrix models a "classical" material, *i.e.*, only using permittivity and permeability,

$$\mathsf{M} = \begin{pmatrix} \boldsymbol{\epsilon} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\mu} \end{pmatrix} \tag{3.2}$$

The second order equations then decouple into

$$(\nabla_{\perp} + i\beta\hat{z}) \times [\boldsymbol{\mu}^{-1}(\nabla_{\perp} + i\beta\hat{z}) \times \widehat{\boldsymbol{E}}] = \omega^{2}\epsilon\widehat{\boldsymbol{E}}$$
(3.3)

$$(\nabla_{\perp} + i\beta\hat{\boldsymbol{z}}) \times [\boldsymbol{\epsilon}^{-1}(\nabla_{\perp} + i\beta\hat{\boldsymbol{z}}) \times \widehat{\boldsymbol{H}}] = \omega^{2}\boldsymbol{\mu}\widehat{\boldsymbol{H}}$$
(3.4)

Further assuming the material is isotropic, *i.e.*, $\boldsymbol{\epsilon} = \boldsymbol{\epsilon} \mathbf{I}$ and $\boldsymbol{\mu} = \boldsymbol{\mu} \mathbf{I}$, the left hand side of the first equation becomes proportional to

$$(\nabla_{\perp} + i\beta\hat{\boldsymbol{z}}) \times [(\nabla_{\perp} + i\beta\hat{\boldsymbol{z}}) \times \widehat{\boldsymbol{E}}]$$

= $(\nabla_{\perp} + i\beta\hat{\boldsymbol{z}})[(\nabla_{\perp} + i\beta\hat{\boldsymbol{z}}) \cdot \widehat{\boldsymbol{E}}] - (\nabla_{\perp}^{2} - \beta^{2})\widehat{\boldsymbol{E}} = -\nabla_{\perp}^{2}\widehat{\boldsymbol{E}} + \beta^{2}\widehat{\boldsymbol{E}}$ (3.5)

where the last equality follows since the divergence of \hat{E} is zero from the original equation. By ∇_{\perp}^2 we denote the Laplace operator in the xy variables, $\nabla_{\perp}^2 = \partial_x^2 + \partial_y^2$. A similar expression holds for the magnetic field, and we obtain

$$-\nabla_{\perp}^{2}\widehat{\boldsymbol{E}} = (\omega^{2}\epsilon\mu - \beta^{2})\widehat{\boldsymbol{E}}$$
(3.6)

$$-\nabla_{\perp}^{2}\widehat{\boldsymbol{H}} = (\omega^{2}\epsilon\mu - \beta^{2})\widehat{\boldsymbol{H}}$$
(3.7)

We see that by treating $\omega^2 \epsilon \mu - \beta^2$ as a new eigenvalue λ , an eigenvalue problem independent of both ω and β can be formulated and precomputed, which provides us with dispersion relations as $\omega = W_n(\beta) = \sqrt{(\lambda_n + \beta^2)/(\epsilon\mu)}$, where λ_n depends only on the shape of the boundary. Usually two different eigenvalue problems are formulated: one for the z component of the electric field with Dirichlet conditions $\widehat{E}_z = 0$ on the boundary (TM modes), and one for the z component of the magnetic field with Neumann conditions $\hat{n} \cdot \nabla_{\perp} \widehat{H}_z = 0$ on the boundary (TE modes).

The dispersion relation $\omega = \sqrt{(\lambda_n + \beta^2)/(\epsilon\mu)}$ immediately demonstrates the important phenomenon of a cutoff frequency. For a hollow waveguide (consisting of a simply connected region Ω enclosed by PEC walls), the smallest eigenvalue λ_0 is always positive. This means that there exists a cutoff frequency $\omega_c = \sqrt{\lambda_0/(\epsilon\mu)}$, below which there can be no fixed frequency propagating waves (corresponding to real wave numbers β).

4 Bianisotropic materials

It is very difficult, maybe impossible, to derive an eigenvalue problem independent of both ω and β for a general bianisotropic material. In Appendix A we derive a second order differential equation which may be suitable for special cases, for instance when the material has an optical axis along the waveguide axis. However, in the general case, when nothing is *a priori* known about the structure of the material, this formulation offers little simplification.

Equation (2.8) can be used as an eigenvalue problem determining ω for a fixed β , but in most practical applications it is more relevant to study a fixed frequency ω . In this case, we assume a z dependence on the form $e^{\gamma z}$, where $\gamma = \alpha + i\beta$ is a complex number. Since $\nabla(f(x, y)e^{\gamma z}) = e^{\gamma z}(\nabla_{\perp} + \gamma \hat{z})f(x, y)$, we postulate an eigenvalue problem for the propagation constant γ as

$$\gamma_m \hat{\boldsymbol{z}} \times \mathbf{J} \hat{\mathbf{e}}_m = (-\nabla_\perp \times \mathbf{J} + \mathbf{i}\omega \mathbf{M}) \,\hat{\mathbf{e}}_m \tag{4.1}$$

This almost looks like an eigenvalue problem on generalized standard form, *i.e.*, $Au = \lambda Bu$, except that the mass matrix $B = \hat{z} \times J$ is not positive definite, which is usually required. The eigenvalues of the matrix $\hat{z} \times J$ are -1, 0, 1, all with double multiplicity. The mathematical problem of showing that this problem is well posed seems to be an open issue, but we assume this does not cause any problems.

The idea with this eigenvalue problem is to expand the electromagnetic field in the eigenmodes, and insert them into the z-dependent Maxwell's equations which then produces ordinary differential equations for the expansion coefficients. It then turns out that the solution is simply an expansion in these modes multiplied by exponential functions $e^{\gamma_n z}$, and the expansion coefficients can be determined from the boundary condition that the total transverse electromagnetic field is continuous.

We now demonstrate some general properties for the solutions of the eigenproblem (4.1). We use the following short hand notation for the integral over the cross section:

$$(\mathbf{e}, \mathbf{d}) = \int_{\Omega} \mathbf{e} \cdot \mathbf{d}^* \, \mathrm{d}S = \int_{\Omega} \left(\boldsymbol{E} \cdot \boldsymbol{D}^* + \boldsymbol{H} \cdot \boldsymbol{B}^* \right) \mathrm{d}S \tag{4.2}$$

which satisfies $(\mathbf{e}, \mathbf{d}) = (\mathbf{d}, \mathbf{e})^*$, *i.e.*, it is a scalar product for the fields. A lossless material is characterized by a hermitian symmetric material matrix, $\mathbf{M} = \mathbf{M}^{\mathrm{H}}$. As we shall see, it is convenient to have a means of characterizing the losses in a general material matrix \mathbf{M} . This is related to the anti-hermitian part, and we use the notation

$$\boldsymbol{\sigma}_{\mathsf{M}} = -\mathrm{i}\omega \frac{\mathsf{M} - \mathsf{M}^{\mathsf{H}}}{2} \tag{4.3}$$

The matrix σ_{M} is postulated to be non-negative hermitian symmetric. The notation is motivated by the following example. Consider an isotropic medium with electric conductivity:

$$\mathsf{M} = \begin{pmatrix} (\epsilon + \frac{\sigma}{-\mathrm{i}\omega})\mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mu\mathbf{I} \end{pmatrix} \implies \boldsymbol{\sigma}_{\mathsf{M}} = \begin{pmatrix} \sigma\mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}$$
(4.4)

