Appl. Phys. B 44, 205–209 (1987)

Applied Physics B Photophysics and Laser Chemistry

Bisection Algorithm to Calculate Hybrid Modes of Birefringent Planar Graded Index Waveguides

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Received 6 August 1987/Accepted 15 September 1987

Abstract. Guided modes of a planar dielectric waveguide which encounter a nondiagonal permittivity tensor are neither TE nor TM, but hybrid. They are described by a pair of coupled second-order differential equations for the transversal electric and magnetic field components. We construct a real-valued function which plays the role of the transversal electric or magnetic field in the uncoupled Sturm-Liouville differential equation for TE or TM modes. The number of zeroes, or nodes, of this function labels the modes. The nodes increase with the prospective propagation constant. This fact is proven by constructing suitable self-adjoint operators and referring to the minimax principle. The nodal properties allow to formulate an efficient bisection algorithm for effective indices and field distributions of guided hybrid modes.

PACS: 42.80, 42.82

Linear or planar dielectric waveguides are the key components of integrated optical devices. They serve to guide light waves along a strip or within a layer upon appropriate substrates. Waveguiding regions of increased permittivity, i.e. permittivity profiles, have been produced by exchange, implantation, in- or outdiffusion of suitable ions, or by combinations of such procedures.

Most applications are based on electro- or magnetooptic properties of the substrates and require single domain, optically anisotropic crystals. $LiNbO_3$ is a well-known example. For such media, not only the bulk permittivities, but also the permittivity profiles on top of them must be described by tensors. The resulting mode equations are rather complicated, even for planar waveguides. If, however, the crystal is cut perpendicular to an (optical) symmetry axis and if the propagation direction coincides with another (optical) symmetry axis the mode equations decouple and allow for simple TE or TM solutions.

There are various reasons to investigate hybrid modes in planar dielectric waveguides.

In some applications the propagation constants of different modes must coincide in order to have phase matching over a long interaction length (generation of second and higher harmonics, TE/TM mode conversion, etc.). This may be achieved by selecting an appropriate angle between symmetry axis and propagation direction.

Another domain is holography in planar waveguides. Here two or more surface waves are superimposed to generate an interference pattern which is to be recorded, fixed, and reconstructed. It is not possible, in general, that all waves travel along a symmetry axis, some or all are necessarily hybrid.

A third reason to study hybrid modes is the so-called inverse problem. Mode propagation constants are measured in an effort to reconstruct the guiding permittivity profiles. By investigating pure TE or TM modes only a few *numbers* – the propagation constants β_m – are to determine two or three permittivity *profiles*. If we take hybrid modes into consideration as well we have to fit *curves* $\beta_m(\theta)$, where θ is the angle between a symmetry axis and the mode propagation direction. It is evident: the more data to be fitted the less ambiguous the reconstructed profiles.

Yamamoto et al. [1] investigated an anisotropic and gyrotropic slab waveguide. The non-diagonal elements of the permittivity tensor were treated as perturbations. Burns and Warner [2] derived a closed expression for the dispersion equation of hybrid modes. They assumed isotropic cover layers and specialized to a coplanar optical axis in the waveguiding slab. Marcuse [3] analysed hybrid modes if the optical axis is not in the slab plane, and anisotropic covers were examined by Marcuse and Kaminow [4]. Čtyroký and Čada [5] tackled the anisotropic graded index waveguide by a generalized WKB method, Kolosovskiĭ et al. [6] by Runge-Kutta integration, Koshiba et al. [7] by a finite element calculation.

If the profiles are broad the WKB method can provide rather accurate effective indices, but no field distributions. The finite-element method, on the other hand, is versatile but, in general, difficult to implement. Guided modes have to fall off on both sides of the surface: this is a boundary value problem for which the finite element method is the appropriate tool. In the cover region, however, the mode equations can be solved analytically, and the corresponding initial/boundary value problem is much simpler. The effective index, or the propagation constant β, appears as a parameter in the differential equations and in the initial conditions. It has to be determined such that the boundary condition on the substrate side is met. Kolosovskiĭ et al. have to scan the whole range of possible β values. We present a much simpler and faster method.

