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Mode Tracking for Parametrized Eigenvalue Problems in Computational Electromagnetics

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***Abstract*—An algorithm to perform a mode tracking for parameter dependent eigenvalue problems in computational electromagnetics is presented. It is based on a Taylor expansion using the derivatives of the eigenvalue and the eigenvector and allows distinguishing between intersection and touching points in the eigenvalue curves. The method is applied to discretizations with both the finite integration technique (FIT) and the finite element method (FEM), leading to simple and generalized eigenvalue problems, respectively. The applications include the calculation of the Brillouin diagram for a periodic structure and the variation of a material parameter in a filter structure.**

***Keywords*—Eigenvalue Derivatives, Finite Element Method, Finite Integration Technique, Mode Tracking, Parametrized Eigenvalue Problems.**

I. Introduction

Within the last decades a number of efficient algorithms for the solution of eigenvalue problems (EVP) in electromagnetic field simulation have been proposed. A particular class are EVP with a dependency of one or more parameters such as material constants, geometric properties, or the phase shift of Floquet modes [1] in periodic structures. In most cases, we can assume a continuous relation between the parameter and the eigenmodes, and it is desirable to reflect this fact also in the solution approach, i.e., to provide algorithms which are able to track an eigenvalue along the variation of the parameter within a certain range. As a special challenge for such a mode tracking method it should be able to follow the eigenvalue curves also in the vicinity of intersection and touching points, where the curves of two eigensolutions come close to each other.

In this paper, we present a mode tracking algorithm for parametrized EVP which uses the sensitivity of eigenvalues *and eigenvectors* w.r.t. the parameter, described by their derivatives. It is applied to two generic types of applications given by a traveling wave tube with periodic boundary conditions and a dielectric filter with a sweep of the permittivity in a specific part of the structure.

A first efficient method for the calculation of eigenvalue and eigenvector derivatives has been published by Nelson in 1976 [2] and was extended for non-simple eigenvalues by Dailey in 1989 [3]. A simple sensitivity analysis of a waveguide has been calculated in [4]. In [5] it was shown how to extend this method to higher-order derivatives and it was applied to periodic structures, where the parameter is defined by the phase advance between two boundaries. A related mode tracking technique for the calculation of band structures in photonic crystals has been presented in [6].

The new mode tracking algorithm presented in this paper combines all these ideas and can be applied to a general parameter dependency of an EVP. It is based on a point by point sampling using Taylor expansions, and a correlation factor is introduced to distinguish the different eigenmodes near intersection and touching points. To broaden the application range of the method, an extension for generalized eigenvalue problems (GEVP) is shown.

The paper is organized as follows: In Sect. II a short overview of the basic formulas and an extension for the eigenvalue and eigenvector derivatives of GEVP is given, followed by the introduction of the mode tracking algorithm in Sect. III. In Sect. IV we introduce the physical background of our eigenvalue formulations and discuss the numerical results for two different applications: The Brillouin diagram of a periodic structure is based on a model using the finite integration technique (FIT), leading to mode tracking for a simple EVP. In the second example the eigenmodes in a dielectric filter are calculated for a variation of some permittivity values. Here, we use a finite element (FEM) model, resulting in the mode tracking algorithm for a GEVP. Finally, a conclusion and outlook for further improvements are given in Sect. V.

II. Eigenvalue Derivatives

A. Simple Eigenvalue Problems

We start with the left and right EVP,

$$\mathbf{y}^H(\mathbf{A}-\lambda\mathbf{I})=0, \qquad (\mathbf{A}-\lambda\mathbf{I})\,\mathbf{x}=0, \tag{1}$$

where $\mathbf{I}$ is the identity matrix, and the matrix $\mathbf{A}$ as well as the eigensolution $\{\mathbf{x},\mathbf{y}^H,\lambda\}$ depend on the parameter p. The eigenvectors fulfill the relation $\mathbf{y}^H\mathbf{x}=1$. Differentiating n times w.r.t. the parameter p and applying some algebraic

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transformations yields the n-th order eigenvalue derivative (denoted by $.^{(n)}$, for details of this derivation see [5]):

$$\lambda^{(n)} = \mathbf{y}^H \mathbf{A}^{(n)} \mathbf{x} + \sum_{k=1}^{n-1} \binom{n}{k} \mathbf{y}^H \left(\mathbf{A}^{(n-k)} - \lambda^{(n-k)} \mathbf{I} \right) \mathbf{x}^{(k)}. \quad (2)$$

Note, that for the n-th order derivative in (2) all previous derivatives of the eigenvalue, eigenvector and system matrix are required. However, once this information is available, the formula can be evaluated with very little effort just by matrix vector multiplications.