We now derive the important quasi-orthogonality relation for the modes. Multiplying the equation (4.1) with the solution corresponding to another eigenvalue γ_n and integrating over the cross section, we obtain

$$\gamma_{m}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathbf{e}}_{m}, \hat{\mathbf{e}}_{n}) = ((-\nabla_{\perp} \times \mathsf{J} + \mathrm{i}\omega\mathsf{M})\hat{\mathbf{e}}_{m}, \hat{\mathbf{e}}_{n})$$

$$= ((-\nabla_{\perp} \times \mathsf{J} + \mathrm{i}\omega\mathsf{M}^{\mathrm{H}})\hat{\mathbf{e}}_{m}, \hat{\mathbf{e}}_{n}) + (\mathrm{i}\omega(\mathsf{M} - \mathsf{M}^{\mathrm{H}})\hat{\mathbf{e}}_{m}, \hat{\mathbf{e}}_{n})$$

$$= (\hat{\mathbf{e}}, -(-\nabla_{\perp} \times \mathsf{J} + \mathrm{i}\omega\mathsf{M})\hat{\mathbf{e}}) + \underbrace{\oint_{\partial\Omega} (-\hat{\boldsymbol{n}} \times \mathsf{J}\hat{\mathbf{e}}) \cdot \hat{\mathbf{e}}^{*} \mathrm{d}l}_{=0} - 2(\boldsymbol{\sigma}_{\mathsf{M}}\hat{\mathbf{e}}_{m}, \hat{\mathbf{e}}_{n})$$

$$= -(\hat{\mathbf{e}}_{m}, \gamma_{n}\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathbf{e}}_{n}) - 2(\boldsymbol{\sigma}_{\mathsf{M}}\hat{\mathbf{e}}_{m}, \hat{\mathbf{e}}_{n}) = -\gamma_{n}^{*}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathbf{e}}_{m}, \hat{\mathbf{e}}_{n}) - 2(\boldsymbol{\sigma}_{\mathsf{M}}\hat{\mathbf{e}}_{m}, \hat{\mathbf{e}}_{n}) \quad (4.5)$$

This implies the quasi-orthogonality relation (see also [4])

$$(\gamma_m + \gamma_n^*)(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_m, \hat{\mathsf{e}}_n) = -2(\boldsymbol{\sigma}_{\mathsf{M}}\hat{\mathsf{e}}_m, \hat{\mathsf{e}}_n)$$
(4.6)

The number $(\hat{z} \times J\hat{e}_m, \hat{e}_n)$ represents the time average of the mutual power flow in the z direction, since

$$(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathbf{e}}_m, \hat{\mathbf{e}}_n) = \int_{\Omega} \hat{\boldsymbol{z}} \cdot (\widehat{\boldsymbol{E}}_m \times \widehat{\boldsymbol{H}}_n^* + \widehat{\boldsymbol{E}}_n^* \times \widehat{\boldsymbol{H}}_m) \,\mathrm{d}S$$
(4.7)

Setting m = n in (4.6), we have $\gamma_n + \gamma_n^* = 2 \operatorname{Re}(\gamma_n)$ and find

$$\operatorname{Re}(\gamma_n)(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_n, \hat{\mathsf{e}}_n) = -(\boldsymbol{\sigma}_{\mathsf{M}}\hat{\mathsf{e}}_n, \hat{\mathsf{e}}_n)$$
(4.8)

A lossless waveguide is characterized by $\boldsymbol{\sigma}_{\mathsf{M}} = \mathbf{0}$. In this case, either $\operatorname{Re}(\gamma_n) = \alpha_n$ is equal to zero, *i.e.*, the mode propagates undamped with $\gamma_n = \mathrm{i}\beta_n$, or the time average of the power flow in the *z* direction, $(\hat{\boldsymbol{z}} \times \mathrm{J}\hat{\mathbf{e}}_n, \hat{\mathbf{e}}_n)$, is zero. In a lossy waveguide, the sign of $\operatorname{Re}(\gamma_n)$ is the opposite of the sign of the power flow $(\hat{\boldsymbol{z}} \times \mathrm{J}\hat{\mathbf{e}}_n, \hat{\mathbf{e}}_n)$, since $\boldsymbol{\sigma}_{\mathsf{M}}$ is non-negative. This last property implies that we can split the modes according to the signs of $\operatorname{Re}(\gamma_n)$ and $(\hat{\boldsymbol{z}} \times \mathrm{J}\mathbf{e}_n, \mathbf{e}_n)$,

$$\mathbf{e}_n = \mathbf{e}_n^+$$
 if $\operatorname{Re}(\gamma_n) \le 0$ and $(\hat{\mathbf{z}} \times \mathsf{Je}_n, \mathbf{e}_n) \ge 0$ (4.9)

$$\mathbf{e}_n = \mathbf{e}_n^-$$
 if $\operatorname{Re}(\gamma_n) \ge 0$ and $(\hat{\mathbf{z}} \times \mathsf{Je}_n, \mathbf{e}_n) \le 0$ (4.10)

This splitting is unique in lossy waveguides, and can be introduced in lossless waveguides by considering the modes as limits of modes in lossy waveguides when the loss $\sigma_{\rm M} \rightarrow 0$. We use this splitting when analyzing the scattering problems.

In lossless waveguides, the quasi-orthogonality relation (4.6) demonstrates that the mutual power flow $(\hat{z} \times J\hat{e}_m, \hat{e}_n)$ can be non-zero only if $\gamma_m + \gamma_n^* = 0$. This is achieved when m = n for propagating modes, $\gamma_n = i\beta_n$, but also for pairs of evanescent modes where $\gamma_m = \alpha$ and $\gamma_n = -\alpha$. This condition demonstrates how evanescent modes decaying in opposite directions can couple and carry power through a structure, which is known as the tunnelling effect in quantum mechanics. These modes are called twin-conjugate modes in [4].



Figure 2: The scattering geometry in the waveguide. The material under test (MUT) is confined to the region 0 < z < d with material parameters M, and the surrounding parts of the waveguide are filled with material M₀, usually air.

5 The forward scattering problem

The purpose of this section is to provide a formulation for the forward scattering problem that can be used to solve the inverse scattering problem. We assume a scattering geometry as in Figure 2. The time harmonic field amplitudes in the different regions can then be expanded as

$$\sum_{n=1}^{N} \left(A_n^+ \hat{\mathbf{e}}_{n0}^+ \mathbf{e}^{\mathbf{i}\beta_{n0}z} + A_n^- \hat{\mathbf{e}}_{n0}^- \mathbf{e}^{-\mathbf{i}\beta_{n0}z} \right) + \sum_{n=N+1}^{\infty} A_n^- \hat{\mathbf{e}}_{n0}^- \mathbf{e}^{\alpha_{n0}z} \qquad z < 0 \qquad (5.1)$$

$$\sum_{n=1}^{\infty} \left(f_n^+ \hat{\mathbf{e}}_n^+ \mathbf{e}_n^{\gamma_n^+ z} + f_n^- \hat{\mathbf{e}}_n^- \mathbf{e}_n^{\gamma_n^- z} \right) \qquad 0 < z < d \quad (5.2)$$

$$\sum_{n=1}^{N} \left(B_n^+ \hat{\mathbf{e}}_{n0}^+ e^{i\beta_{n0}(z-d)} + B_n^- \hat{\mathbf{e}}_{n0}^- e^{-i\beta_{n0}(z-d)} \right) + \sum_{n=N+1}^{\infty} B_n^+ \hat{\mathbf{e}}_{n0}^+ e^{-\alpha_{n0}(z-d)} \quad d < z$$
(5.3)

Here, we have explicitly splitted the modes in the surrounding lossless waveguide in propagating and evanescent waves. Note that the reference plane for the Bcoefficients is chosen to be the right boundary through the shift $z \to z - d$ in the exponentials.