Pure TE or TM modes are described by a Sturm-Liouville problem for which there is an efficient algorithm: guess an eigenvalue, integrate the differential equation, count the number of zeroes and decide whether the guessed value was too high or too low. Repeated bisections allow any desired accuracy. We show that this strategy can be applied to hybrid modes as well. Although a system of two coupled second-order differential equations is encountered we exhibit a real-valued node function such that its zeroes behave just as in the pure TE or TM case: if the prospective propagation constant is lowered the nodes move away from infinity, and each time a new node creeps in at infinity, an eigenvalue has been found.

In the following section we set up the differential equations for hybrid modes as well as the appropriate boundary conditions and introduce nodes. We present an equivalent Hilbert space formulation in Sect. 2 and prove that nodes move away from infinity if the propagation constant is lowered. Counting nodes, as outlined in Sect. 3, allows to formulate a bisection algorithm which serves to calculate the propagation constants β_m and field distributions for guided modes.

1. Differential Equations

In order to simplify notation we shall rescale the electric displacement and the magnetic field strength such that they are comparable with the electric field strength. We replace D/ε_0 by the symbol D, $\mu_0 c_0 H$ by H, and $c_0 B$ by B. Likewise dimensionless coordinates are used. With ω as light wave frequency and $k_0=\omega/c_0$ as corresponding vacuum wave number we replace $k_0 x$ by x, etc.

Let us introduce Cartesian coordinates such that the x-axis is normal to the waveguide surface, and mode propagation is along the z-axis. All fields are of the form

$$F(x,y,z,t)=F(x)\,e^{i(\beta z-\omega t)}. \tag{1}$$

We have a dielectric waveguide which is described by

$$D_j(x)=\sum_{k=1}^{3}\varepsilon_{jk}(x)E_k(x) \quad\text{and}\quad B_i(x)=H_i(x). \tag{2}$$

The permittivities $\varepsilon_{jk}(x)$ are constant in the cover region $x<0$. In the substrate region $x>0$ they are assumed to be smooth functions which converge sufficiently rapidly towards the bulk values with $x\to\infty$. The permittivities will jump at the cover/substrate interface.

Maxwell's equations reduce to identities between field components and to first-order differential equations. The identities are

$$D_1=\beta H_2, \qquad H_1=-\beta E_2. \tag{3}$$

Together with (2) we may express D_i, E_1, and H_1 in terms of E_2, E_3, H_2, and H_3. The differential equations are

$$\begin{aligned}
iE_2' &= -H_3,\\
iH_3' &= \frac{\beta\varepsilon_{12}}{\varepsilon_{11}}E_2+\frac{\beta_{13}}{\varepsilon_{11}}E_3+\left(1-\frac{\beta^2}{\varepsilon_{11}}\right)H_2,\\
iH_2' &= \left(\varepsilon_{32}-\frac{\varepsilon_{12}\varepsilon_{31}}{\varepsilon_{11}}\right)E_2\\
&\quad+\left(\varepsilon_{33}-\frac{\varepsilon_{13}\varepsilon_{31}}{\varepsilon_{11}}\right)E_3+\frac{\beta\varepsilon_{31}}{\varepsilon_{11}}H_2,\\
iH_3' &= \left(\beta^2-\varepsilon_{22}+\frac{\varepsilon_{12}\varepsilon_{21}}{\varepsilon_{11}}\right)E_2\\
&\quad+\left(-\varepsilon_{23}+\frac{\varepsilon_{21}\varepsilon_{13}}{\varepsilon_{11}}\right)E_3-\frac{\beta\varepsilon_{21}}{\varepsilon_{11}}H_2.
\end{aligned} \tag{4}$$

Note that E_2, E_3, H_2, and H_3 are tangential components of the electric and magnetic fields. They must be continuous at the cover/substrate interface at $x=0$. By (3) the normal components of magnetic induction and electric displacement then are continuous as well.