The n-th order eigenvector derivative is given by a similar formula:

$$(\mathbf{A} - \lambda \mathbf{I}) \mathbf{x}^{(n)} = - \sum_{k=0}^{n-1} \binom{n}{k} \left(\mathbf{A}^{(n-k)} - \lambda^{(n-k)} \mathbf{I} \right) \mathbf{x}^{(k)}. \quad (3)$$

Here, a linear system with rank defect has to be solved, appropriate techniques are given, e.g., in [2], [3]. Since the matrix to be inverted in (3) remains the same for each n, a matrix decomposition technique is efficient if higher order derivatives are required. Further, such techniques can be combined with model order reduction for a faster calculation as described in [5].

B. Generalized Eigenvalue Problems

To extend the formulas above to a GEVP we start again with the eigensolution $\{\mathbf{x}, \mathbf{y}^H, \lambda\}$ of the left and right GEVP,

$$\mathbf{y}^H (\mathbf{A} - \lambda \mathbf{B}) = 0, \qquad (\mathbf{A} - \lambda \mathbf{B}) \mathbf{x} = 0, \quad (4)$$

respectively, with $\mathbf{y}^H \mathbf{B} \mathbf{x} = 1$. The eigensolution as well as both system matrices $\mathbf{A}$ and $\mathbf{B}$ might have a dependency of the parameter p. Differentiating the GEVP w.r.t. this parameter using the chain rule leads to some additional terms compared to the case of a simple EVP. Still, the approach is very similar to the one for simple EVP in [5]. The right GEVP is differentiated n times, and by reordering the terms we obtain the formula for the eigenvector derivative as:

$$(\mathbf{A} - \lambda \mathbf{B}) \mathbf{x}^{(n)} = - \sum_{k=1}^{n} \binom{n}{k} \left(\mathbf{A}^{(k)} - \sum_{j=0}^{k} \binom{k}{j} \lambda^{(j)} \mathbf{B}^{(k-j)} \right) \mathbf{x}^{(n-k)}. \quad (5)$$

Multiplying from the left with the left eigenvector y^H the highest order derivative of the eigenvector vanishes, and by reordering the terms we find the derivative of the eigenvalue:

$$\lambda^{(n)} = \sum_{k=1}^{n-1} \binom{n}{k} \left(\mathbf{y}^H \mathbf{A}^{(k)} \mathbf{x}^{(n-k)} - \left[\sum_{j=0}^{k-1} \binom{k}{j} \lambda^{(j)} \mathbf{y}^H \mathbf{B}^{(k-j)} \mathbf{x}^{(n-k)} + \lambda^{(k)} \mathbf{y}^H \mathbf{B} \mathbf{x}^{(n-k)} \right] \right) + \mathbf{y}^H \mathbf{A}^{(n)} \mathbf{x} - \sum_{j=0}^{n-1} \binom{n}{j} \lambda^{(j)} \mathbf{y}^H \mathbf{B}^{(n-j)} \mathbf{x}. \quad (6)$$

Again, this long formula only contains matrix vector multiplications and can therefore be calculated with little effort. As a cross check, (6) simplifies to (2) if $\mathbf{B} = \mathbf{I}$ and $\mathbf{B}^{(i)} = 0$ $(\forall i > 0)$ are chosen as in the case of a simple EVP. The same holds for (5) compared to (3). Moreover, and analogously to the simple EVP in (3), the matrix to be inverted in (5) remains the same for each order n, allowing similar techniques for an efficient implementation as described above.

C. Polynomial and Nonlinear Eigenvalue Problems

With its extension to GEVP, there is also the possibility to apply this algorithm to polynomial eigenvalue problems (PEVP), where higher powers of the eigenvalue λ appear in the formulation. Such PEVP (quadratic, cubic, etc.) arise, e.g., from discrete models including dispersive materials (with rational functions in ω for the permittivity) or a perfectly matched layer (PML) boundary condition in its classical form. A couple of such problems are described in [7]. In principle, a PEVP can always be transformed into a GEVP with larger dimension, which allows its solution using the presented mode tracking algorithm. However, more efficient approaches without doubling the matrix dimensions may exist.