The boundary conditions are that the tangential \boldsymbol{E} and \boldsymbol{H} fields should be continuous. This is ensured by requiring the following equations to hold, where we have made extensive use of the quasi-orthogonality relations (4.6) in the surrounding lossless medium (remember that for evanescent waves $(\hat{\boldsymbol{z}} \times \mathsf{J} \hat{\mathbf{e}}_{m0}^{\pm}, \hat{\mathbf{e}}_{m0}^{\pm}) = 0$, but the combination $(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{m0}^{\pm}, \hat{\mathsf{e}}_{m0}^{\mp})$ may be nonzero)

$$A_{m}^{+}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{m0}^{+}, \hat{\mathsf{e}}_{m0}^{+}) = \sum_{n=1}^{\infty} \left(f_{n}^{+}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{n}^{+}, \hat{\mathsf{e}}_{m0}^{+}) + f_{n}^{-}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{n}^{-}, \hat{\mathsf{e}}_{m0}^{+}) \right)$$
(5.4)

$$A_{m}^{-}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{m0}^{-}, \hat{\mathsf{e}}_{m0}^{-}) = \sum_{n=1}^{\infty} \left(f_{n}^{+}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{n}^{+}, \hat{\mathsf{e}}_{m0}^{-}) + f_{n}^{-}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{n}^{-}, \hat{\mathsf{e}}_{m0}^{-}) \right)$$
(5.5)

$$A_{m}^{-}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{m0}^{-}, \hat{\mathsf{e}}_{m0}^{+}) = \sum_{n=1}^{\infty} \left(f_{n}^{+}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{n}^{+}, \hat{\mathsf{e}}_{m0}^{+}) + f_{n}^{-}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{n}^{-}, \hat{\mathsf{e}}_{m0}^{+}) \right)$$
(5.6)

$$0 = \sum_{n=1}^{\infty} \left(f_n^+ (\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_n^+, \hat{\mathsf{e}}_{m0}^-) + f_n^- (\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_n^-, \hat{\mathsf{e}}_{m0}^-) \right)$$
(5.7)

$$B_{m}^{+}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{m0}^{+}, \hat{\mathsf{e}}_{m0}^{+}) = \sum_{n=1}^{\infty} \left(f_{n}^{+} \mathrm{e}^{\gamma_{n}^{+}d}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{n}^{+}, \hat{\mathsf{e}}_{m0}^{+}) + f_{n}^{-} \mathrm{e}^{\gamma_{n}^{-}d}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{n}^{-}, \hat{\mathsf{e}}_{m0}^{+}) \right)$$
(5.8)

$$B_{m}^{-}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{m0}^{-}, \hat{\mathsf{e}}_{m0}^{-}) = \sum_{n=1}^{\infty} \left(f_{n}^{+} \mathrm{e}^{\gamma_{n}^{+}d}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{n}^{+}, \hat{\mathsf{e}}_{m0}^{-}) + f_{n}^{-} \mathrm{e}^{\gamma_{n}^{-}d}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{n}^{-}, \hat{\mathsf{e}}_{m0}^{-}) \right)$$
(5.9)

$$B_{m}^{+}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{m0}^{+}, \hat{\mathsf{e}}_{m0}^{-}) = \sum_{n=1}^{\infty} \left(f_{n}^{+} \mathrm{e}^{\gamma_{n}^{+}d}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{n}^{+}, \hat{\mathsf{e}}_{m0}^{-}) + f_{n}^{-} \mathrm{e}^{\gamma_{n}^{-}d}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{n}^{-}, \hat{\mathsf{e}}_{m0}^{-}) \right)$$
(5.10)

$$0 = \sum_{n=1}^{\infty} \left(f_n^+ e^{\gamma_n^+ d} (\hat{\boldsymbol{z}} \times \mathsf{J} \hat{\mathsf{e}}_n^+, \hat{\mathsf{e}}_{m0}^+) + f_n^- e^{\gamma_n^- d} (\hat{\boldsymbol{z}} \times \mathsf{J} \hat{\mathsf{e}}_n^-, \hat{\mathsf{e}}_{m0}^+) \right) \quad (5.11)$$

The equations for $\{A_m^{\pm}, B_m^{\pm}\}$ (propagating modes, *i.e.*, (5.4), (5.5), (5.8), and (5.9)) are valid for $1 \leq m \leq N$, and the others (evanescent modes, *i.e.*, (5.7), (5.6), (5.10), and (5.11)) are valid for m > N.

In the forward scattering problem, the coefficients $\{A_n^+\}_{n=1}^N$ and $\{B_n^-\}_{n=1}^N$ are known, and the remaining coefficients are to be determined assuming full knowledge of the modes inside and outside the MUT. Based on the reasoning that equations (5.7) and (5.11) span all degrees of freedom except the 2N propagating modes in the surrounding medium, we assume that they can be used to eliminate all of the modes in the material except 2N ones (the first N plus modes and the first N minus modes inside the MUT), *i.e.*,

$$f_p^+ = \sum_{n=1}^N \left(Q_{pn}^A f_n^+ + R_{pn}^A f_n^- \right), \qquad p > N \qquad (5.12)$$

$$f_{p}^{-} e^{\gamma_{p}^{-} d} = \sum_{n=1}^{N} \left(R_{pn}^{B} f_{n}^{+} e^{\gamma_{n}^{+} d} + Q_{pn}^{B} f_{n}^{-} e^{\gamma_{n}^{-} d} \right), \qquad p > N \qquad (5.13)$$

Inserting the relations (5.12) and (5.13) into (5.4), we find

$$A_{m}^{+}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathbf{e}}_{m0}^{+}, \hat{\mathbf{e}}_{m0}^{+}) = \sum_{n=1}^{\infty} \left(f_{n}^{+}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathbf{e}}_{n}^{+}, \hat{\mathbf{e}}_{m0}^{+}) + f_{n}^{-}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathbf{e}}_{n}^{-}, \hat{\mathbf{e}}_{m0}^{+}) \right)$$
$$= \sum_{n=1}^{N} \left\{ f_{n}^{+} \left[(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathbf{e}}_{n}^{+}, \hat{\mathbf{e}}_{m0}^{+}) + \sum_{p=N+1}^{\infty} Q_{pn}^{A}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathbf{e}}_{p}^{+}, \hat{\mathbf{e}}_{m0}^{+}) \right] + f_{n}^{-} \left[(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathbf{e}}_{n}^{-}, \hat{\mathbf{e}}_{m0}^{+}) + \sum_{p=N+1}^{\infty} R_{pn}^{A}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathbf{e}}_{p}^{-}, \hat{\mathbf{e}}_{m0}^{+}) \right] \right\} \quad (5.14)$$

and a corresponding expression for (5.9), both valid for $1 \leq m \leq N$. This corresponds to two $N \times N$ systems of linear equations, from which $\{f_n^+, f_n^-\}_{n=1}^N$ can be determined from $\{A_m^+, B_m^-\}_{n=1}^N$.