If the permittivity tensor were diagonal the four coupled first order differential equations (4) would give rise to two independent second-order equations. With

$\varepsilon_2 = \varepsilon_{22}$ we may write

$$E'' + (\varepsilon_2 - \beta^2)E = 0. \tag{5}$$

This equation describes transverse electric, or TE modes. Solutions are of the form

$$\begin{aligned} &E_1 = 0, \quad E_2 = E, \quad E_3 = 0, \\ &H_1 = -\beta E, \quad H_2 = 0, \quad H_3 = -iE'. \end{aligned} \tag{6}$$

The second equation is

$$\varepsilon_1 \left(\frac{1}{\varepsilon_3} H' \right)' + (\varepsilon_1 - \beta^2) H = 0. \tag{7}$$

Again we have set $\varepsilon_1 = \varepsilon_{11}$ and $\varepsilon_3 = \varepsilon_{33}$. (7) describes transverse magnetic, or TM modes which are of the form

$$\begin{aligned} &E_1 = \frac{\beta H}{\varepsilon_1}, \quad E_2 = 0, \quad E_3 = \frac{iH'}{\varepsilon_3}, \\ &H_1 = 0, \quad H_2 = H, \quad H_3 = 0. \end{aligned} \tag{8}$$

We have to deal with pure TE and TM modes if the waveguide surface is perpendicular to an optical symmetry axis and if the mode propagates along another symmetry axis. We now allow for an angle θ between the propagation direction (our z-axis) and the optical symmetry axis in the surface plane. The diagonal permittivity tensor with profiles ε_1, ε_2, and ε_3 must be rotated by an angle θ around the x-axis. The result is

$$\varepsilon_{jk} = \begin{pmatrix} \varepsilon_1 & 0 & 0 \\ 0 & \varepsilon_2 \cos^2\theta + \varepsilon_3 \sin^2\theta & (\varepsilon_2 - \varepsilon_3)\cos\theta \sin\theta \\ 0 & (\varepsilon_2 - \varepsilon_3)\cos\theta\sin\theta & \varepsilon_2 \sin^2\theta + \varepsilon_3 \cos^2\theta \end{pmatrix}. \tag{9}$$

Just as above fields can be expressed in terms of the two transversal components:

$$\begin{aligned} &E_1 = \frac{\beta H}{\varepsilon_1}, \quad E_2 = E, \quad E_3 = \frac{\mathrm{i}H' - \varepsilon_{32}E}{\varepsilon_{33}}, \\ &H_1 = -\beta E, \quad H_2 = H, \quad H_3 = -\mathrm{i}E'. \end{aligned} \tag{10}$$

E and H must obey the following system of coupled second-order differential equations:

$$\begin{aligned} &E'' + \left(\varepsilon_{22} - \frac{\varepsilon_{23}\varepsilon_{32}}{\varepsilon_{33}} \right) E + \mathrm{i}\frac{\varepsilon_{23}H'}{\varepsilon_{33}} = \beta^2 E, \\ &\varepsilon_1 \left(\frac{H'}{\varepsilon_{33}} \right)' + \varepsilon_1 H + \mathrm{i}\varepsilon_1 \left(\frac{\varepsilon_{32}E}{\varepsilon_{33}} \right)' = \beta^2 H. \end{aligned} \tag{11}$$

In the cover region the permittivities are constant, and in order not to obscure the discussion we assume optical isotropy,

$$\varepsilon_{jk}(x) = \varepsilon_{\mathrm{cov}} \delta_{jk} \quad \text{for} \quad x < 0. \tag{12}$$

The non-exploding solutions of (11) in $x < 0$ are

$$E(x) = E_0 e^{\kappa x}, \quad H(x) = H_0 e^{\kappa x} \quad \text{where} \quad \kappa = \sqrt{\beta^2 - \varepsilon_{\mathrm{cov}}}. \tag{13}$$

Since E, E', H, and $(H' + \mathrm{i}\varepsilon_{32}E)/\varepsilon_{33}$ are to be continuous we have the following initial conditions at the substrate side of the waveguide surface:

$$\begin{aligned} &E(0) = E_0, \quad E'(0) = \kappa E_0, \\ &H(0) = H_0, \quad H'(0) = -\mathrm{i}\varepsilon_{32}(0)E_0 + \kappa \frac{\varepsilon_{33}(0)}{\varepsilon_{\mathrm{cov}}} H_0. \end{aligned} \tag{14}$$

β in (11) is the propagation constant of a guided mode if a pair of amplitudes E_0, H_0 can be chosen such that the initial condition (14) and the coupled-mode equations (11) produce fields E, H vanishing with $x \to +\infty$.