The next step of generalization are *nonlinear* EVP with an arbitrary, non-polynomial dependency of the eigenvalue in the formulation. Such problems appear, e.g., for models with a special radiation boundary condition for waveguide problems and have been briefly discussed in [8]. Of course a general expression for the eigenvalue derivative of such formulations is not available. However, they may be tackled using linearization approaches in an expansion point with a limited range of validity, which again makes the method presented here a candidate for mode tracking. However, the general properties of such non-linear EVP can be quite different from the standard case, and thus this scenario still needs to be tested.

III. Mode Tracking Algorithm

The mode tracking algorithm can best be explained by Fig. 1. First a starting point is chosen at an arbitrary $p \in [p_{min}, p_{max}]$. In this point, the EVP is solved and the mode k for the tracking is selected. (For simplicity, the index k for the chosen mode is omitted in most of the following formulas.)

As an initialization step, the derivatives of the system matrices $\mathbf{A}^{(i)}, \mathbf{B}^{(i)}$ of the EVP as well as the derivatives of the eigensolution $\{\mathbf{x}^{(i)}, \lambda^{(i)}\}$ are required. Note that for some simulation models the matrix derivatives can be computed analytically (such as in our first example in Fig. 2, see below). If no analytical formulas are available, some additional computational effort is necessary to calculate the matrix derivatives numerically, using, e.g., a simple finite difference approach (such as for our second example, Fig. 4). Once the derivatives of the system matrices are available, formulas (2) and (3) for the simple EVP, or (6) and (5) for the GEVP, respectively, can be evaluated.

In the next step, a step width Δp is determined, depending on the derivatives of the eigenvalue and eigenvector. The smaller the derivatives are, the larger the step width can be

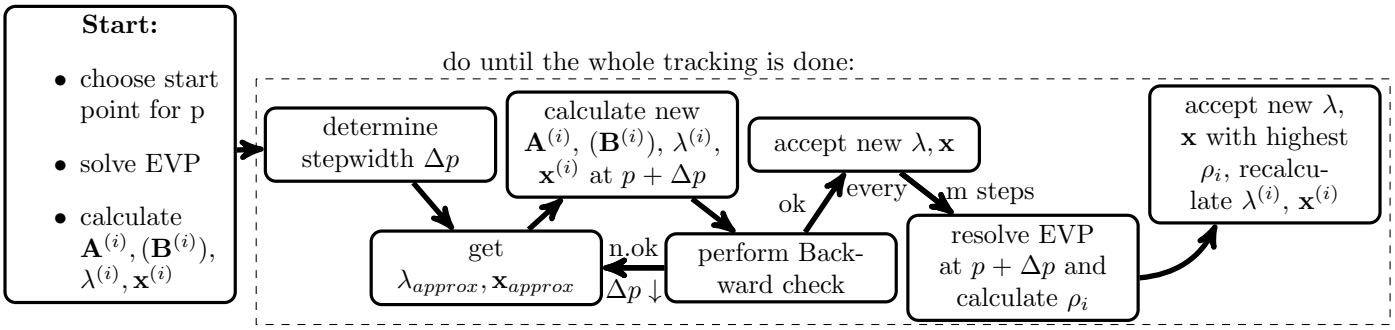

Fig. 1. Flowchart of the mode tracking algorithm.

chosen and vice versa. This step width control is important to prevent errors due to a too high step width at intersection or touching points, where the eigenvector derivatives are typically huge. On the other hand, a too small step width can considerably increase the numerical effort.

After the step width Δp has been chosen, approximations λ_{approx} of the eigenvalue and $\mathbf{x}_{approx}$ of the eigenvector at the point $p + \Delta p$ are computed, using the eigensolutions at p and the Taylor expansions:

$$\lambda_{approx} = f\left(p, \lambda, ..., \frac{\partial^n}{\partial p^n}\lambda\right), \tag{7}$$

$$\mathbf{x}_{approx} = f\left(p, \mathbf{x}, ..., \frac{\partial^n}{\partial p^n}\mathbf{x}\right). \tag{8}$$

Using these approximations, the new derivatives of this eigenpair at $p + \Delta p$ can be calculated. To do so, the new matrix derivatives at $p + \Delta p$ have to be computed first as explained above.