When all the modes in the MUT contribute to the coupling between the interfaces, the coefficients $Q_{pn}^{A,B}$ and $R_{pn}^{A,B}$ depend on all the propagation constants γ_n^{\pm} and the length d of the slab, but not on the excitation. However, if the number of propagating modes inside the MUT is equal to the number of propagating modes outside, N, and the length is large enough so that only the propagating modes contribute to the coupling (the evanescent modes are sufficiently damped when reaching the opposite interface), the equations (5.7) and (5.11) take the following form:

$$\sum_{n=N+1}^{\infty} f_n^+(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_n^+, \hat{\mathsf{e}}_{m0}^-) = -\sum_{n=1}^N \left(f_n^+(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_n^+, \hat{\mathsf{e}}_{m0}^-) + f_n^-(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_n^-, \hat{\mathsf{e}}_{m0}^-) \right) \quad (5.15)$$
$$\sum_{n=N+1}^{\infty} f_n^- \mathrm{e}^{\gamma_n^- d}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_n^-, \hat{\mathsf{e}}_{m0}^+) = -\sum_{n=1}^N \left(f_n^+ \mathrm{e}^{\gamma_n^+ d}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_n^+, \hat{\mathsf{e}}_{m0}^+) + f_n^- \mathrm{e}^{\gamma_n^- d}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_n^-, \hat{\mathsf{e}}_{m0}^+) \right)$$

(5.16)

From this it is deduced that the matrices $Q_{pn}^{A,B}$ and $R_{pn}^{A,B}$ are independent of the propagation constants and the slab length in this approximation, since each equation can be solved independently.

6 The inverse scattering problem

In the inverse scattering problem the aim is to infer information on the scattering system from scattering data. In our case, the ultimate goal is to determine the material matrix M from reflection and transmission coefficients, or S-parameters, which can be measured using a network analyzer. This is very difficult, but we can at least obtain partial information on the wave propagation characteristics.

Assume that in the full problem, the interfaces are so widely separated that only propagating modes contribute to the coupling between the interfaces. Further assume the number of propagating modes in the MUT is the same as in the surrounding medium, that is, N. From Section 5 we then have the following equations

$$A_{m}^{\pm}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{m0}^{\pm}, \hat{\mathsf{e}}_{m0}^{\pm}) = \sum_{n=1}^{N} f_{n}^{+} \left[(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{n}^{+}, \hat{\mathsf{e}}_{m0}^{\pm}) + \sum_{p=N+1}^{\infty} Q_{pn}^{A}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{p}^{+}, \hat{\mathsf{e}}_{m0}^{\pm}) \right] \\ + \sum_{n=1}^{N} f_{n}^{-} \left[(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{n}^{-}, \hat{\mathsf{e}}_{m0}^{\pm}) + \sum_{p=N+1}^{\infty} R_{pn}^{A}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{p}^{-}, \hat{\mathsf{e}}_{m0}^{\pm}) \right]$$
(6.1)

$$B_{m}^{\pm}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{m0}^{\pm}, \hat{\mathsf{e}}_{m0}^{\pm}) = \sum_{n=1}^{N} f_{n}^{+} \mathrm{e}^{\gamma_{n}^{+}d} \left[(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{n}^{+}, \hat{\mathsf{e}}_{m0}^{\pm}) + \sum_{p=N+1}^{\infty} R_{pn}^{B}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{p}^{+}, \hat{\mathsf{e}}_{m0}^{\pm}) \right] \\ + \sum_{n=1}^{N} f_{n}^{-} \mathrm{e}^{\gamma_{n}^{-}d} \left[(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{n}^{-}, \hat{\mathsf{e}}_{m0}^{\pm}) + \sum_{p=N+1}^{\infty} Q_{pn}^{B}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{p}^{-}, \hat{\mathsf{e}}_{m0}^{\pm}) \right]$$
(6.2)

As explained in the discussion of the forward problem, the matrices Q_{pn}^A and Q_{pn}^B are strongly related to each other, as are R_{pn}^A and R_{pn}^B . The coefficients $\{A_m^\pm, B_m^\pm\}_{m=1}^N$ can be determined from measurements, and the expressions inside the square brackets and the propagation constants $\{\gamma_n^\pm\}_{n=1}^N$ are independent of the excitations. This means the equations can be written

$$A_m^{\pm}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{m0}^{\pm}, \hat{\mathsf{e}}_{m0}^{\pm}) = \sum_{n=1}^N \left(f_n^+ a_{mn}^{\pm} + f_n^- b_{mn}^{\pm} \right)$$
(6.3)

$$B_m^{\pm}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{m0}^{\pm}, \hat{\mathsf{e}}_{m0}^{\pm}) = \sum_{n=1}^N \left(f_n^+ \mathrm{e}^{\gamma_n^+ d} c_{mn}^{\pm} + f_n^- \mathrm{e}^{\gamma_n^- d} d_{mn}^{\pm} \right)$$
(6.4)

If $Q_{pn}^A = Q_{pn}^B = R_{pn}^A = R_{pn}^B = 0$, it is seen that $a_{mn}^{\pm} = c_{mn}^{\pm}$ and $b_{mn}^{\pm} = d_{mn}^{\pm}$. For a fixed n, assume the A-coefficients are chosen so that only the coefficient f_n^+ is nonzero. The B-coefficients are then equal to the A-coefficients multiplied by $e^{\gamma_n^{\pm}d}$. This means the exponential factors $e^{\gamma_n^{\pm}d}$ are the eigenvalues of the operator mapping A-coefficients to B-coefficients, and the vectors $a_{mn}^{\pm} = (\hat{z} \times J \hat{e}_n^+, \hat{e}_{m0}^{\pm})$ etc are the eigenvectors. This is the case for isotropic media, and possibly some more special cases. Thus, for these cases, it is sufficient to determine the operator between A-and B-coefficients to determine the propagations constants. With no assumptions on the material, we need to generalize this idea.

6.1 Determining the dispersion relations and modes

In what remains of this section, we use an index q to denote summation over the \pm index. Thus, instead of writing a_{mn}^{\pm} , we write a_{mn}^{q} , where the only possibilities for q are q = + or q = -.