A position $\xi > 0$ is called a node if there are amplitudes E_0 and H_0 for which $E(\xi) = H(\xi) = 0$. The nodes clearly depend on the parameter β in (11). They are labelled in increasing order, $0 < \xi_0(\beta) < \xi_1(\beta) < \dots$. Note that the differential equations (11) for $x > 0$ as well as the corresponding initial conditions (14) depend analytically on β (we stay well away from $\varepsilon_{\mathrm{cov}}$). By standard theorems for systems of ordinary linear differential equations the solutions then depend likewise analytically on such parameters. We conclude that $\beta \mapsto \xi_m(\beta)$ are continuous functions, and $\xi_m(\beta_m) = \infty$ determines the propagation constants β_m of guided modes.

We will show in the next section that $\beta \mapsto \xi_m(\beta)$ are strictly increasing functions. These nodal properties – upon which our bisection algorithm is based – cannot be read off directly from the differential equations. We have to resort to Hilbert space methods to prove them.

2. Hilbert Space Formulation

In this section a field $\phi = \{E, H\}$ is described by two square integrable complex valued functions E and H defined on the real axis. The scalar product of two fields ϕ and $\tilde{\phi}$ is defined by

$$(\phi, \tilde{\phi}) = \int dx E^* \tilde{E} + \int \frac{dx}{\varepsilon_1} H^* \tilde{H}. \tag{15}$$

This definition is motivated by demanding that the energy flux per unit lateral waveguide extension should be finite,

$$\begin{aligned} \int dx S_z &= \int dx (E_1^* H_2 - E_2^* H_1) \\ &= \beta \int dx \left(|E|^2 + \frac{|H|^2}{\varepsilon_1} \right) < \infty. \end{aligned} \tag{16}$$

The Hilbert space $\mathscr{H}_\xi$ is equipped with the above scalar product. It contains all fields vanishing for $x > \xi$ and having a finite norm, $\|\phi\|^2 = (\phi, \phi) < \infty$.

$\mathscr{D}_\xi \subset \mathscr{H}_\xi$ contains all fields $\phi = \{E, H\}$ which

1) are twice continuously differentiable in $0 < x < \xi$,
2) are twice continuously differentiable in $x < 0$,
3) are tied together by E, E', H, and $(H' + i\varepsilon_{32}E)/\varepsilon_{33}$ being continuous at $x = 0$,
4) vanish at $x = \xi$.

We define the operator M_ξ on $\mathscr{D}_\xi$ by the left-hand side of (11). The first line defines the E-component of $M_\xi\phi$, the second line the H-component. Permittivities are either constant (for $x < 0$) or smoothly varying (i.e. at least continuously differentiable for $x > 0$). Hence M_ξ is well-defined on $\mathscr{D}_\xi$.

The M_ξ are symmetric operators. Besides $\varepsilon_{jk} = \varepsilon_{kj}^*$ the continuity properties at $x = 0$ of $\mathscr{D}_\xi$ are required as well as $E = H = 0$ at $x = \xi$ and $x = -\infty$. With M_ξ we associate a quadratic form μ_ξ by

$$\mu_\xi(\phi) = (\phi, M_\xi\phi) = -\int dx|E'|^2 + \int dx\varepsilon_{22}|E|^2 - \int \frac{dx}{\varepsilon_{33}}|H' + i\varepsilon_{32}E|^2 + \int dx|H|^2 . \tag{17}$$

This form is defined on $\mathscr{D}_\xi$.

Let $\varepsilon_{\max}$ be the maximum of the two permittivity profiles $\varepsilon_{22}(x)$ and $\varepsilon_1(x)$. From (17) we deduce $\mu_\xi(\phi) \leqq \varepsilon_{\max}\|\phi\|^2$. We conclude that $\varepsilon_{\max}$ is an upper bound to the form μ_ξ as well as to the operator M_ξ.

M_ξ is a densely defined symmetric operator bounded from above, therefore the associated quadratic form is closable [8]. We denote the closure by μ_ξ^C, defined on $\mathscr{D}_\xi^C \subset \mathscr{H}_\xi$. μ_ξ^C is the quadratic form associated with a certain self-adjoint operator M_ξ^F, the so-called Friedrichs extension of M_ξ. Its domain of definition $\mathscr{D}_\xi^F \subset \mathscr{H}_\xi$ is larger than the original domain and smaller than the closed form domain, $\mathscr{D}_\xi \subset \mathscr{D}_\xi^F \subset \mathscr{D}_\xi^C$.

The eigenvalues of the Friedrichs extension can be calculated from its associated form by the minimax principle [9]. For $m = 0, 1, \ldots$ we define

$$\Lambda_{\xi,m} = \sup_{\substack{S \subset \mathscr{D}_\xi^C \\ \dim S = m}} \ \inf_{\substack{\phi \in S \\ \|\phi\| = 1}} \mu_\xi^C(\phi) . \tag{18}$$

This means: find the infimum of the form in an m-dimensional subspace, and take the supremum over all such subspaces. $\Lambda_{\xi,m}$ are those eigenvalues of M_ξ^F which are above the continuous part of its spectrum. They are arranged in decreasing order, multiple eigenvalues occur repeatedly.

For $\xi < \infty$ the continuous spectrum consists of $\Lambda \leqq \varepsilon_{\text{cov}}$. For $\xi = \infty$, i.e. if the support of fields is not restricted, the continuous spectrum is made up of $\Lambda \leqq \varepsilon_{\max}^\infty$. Either $\varepsilon_1(\infty)$ or $1/(\varepsilon^{-1})_{22}(\infty)$ determine the onset of leakage in this case, and $\varepsilon_{\max}^\infty$ is the larger of the two. These properties may be read off from (17) when inserting trial functions of very long wavelength. (18) yields all eigenvalues above ε_{cov}, but only those above $\varepsilon_{\max}^\infty$ are of interest here. We will prove now that the eigenvalues increase with the support.

Assume $\xi \leqq \eta$. Since the fields for which μ_ξ^C is defined are absolutely continuous we conclude $\mathscr{D}_\xi^C \subset \mathscr{D}_\eta^C$. Note that $\mu_\xi^C(\phi) = \mu_\eta^C(\phi)$ for $\phi \in \mathscr{D}_\xi^C$. Therefore

$$\Lambda_{\xi,m} = \sup_{\substack{S \subset \mathscr{D}_\xi^C \\ \dim S = m}} \ \inf_{\substack{\phi \in S \\ \|\phi\| = 1}} \mu_\eta^C(\phi) \leqq \Lambda_{\eta,m} \tag{19}$$

holds which means that $\xi \mapsto \Lambda_{\xi,m}$ is an increasing function.

We did not – and need not – show that all eigenvalues of the Friedrichs extension are also eigenvalues of the original mode operator. For our purpose it is sufficient to know that each eigenvalue β_m^2 of M_ξ is also an eigenvalue of M_ξ^F. Hence β_m and ξ grow simultaneously.

Since $\xi \mapsto \beta_m(\xi)$ increases there is an inverse function $\beta \mapsto \xi_m(\beta)$. The former function may jump at certain points, and the inverse function then would be constant within a certain interval. This, however, is impossible since $\xi_m(\beta)$ depends analytically on β. We conclude that it is strictly increasing.

3. Bisection Algorithm

The second-order equations (11) allow for rapid identification with symmetric operators. From a numerical point of view the first-order equations (4) are better suited. We specialize to the permittivity tensor (9) because nodal properties could be established for $\varepsilon_{12} = \varepsilon_{13} = 0$ only. Moreover, if $\varepsilon_{23} = \varepsilon_{32}$ is real we get away with real-valued functions.

Let us identify $y_1 \ldots y_4$ with E_2, E_3, iH_2, and iH_3, respectively. The following differential equations

$$y_1' = y_4 , \quad y_2' = \left(\frac{\beta^2}{\varepsilon_1} - 1\right) y_3 , \quad y_3' = \varepsilon_{23}y_1 + \varepsilon_{33}y_2 , \quad y_4' = (\beta^2 - \varepsilon_{22})y_1 - \varepsilon_{23}y_2 \tag{20}$$

must be solved. With

$$y_1(0) = 1, \quad y_2(0) = 0, \quad y_3(0) = 0, \quad y_4(0) = \kappa \tag{21}$$

the mode vanishes at $x \to -\infty$ and is TE polarized in the cover region. Recall that κ stands for $\sqrt{\beta^2 - \varepsilon_{\text{cov}}}$, where ε_{cov} is the cover permittivity.