With *n* fixed, and *m* and *q* free indices, we identify a_{mn}^q as a vector in \mathbb{C}^{2N} . We then assume that the 2*N* vectors $\{a_{mn}^q, b_{mn}^q\}_{n=1}^N$ are linearly independent. An adjoint basis $\{a_{mn}^{q\dagger}, b_{mn}^{q\dagger}\}_{n=1}^N$ can then be defined, such that [9, p. 12]

$$\sum_{m,q} a_{mn}^{q\dagger} a_{mn'}^q = \delta_{nn'}, \quad \sum_{m,q} b_{mn}^{q\dagger} b_{mn'}^q = \delta_{nn'}, \quad \sum_{m,q} a_{mn}^{q\dagger} b_{mn'}^q = \sum_{m,q} b_{mn}^{q\dagger} a_{mn'}^q = 0, \quad (6.5)$$

where $\delta_{nn'}$ is the Kronecker delta, *i.e.*, $\delta_{nn'} = 0$ if $n \neq n'$ and $\delta_{nn} = 1$. Multiplying (6.4) by vectors from this adjoint basis, this means the mode coefficients in the material can be expressed as

$$f_n^+ e^{\gamma_n^+ d} = \sum_{m,q} c_{mn}^{q\dagger} B_m^q (\hat{\boldsymbol{z}} \times \mathsf{J} \hat{\mathsf{e}}_{m0}^q, \hat{\mathsf{e}}_{m0}^q)$$
(6.6)

$$f_n^- \mathrm{e}^{\gamma_n^- d} = \sum_{m,q} d_{mn}^{q\dagger} B_m^q (\hat{\boldsymbol{z}} \times \mathsf{J} \hat{\mathsf{e}}_{m0}^q, \hat{\mathsf{e}}_{m0}^q)$$
(6.7)

and we have the following relation between the A- and B-coefficients from (6.3)

$$A_{m}^{q}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{m0}^{q}, \hat{\mathsf{e}}_{m0}^{q}) = \sum_{m',q'} \left[\sum_{n=1}^{N} \mathrm{e}^{-\gamma_{n}^{+}d} a_{mn}^{q} c_{m'n}^{q'\dagger} + \mathrm{e}^{-\gamma_{n}^{-}d} b_{mn}^{q} d_{m'n}^{q'\dagger} \right] B_{m'}^{q'}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{m'0}^{q'}, \hat{\mathsf{e}}_{m'0}^{q'}) = \sum_{m',q'} T_{mm'}^{qq'} B_{m'}^{q'}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{m'0}^{q'}, \hat{\mathsf{e}}_{m'0}^{q'}) \quad (6.8)$$

The matrix $T_{mm'}^{qq'}$ is independent of the excitation. By varying the input coefficients $\{A_m^+, B_m^-\}_{m=1}^N$ and measuring the response coefficients $\{A_m^-, B_m^+\}_{m=1}^N$, the *S*-parameters describing the mapping $\{A_m^+, B_m^-\}_{m=1}^N \to \{A_m^-, B_m^+\}_{m=1}^N$ can be determined. This is what a network analyzer typically measures. The *T*-parameters are then found by rearranging the *S*-parameters to obtain the mapping $\{B_m^+, B_m^-\}_{m=1}^N \to \{A_m^-, A_m^-\}_{m=1}^N$. An example of this procedure for the single-mode case is given in Section 7.

Performing this procedure for two different sample lengths d_1 and d_2 , we can determine two matrices $T(d_1)$ and $T(d_2)$. Now consider the linear combination $T(d_1) - \lambda T(d_2)$, where λ is a complex scalar. From the definition of the adjoint basis vectors $\{c_{mn}^{q\dagger}, d_{mn}^{q\dagger}\}_{n=1}^{N}$, we see that

$$\sum_{m',q'} [T_{mm'}^{qq'}(d_1) - \lambda T_{mm'}^{qq'}(d_2)] c_{m'n}^{q'} = (e^{-\gamma_n^+ d_1} - \lambda e^{-\gamma_n^+ d_2}) a_{mn}^q$$
(6.9)

This means that the matrix $T(d_1) - \lambda T(d_2)$ has a null space for $\lambda = e^{\gamma_n^+(d_2-d_1)}$. This means we can determine the propagation constant γ_n^+ by searching for λ such that this matrix has a null space, which is equivalent to solving the eigenvalue problem

$$T(d_2)^{-1}T(d_1)u_n = \lambda_n u_n \tag{6.10}$$

which is a well-defined numerical procedure once the matrices $T(d_1)$ and $T(d_2)$ are given. Following the previous reasoning, the eigenvalues and eigenvectors are

$$\lambda_n = \{ e^{\gamma_n^+(d_2 - d_1)}, e^{\gamma_n^-(d_2 - d_1)} \}, \quad u_n = \{ c_{mn}^\pm, d_{mn}^\pm \}$$
(6.11)

Another eigenvalue problem can be defined by

$$T(d_1)T(d_2)^{-1}v_n = \kappa_n v_n \tag{6.12}$$

where the eigenvalues and eigenvectors are

$$\kappa_n = \{ e^{\gamma_n^+(d_2 - d_1)}, e^{\gamma_n^-(d_2 - d_1)} \}, \quad v_n = \{ a_{mn}^\pm, b_{mn}^\pm \}$$
(6.13)

The eigenvectors are determined only up to a multiplicative constant. This corresponds to the normalization of the modes $\hat{\mathbf{e}}_n^{\pm}$, which we have left undefined since we do not need it. The idea for employing this data in determining the material, as discussed at the end of Section 6.2, does not seem to need such a normalization either.

We finally note that if we are only interested in obtaining the propagation constants, *i.e.*, the eigenvalues of $T(d_2)^{-1}T(d_1)$, the reference plane for the measurement does not need to be at the material boundary. This is due to the fact that a shift of reference plane in a lossless waveguide simply corresponds to $T \to UTV^{\rm H}$, where Uand V are unitary matrices. This means

$$T(d_2)^{-1}T(d_1) \to VT(d_2)^{-1}U^{\mathrm{H}}UT(d_1)V^{\mathrm{H}} = VT(d_2)^{-1}T(d_1)V^{\mathrm{H}}$$
 (6.14)

which does not change the eigenvalues, only the eigenvectors. Thus, if we are only interested in the propagation constants, the reference plane on each side of the sample is arbitrary as long as it is the same for both samples. But if we want information related to the eigenvectors, it is necessary to calibrate the reference plane to be at the material boundary.

The same reasoning also applies to the circumstance that we do not really measure the mode coefficient, but rather how this mode couples to a probe and is fed back in a cable; such transformations are modeled by transformations of the kind $T \rightarrow FTG^{-1}$, where F and G are matrices (or error boxes) modeling the probes at each end. Obviously, this does not change the situation compared to the previous paragraph.

6.2 Determining the material

From the previous subsection, we conclude that under the assumptions

- There are precisely N propagating modes inside and outside the MUT.
- Measurements are performed for two sample lengths d_1 and d_2 where each sample is sufficiently long so that only the first N modes inside the MUT contribute to the coupling between the interfaces.
- The measurements are versatile enough to explore all available degrees of freedom, *i.e.*, determine the matrices $T(d_1)$ and $T(d_2)$.

the propagation constants $\{\gamma_n^{\pm}\}_{n=1}^N$ and numerical vectors proportional to the following quantities can be determined (with m and q as free indices):

$$a_{mn}^{q} = (\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{n}^{+}, \hat{\mathsf{e}}_{m0}^{q}) + \sum_{p=N+1}^{\infty} Q_{pn}^{A} (\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{p}^{+}, \hat{\mathsf{e}}_{m0}^{q})$$
(6.15)

$$b_{mn}^q = (\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_n^-, \hat{\mathsf{e}}_{m0}^q) + \sum_{p=N+1}^{\infty} R_{pn}^A (\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_p^-, \hat{\mathsf{e}}_{m0}^q)$$
(6.16)

$$c_{mn}^{q} = (\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{n}^{+}, \hat{\mathsf{e}}_{m0}^{q}) + \sum_{p=N+1}^{\infty} R_{pn}^{B}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{p}^{+}, \hat{\mathsf{e}}_{m0}^{q})$$
(6.17)

$$d_{mn}^{q} = (\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{n}^{-}, \hat{\mathsf{e}}_{m0}^{q}) + \sum_{p=N+1}^{\infty} Q_{pn}^{B}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{p}^{-}, \hat{\mathsf{e}}_{m0}^{q})$$
(6.18)

This is all information that can be determined from this kind of measurements, since this represents a complete description of the N-port scattering matrix. These quantities can be used as follows to determine an interesting quantity, containing information on M. The modes inside and outside the MUT are defined by the equations

$$\gamma_n^q \hat{\boldsymbol{z}} \times \mathsf{J} \hat{\mathsf{e}}_n^q = (-\nabla_\perp \times \mathsf{J} + \mathrm{i}\omega\mathsf{M})\hat{\mathsf{e}}_n^q \tag{6.19}$$

$$\gamma_{m0}^{q'} \hat{\boldsymbol{z}} \times \mathsf{J} \hat{\mathsf{e}}_{m0}^{q'} = (-\nabla_{\perp} \times \mathsf{J} + \mathrm{i}\omega \mathsf{M}_0) \hat{\mathsf{e}}_{m0}^{q'}$$
(6.20)

This implies

$$\begin{split} \gamma_{n}^{q}(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{n}^{q}, \hat{\mathsf{e}}_{m0}^{q'}) &= ((-\nabla_{\perp} \times \mathsf{J} + \mathrm{i}\omega\mathsf{M})\hat{\mathsf{e}}_{n}^{q}, \hat{\mathsf{e}}_{m0}^{q'}) \\ &= (\mathrm{i}\omega(\mathsf{M} - \mathsf{M}_{0})\hat{\mathsf{e}}_{n}^{q}, \hat{\mathsf{e}}_{m0}^{q'}) + ((-\nabla_{\perp} \times \mathsf{J} + \mathrm{i}\omega\mathsf{M}_{0})\hat{\mathsf{e}}_{n}^{q}, \hat{\mathsf{e}}_{m0}^{q'}) \\ &= (\mathrm{i}\omega(\mathsf{M} - \mathsf{M}_{0})\hat{\mathsf{e}}_{n}^{q}, \hat{\mathsf{e}}_{m0}^{q'}) - (\hat{\mathsf{e}}_{n}^{q}, (-\nabla_{\perp} \times \mathsf{J} + \mathrm{i}\omega\mathsf{M}_{0})\hat{\mathsf{e}}_{m0}^{q'}) \\ &= (\mathrm{i}\omega(\mathsf{M} - \mathsf{M}_{0})\hat{\mathsf{e}}_{n}^{q}, \hat{\mathsf{e}}_{m0}^{q'}) - (\hat{\mathsf{e}}_{n}^{q}, \gamma_{m0}^{q'}\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_{m0}^{q'}) \quad (6.21) \end{split}$$

or

$$(\gamma_n^q + (\gamma_{m0}^{q'})^*)(\hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathsf{e}}_n^q, \hat{\mathsf{e}}_{m0}^{q'}) = (\mathrm{i}\omega(\mathsf{M} - \mathsf{M}_0)\hat{\mathsf{e}}_n^q, \hat{\mathsf{e}}_{m0}^{q'})$$
(6.22)

Since the propagation constants are known, we see that information on the scalar product $(\hat{z} \times J\hat{e}_n^q, \hat{e}_{m0}^{q'})$ implies information on the scalar product $(i\omega(M-M_0)\hat{e}_n^q, \hat{e}_{m0}^{q'})$, which is directly linked to the material matrix M. Using this relation in (6.15) produces

$$(\gamma_n^+ + (\gamma_{m0}^q)^*)a_{mn}^q = \left(\mathrm{i}\omega(\mathsf{M} - \mathsf{M}_0)\left[\hat{\mathsf{e}}_n^+ + \sum_{p=N+1}^\infty Q_{pn}^A \frac{\gamma_n^+ + (\gamma_{m0}^q)^*}{\gamma_p^+ + (\gamma_{m0}^q)^*}\hat{\mathsf{e}}_p^+\right], \hat{\mathsf{e}}_{m0}^q\right) \quad (6.23)$$

with similar equations for the b, c, and d vectors. The left hand side is known from the eigenvalue problems formulated from measurement data, which means we have an indirect way of calculating the right hand side. With more information on the modes \hat{e}_n , this can be used to determine at least parts of the material matrix M. However, this problem is left for subsequent papers.



Figure 3: The geometry and mesh of the numerical examples. The two surrounding waveguides are designed for X-band operation (8.2–12.4 GHz, cutoff frequency 6.55 GHz), with cross section $2.29 \times 1.02 \text{ cm}$ and length 5.00 cm. Each open end is used as a port for the TE₁₀ mode. A waveguide section of cross section $1.25 \times 1.02 \text{ cm}$ and length 4.00 cm or 5.00 cm is filled with the material under test. The mesh uses 3514 tetrahedral elements.

7 Numerical examples

To illustrate the algorithm for the inverse scattering problem, we apply it to numerically simulated data. The results in this section can be transformed to other frequency regions by simultaneously scaling the dimensions of the waveguide and the frequency.

The waveguide setup is shown in Figure 3. The center part of the waveguide, containing the MUT, has different physical dimensions from the surrounding waveguides. This is in order to limit the number of propagating modes in the MUT.

The simulations were made with the program Comsol Multiphysics version 3.3, which is based on the Finite Element Method. The cutoff frequency for the TE₁₀ mode of the air-filled waveguides is 6.55 GHz, and the frequency interval for simulation was chosen as 7–15 GHz. The central waveguide part was filled with a non-magnetic isotropic material with relative permittivity $\epsilon_r = 4$ and conductivity $\sigma = 0.1 \text{ S/m}$, implying a dispersive complex relative permittivity $\epsilon(\omega) = \epsilon_r + \frac{\sigma}{i\omega\epsilon_0}$, where ϵ_0 is the permittivity of vacuum. The calculations were made for the two lengths $d_1 = 4.00 \text{ cm}$ and $d_2 = 5.00 \text{ cm}$. The program generates S-parameters for the structure with reference planes at the ports, and they are shown in Figure 4. The S-parameters are defined from

$$\begin{pmatrix} A^{-} \\ B^{+} \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} A^{+} \\ B^{-} \end{pmatrix}$$
(7.1)

whereas we want to use the relation

$$\begin{pmatrix} A^+ \\ A^- \end{pmatrix} = \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} \begin{pmatrix} B^+ \\ B^- \end{pmatrix}$$
(7.2)

in the algorithm determining the propagation constants. These are the T-parameters, which are closely related to the ABCD-parameters; the T-parameters map the in- and outgoing waves on each side to each other, whereas the ABCD-parameters map the total voltages and currents on each side of a two-port network to each other. The T-parameters are easily expressed in terms of the S-parameters as [8]

$$T_{11} = 1/S_{21} \tag{7.3}$$

$$T_{12} = -S_{22}/S_{21} \tag{7.4}$$

$$T_{21} = S_{11}/S_{21} \tag{7.5}$$

$$T_{22} = (S_{12}S_{21} - S_{11}S_{22})/S_{21} \tag{7.6}$$

After using this transformation, we can find the propagation constants from the eigenvalues of the matrix $T(d_2)^{-1}T(d_1)$. In this procedure, it is necessary to unwrap the phase (remove discontinuities $\geq \pi$ in the imaginary part) in order to avoid discontinuities in the propagation constants as functions of ω . The complex permittivity is then determined by inverting the relation $\beta^2 = \epsilon(\omega)\omega^2/c_0^2 - \lambda$, where $\lambda = (\pi/a)^2$, with *a* being the width of the center waveguide. The resulting quantity is plotted in Figure 5. The code doing this procedure on given *S*-parameter data is only a few lines in Matlab.