We duplicate the system for fields which are TM polarized in the cover region. $y_5 \ldots y_8$ are likewise identified with $E_2 \ldots iH_3$. They obey the same differential equations:

$$y_5' = y_8 , \quad y_6' = \left(\frac{\beta^2}{\varepsilon_1} - 1\right) y_7 , \quad y_7' = \varepsilon_{23}y_5 + \varepsilon_{33}y_6 , \quad y_8' = (\beta^2 - \varepsilon_{22})y_5 - \varepsilon_{23}y_6 . \tag{22}$$

The initial conditions, however, are different:

$$y_5(0)=0, \quad y_6(0)=\frac{\kappa}{\varepsilon_{\text{cov}}}, \quad y_7(0)=1, \quad y_8(0)=0. \tag{23}$$

We integrate the eight first-order differential equations (20, 22) by a Runge-Kutta procedure starting with initial values (21, 23). The TE solution $y_1 \dots y_4$ and the TM solution $y_5 \dots y_8$ must be superimposed with amplitudes A_{TE} and A_{TM} respectively to obtain the generally polarized solution. The transversal electric and magnetic fields at a certain position x in the substrate region are

$$\begin{aligned} E(x) &= y_1(x)A_{\text{TE}} + y_5(x)A_{\text{TM}}, \\ \mathrm{i}H(x) &= y_3(x)A_{\text{TE}} + y_7(x)A_{\text{TM}}. \end{aligned} \tag{24}$$

ξ is a node if, for given β, A_{TE} and A_{TM} can be chosen such that $E(\xi)=H(\xi)=0$. A sufficient and necessary condition for this is that the determinant

$$\Delta_\beta(x) = y_1(x)y_7(x) - y_3(x)y_5(x) \tag{25}$$

vanish at $x=\xi$.

Let us now formulate the bisection algorithm. With every iteration the interval is halved within which β_m must be contained. $\beta_{\text{low}}=\varepsilon_{\max}^{\infty}$ and $\beta_{\text{high}}=\varepsilon_{\max}$ is a safe guess. Recall that $\varepsilon_{\max}$ is an ξ-independent upper bound for the spectrum and $\varepsilon_{\max}^{\infty}$ is the upper limit of the continuous spectrum for $\xi=\infty$. If β_m is already known it may serve as β_{high} for β_{m+1}.

And this is the program for the m^{th} mode:

1) establish an interval $[\beta_{\text{low}}, \beta_{\text{high}}]$ within which to search for β_m,
2) reset the node counter to 0 and try $\beta := \frac{1}{2}(\beta_{\text{high}} + \beta_{\text{low}})$,
3) begin at $x=0$ with (21, 23),
4) integrate (20, 22) step by step,
5) calculate the determinant Δ according to (25),
6) if Δ has crossed the zero line increase the node counter,
7) if m nodes have been found – stop the integration procedure,
8) if a field gets too large – stop the integration procedure,
9) if m nodes have been found set $\beta_{\text{low}} := \beta$ else set $\beta_{\text{high}} := \beta$,
10) repeat the procedure at step 2) until $|\beta_{\text{high}} - \beta_{\text{low}}|$ is sufficiently small.

The most recently found matrix

$$\begin{pmatrix} y_1(\xi) & y_5(\xi) \\ y_3(\xi) & y_7(\xi) \end{pmatrix} \tag{26}$$

allows to determine the amplitudes A_{TE} and A_{TM} such that (24) describes the hybrid mode field distributions.

4. Concluding Remarks

The program we have just described is simple and efficient. With a personal computer it takes at most a few minutes to calculate all hybrid modes for a typical Ti:$LiNbO_3$ waveguide. The Runge-Kutta four-point integration procedure is convenient, but any other method will do as well.

A birefringent cover would cause no problem. Equation (13) has to be replaced by the two appropriate plane wave solutions. Only the initial conditions (21, 23) will change.

If the permittivity tensor becomes non-diagonal because it is rotated it will be real and symmetric. This has been assumed when writing down (20, 22). The discussion in Sect. 2, however, assumes $\varepsilon_{32}=\varepsilon_{23}^{*}$ only. The nodal properties are valid for gyroscopic media as well.

The waveguide normal must be an optical symmetry axis in the substrate. For the general permittivity tensor we could not yet rewrite (4) into an appropriate problem for eigenvalues which increase with the support of field.

Although the operators M_ξ^F and M_∞^F describe leaky modes as well we cannot apply the bisection algorithm in a straightforward way. This method allows to search in a one-dimensional manifold only.

Acknowledgement. This work was performed within the program of SFB 225. We gratefully acknowledge financial support from 'Deutsche Forschungsgemeinschaft.'

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