It is seen that the method can determine the complex permittivity rather accurately. The errors can be attributed to the numerical accuracy of the FEM program generating the data. A full-blown stability analysis of the algorithm is beyond the scope of this paper, but we can at least do some numerical experiments. We perturbed the S-parameters in the simulations by adding noise generated by the Matlab command randn multiplied by three different factors 0.1, 0.01, and 0.001, representing different noise levels. The results are depicted in Figure 6, and it is seen that the algorithm is reasonably stable for this test.

To conclude this section, in Figure 7 we also give the results for an extension to the anisotropic case presented in [6]. There, it is shown that for a non-magnetic, anisotropic dielectric with its principal axis aligned with the walls of a rectangular waveguide, the same dispersion relations apply for the fundamental TE mode as for an isotropic material, *i.e.*, $\beta^2 = \epsilon_{x,y,z}(\omega)\omega^2/c_0^2 - \lambda$. In order to deduce all three principal values, the material sample is rotated so that each principal direction is aligned with the fundamental TE mode in the waveguide.

8 Conclusions

In this paper, we have analyzed the forward and inverse scattering problems of a bianisotropic material sample in a metallic waveguide. Under the assumption that there are as many modes inside the MUT as outside, measurements on two samples with different lengths are enough to determine the propagation constants inside the MUT. Additional information on the modes is available, but the utilization of this information remains a problem for further research.



Figure 4: The S-parameters for the two experiments. Figures a and b refer to sample length $d_1 = 5.00$ cm, and figures c and d are for $d_2 = 4.00$ cm. For reciprocal media we have as usual $S_{11} = S_{22}$ and $S_{21} = S_{12}$.



Figure 5: The complex permittivity computed from the S-parameters by the algorithm in this paper. The circles indicate 10 linearly distributed frequencies in the interval 7–15 GHz, smallest frequencies farthest to the left. Notice that the imaginary part (the y-axis) is scaled by the factor $\omega \epsilon_0$, making it correspond to the conductivity σ . Also observe the tight scales. The relatively large deviation for high frequencies is probably due to multimode propagation.



Figure 6: The complex permittivity computed when perturbing the *S*-parameters by random numbers of typical size 0.1, 0.01, and 0.001, from top to bottom.



Figure 7: Results for an anisotropic material. In this case, the narrow section of the waveguide has principal values $\epsilon_x = 2 + i\sigma/(\omega\epsilon_0)$, $\epsilon_y = 3 + i\sigma/(\omega\epsilon_0)$, and $\epsilon_z = 4 + i\sigma/(\omega\epsilon_0)$, where $\sigma = 0.1$ S/m. The mesh and the frequency range, 7– 15 GHz, are the same as in the other examples, and the errors are largest for higher frequencies. The curve for $\epsilon_x - 2$ starts off with a relatively large error at around (0.0024, 0.0928) for f = 7 GHz in the figure. This is due to that for this principal value the midsection waveguide is then operating below its cutoff frequency, which is 8.5 GHz.

The analysis is very general, and only assumes the material is linear. For instance, nothing in the analysis changes if the material is heterogeneous in the (x, y)plane, but does not depend on the z variable. Indeed, this has been utilized in the numerical example in Section 7, where we used a different cross section of the waveguide containing the sample. Actually, the analysis is applicable to any structure in which the electromagnetic field can be described by an expansion in propagating and evanescent modes.

There is probably a large range of special cases where the proposed formalism reduces significantly in complexity. Most prominently, in waveguides filled with isotropic materials, there is almost no coupling between different modes. Also, as seen from the eigenproblems (A.9) and (A.10) for a general bianisotropic material, there are significant simplifications for materials where an optical axis is along the waveguide axis.

The major assumption in this paper is that the number of propagating modes is the same inside and outside the MUT, or possibly a smaller number inside the MUT. The main reason for this assumption is that it is necessary to be able to explore the degrees of freedom available *inside* the material by varying the degrees of freedom *outside* the material. This is not always easy to achieve: if the surrounding medium is air, the cutoff frequencies inside the MUT are usually lower, implying that there may be more propagating modes inside the material. In order to achieve the same number of propagating modes, we may choose the surrounding material M_0 to obtain a small contrast to the MUT M, or place the MUT in a somewhat narrower waveguide than its surrounding material. The latter strategy was employed in Section 7 of this paper.

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Appendix A A second order eigenproblem

One of the major problems with the well-posedness of the eigenproblem

$$\gamma \hat{\boldsymbol{z}} \times \mathsf{J} \hat{\mathsf{e}} = (-\nabla_{\perp} \times \mathsf{J} + \mathrm{i}\omega\mathsf{M})\hat{\mathsf{e}} \tag{A.1}$$

is that the weight matrix $\hat{z} \times J$ is not positive definite. Indeed, it has the eigenvalues -1, 0, and 1, all with double multiplicity. To eliminate at least the eigenvalue 0, we observe that this is related to the z component of the field (since $\hat{z} \times \hat{z} = 0$), which leads us to the idea to eliminate the z component of the field. The transverse curl operator can be written in terms of its transverse and z parts as

$$\nabla_{\perp} \times \mathbf{J} = -\hat{\mathbf{z}} \times \mathbf{J} \cdot \nabla_{\perp} \hat{\mathbf{z}} - \hat{\mathbf{z}} \nabla_{\perp} \cdot \hat{\mathbf{z}} \times \mathbf{J}$$
(A.2)

We separate the transverse and z component of the electromagnetic field as

$$\hat{\mathbf{e}} = \hat{\mathbf{e}}_{\perp} + \hat{\mathbf{e}}_z \tag{A.3}$$

which splits the eigenvalue problem above in one transverse part and one z part,

$$\gamma \hat{\boldsymbol{z}} \times \mathsf{J} \hat{\mathsf{e}}_{\perp} = \hat{\boldsymbol{z}} \times \mathsf{J} \cdot \nabla_{\perp} \hat{\mathsf{e}}_{z} + \mathrm{i}\omega(\mathsf{M}_{\perp\perp} \hat{\mathsf{e}}_{\perp} + \mathsf{M}_{\perp z} \hat{\mathsf{e}}_{z}) \tag{A.4}$$

$$0 = \nabla_{\perp} \cdot \hat{\boldsymbol{z}} \times \mathsf{J}\hat{\mathbf{e}}_{\perp} + \mathrm{i}\omega(\mathsf{M}_{z\perp}\hat{\mathbf{e}}_{\perp} + \mathsf{M}_{zz}\hat{\mathbf{e}}_{z}) \tag{A.5}$$

From the last equation we eliminate $\hat{\mathbf{e}}_z$ as

$$\hat{\mathbf{e}}_{z} = \mathsf{M}_{zz}^{-1} \left(-\frac{1}{\mathrm{i}\omega} \nabla_{\perp} \cdot \hat{\boldsymbol{z}} \times \mathsf{J} \hat{\mathbf{e}}_{\perp} - \mathsf{M}_{z\perp} \hat{\mathbf{e}}_{\perp} \right)$$
(A.6)

By eliminating the z component of the field, we raise the order of the differential operator and must make sure that all boundary conditions from the original formulation are preserved. Thus, we explicitly require the boundary condition

$$\hat{\mathbf{e}}_{z} = \begin{pmatrix} \hat{E}_{z} \\ \hat{H}_{z} \end{pmatrix} = \begin{pmatrix} 0 \\ \hat{H}_{z} \end{pmatrix} = \mathsf{M}_{zz}^{-1} (-\frac{1}{\mathrm{i}\omega} \nabla_{\perp} \cdot \hat{\mathbf{z}} \times \mathsf{J} \hat{\mathbf{e}}_{\perp} - \mathsf{M}_{z\perp} \hat{\mathbf{e}}_{\perp}), \quad (x, y) \in \partial\Omega \qquad (A.7)$$

For isotropic materials, this corresponds to a Neumann boundary condition for the magnetic field. Had we not required this, we would only have a Dirichlet boundary condition for the electric field, *i.e.*, not enough to specify a unique solution in both electric and magnetic field.

Inserting the expression for $\hat{\mathbf{e}}_z$ in (A.4), we obtain

$$\begin{split} \gamma \hat{\boldsymbol{z}} \times \mathsf{J} \hat{\mathbf{e}}_{\perp} &= \hat{\boldsymbol{z}} \times \mathsf{J} \cdot \nabla_{\perp} \hat{\mathbf{e}}_{z} + \mathrm{i}\omega (\mathsf{M}_{\perp\perp} \hat{\mathbf{e}}_{\perp} + \mathsf{M}_{\perp z} \hat{\mathbf{e}}_{z}) \\ &= \hat{\boldsymbol{z}} \times \mathsf{J} \cdot \nabla_{\perp} \mathsf{M}_{zz}^{-1} (-\frac{1}{\mathrm{i}\omega} \nabla_{\perp} \cdot \hat{\boldsymbol{z}} \times \mathsf{J} \hat{\mathbf{e}}_{\perp} - \mathsf{M}_{z\perp} \hat{\mathbf{e}}_{\perp}) \\ &+ \mathrm{i}\omega \left[\mathsf{M}_{\perp\perp} \hat{\mathbf{e}}_{\perp} + \mathsf{M}_{\perp z} \mathsf{M}_{zz}^{-1} (-\frac{1}{\mathrm{i}\omega} \nabla_{\perp} \cdot \hat{\boldsymbol{z}} \times \mathsf{J} \hat{\mathbf{e}}_{\perp} - \mathsf{M}_{z\perp} \hat{\mathbf{e}}_{\perp}) \right] \\ &= -\frac{1}{\mathrm{i}\omega} \hat{\boldsymbol{z}} \times \mathsf{J} \cdot \nabla_{\perp} \mathsf{M}_{zz}^{-1} \nabla_{\perp} \cdot \hat{\boldsymbol{z}} \times \mathsf{J} \hat{\mathbf{e}}_{\perp} \\ &- \hat{\boldsymbol{z}} \times \mathsf{J} \cdot \nabla_{\perp} \mathsf{M}_{zz}^{-1} \mathsf{M}_{z\perp} \hat{\mathbf{e}}_{\perp} - \mathsf{M}_{\perp z} \mathsf{M}_{zz}^{-1} \nabla_{\perp} \cdot \hat{\boldsymbol{z}} \times \mathsf{J} \hat{\mathbf{e}}_{\perp} \\ &+ \mathrm{i}\omega \left[\mathsf{M}_{\perp\perp} - \mathsf{M}_{\perp z} \mathsf{M}_{zz}^{-1} \mathsf{M}_{z\perp} \right] \hat{\mathbf{e}}_{\perp} \quad (A.8) \end{split}$$

and after multiplying by $-i\omega$ this is

$$-\mathrm{i}\omega\gamma\hat{\boldsymbol{z}}\times\mathsf{J}\hat{\mathsf{e}}_{\perp} = \hat{\boldsymbol{z}}\times\mathsf{J}\cdot\nabla_{\perp}\mathsf{M}_{zz}^{-1}\nabla_{\perp}\cdot\hat{\boldsymbol{z}}\times\mathsf{J}\hat{\mathsf{e}}_{\perp} + \omega^{2}\left[\mathsf{M}_{\perp\perp}-\mathsf{M}_{\perp z}\mathsf{M}_{zz}^{-1}\mathsf{M}_{z\perp}\right]\hat{\mathsf{e}}_{\perp} +\mathrm{i}\omega\left[\hat{\boldsymbol{z}}\times\mathsf{J}\cdot\nabla_{\perp}\mathsf{M}_{zz}^{-1}\mathsf{M}_{z\perp}+\mathsf{M}_{\perp z}\mathsf{M}_{zz}^{-1}\nabla_{\perp}\cdot\hat{\boldsymbol{z}}\times\mathsf{J}\right]\hat{\mathsf{e}}_{\perp} \quad (A.9)$$

For propagating modes in lossless waveguides the eigenvalue is real, $-i\omega\gamma = -i\omega i\beta = \omega\beta$. Observe that significant simplifications occur when the material is symmetric around the z axis, *i.e.*, $M_{z\perp} = M_{\perp z} = 0$.

This problem is still not quite on standard form, since the eigenvalues for $\hat{z} \times J$ are ± 1 (with double multiplicity) when considering only the transverse components

of the field. Though, note that for hermitian symmetric materials $(M = M^{H})$ the operator in the right hand side is self-adjoint due to the extra boundary condition induced by the elimination of the z component.

The same procedure can be applied to formulate a problem in the z-components of the fields instead of the transverse components. The result is

$$-\nabla_{xy}\cdot\hat{\boldsymbol{z}}\times\mathsf{J}(\mathsf{M}_{\perp\perp}-\frac{\gamma}{\mathrm{i}\omega}\hat{\boldsymbol{z}}\times\mathsf{J})^{-1}\hat{\boldsymbol{z}}\times\mathsf{J}\cdot\nabla_{xy}\hat{\mathsf{e}}_{z} = \omega^{2}\left[\mathsf{M}_{zz}-\mathsf{M}_{z\perp}(\mathsf{M}_{\perp\perp}-\frac{\gamma}{\mathrm{i}\omega}\hat{\boldsymbol{z}}\times\mathsf{J})^{-1}\mathsf{M}_{\perp z}\right]\hat{\mathsf{e}}_{z}$$
$$+\left[\nabla_{xy}\cdot\hat{\boldsymbol{z}}\times\mathsf{J}(\mathsf{M}_{\perp\perp}-\frac{\gamma}{\mathrm{i}\omega}\hat{\boldsymbol{z}}\times\mathsf{J})^{-1}\mathsf{M}_{\perp z}+\mathsf{M}_{z\perp}(\mathsf{M}_{\perp\perp}-\frac{\gamma}{\mathrm{i}\omega}\hat{\boldsymbol{z}}\times\mathsf{J})^{-1}\hat{\boldsymbol{z}}\times\mathsf{J}\cdot\nabla_{xy}\right]\hat{\mathsf{e}}_{z}$$
$$(A.10)$$

which does not offer any clear advantage over the previous formulation. Note again the significant simplification which occurs if $M_{z\perp} = M_{\perp z} = 0$.

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