To control the quality of the approximations involved, a backward check is performed (see, e.g., [6]): A Taylor expansion at the new expansion point $p + \Delta p$ is evaluated for the previous point p using the new derivatives at $p + \Delta p$. The deviation between the previous eigenvalue $\lambda(p)$ and the backward approximated eigenvalue $\lambda_{approx,backward}$ from $p+\Delta p$ has to be smaller than some predefined tolerance. When the difference is small enough, the eigenpair approximation as well as their derivatives are considered to be correct, and the point $p + \Delta p$ is used as a new starting point p to continue the tracking procedure. If the backward check for the eigenpair approximation (and their derivatives) fails, i.e., the backward approximated eigenvalue is not close to the original eigenvalue, the step width Δp needs to be corrected. Using a new, smaller step width, the previous steps are repeated until the backward check succeeds.

Up to this point, the algorithm works in a purely recursive manner, and small deviations in every step may sum up to an error which at some point can no longer be tolerated. A suitable indicator to check the quality of the solutions is the residual of the eigenpair at each p. Since no corrector equation is not used here to decrease this error, every couple of steps of this algorithm the EVP has to be solved newly to eliminate this error. Here, the main challenge is to identify the proper eigenmode from this new solution. At some points within the parameter range, a couple of eigenvalues can be very close to each other or may even coincide. To identify the correct eigenpair a correlation factor,

$$\rho_k = \frac{\mathbf{x}_k^H \mathbf{x}_{approx}}{||\mathbf{x}_k||\,||\mathbf{x}_{approx}||}, \tag{9}$$

is introduced as the normalized scalar product between the approximated eigenvector and the eigenvectors from the recalculated EVP. This factor is computed for all candidates from the recalculated solution of the EVP, and the eigenmode with the highest ρ_k is accepted as the proper mode. The new eigenpair is also used as a new starting point for the tracking procedure, and the corresponding derivatives are calculated. In this way, the recursive error is eliminated every couple of steps.

This tracking procedure is repeated until the end of the interval of parameters p is reached. This completes the mode tracking, and solutions for each calculated point on the eigenvalue curve are available. In contrast to the standard procedure with a simple parameter sweep, the number of full EVP solutions can be considerably reduced.

IV. Numerical Results

A. Traveling Wave Tube (TWT)

The first example to test this algorithm is a so-called traveling wave tube (TWT), taken from the library of application examples of the commercial tool CST Microwave Studio [9], see Fig. 2.

The discrete model consists of a small longitudinal section of this TWT, and periodic boundary conditions are used at the front and the back plane. A predefined phase lead for the tangential fields at these boundaries defines the eigenmodes of the model to be 'macroscopic' waves, and the eigenvalues their (squared) angular frequency. Varying this phase angle between 0 and 180 degrees, the correlation of the phase advance and the eigenfrequency defines the dispersion diagram (or Brillouin diagram) of each mode. Additionally, the electric fields (the eigenvectors) are of interest, e.g., to analyze their interaction with charged particles within the TWT.

The standard procedure to compute the Brillouin diagram is to solve the EVP many times for a number of phase angles.

Here, however, we interpret the phase angle as the parameter of a parametrized EVP and apply our mode tracking algorithm.

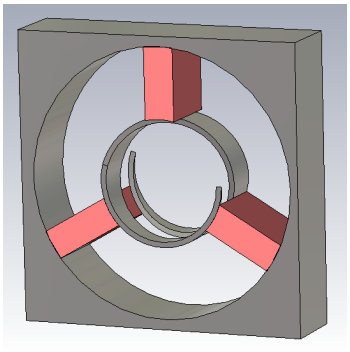

Fig. 2. Simulation setup with periodic boundaries at the front and back plane.

The model is discretized using the finite integration technique (FIT, [1]) on a Cartesian computational grid. The state variables in the FIT are the grid voltages $\widehat{\mathbf{e}}$ and $\widehat{h}$, defined as the line integrals of the electric field and the magnetic fields along the edges of the primary and the dual Grid $G, \tilde{G}$, respectively. Using these definitions, FIT transforms Maxwell's curl equations in frequency domain (for linear, isotropic and non-dispersive materials, and without currents and space charges):

$$\operatorname{curl} \mathbf{E} = -j\omega\mu\mathbf{H}, \qquad \operatorname{curl} \mathbf{H} = j\omega\varepsilon\mathbf{E}, \tag{10}$$

(with ω the angular frequency, $\mathbf{E}, \mathbf{H}$ the electric and magnetic fields, ε, μ the permittivity and the permeability, and j the imaginary unit) into matrix-vector equations, the so-called Maxwell's Grid Equations:

$$\mathbf{C}\widehat{\mathbf{e}} = -j\omega\mathbf{M}_\mu\widehat{\mathbf{h}}, \qquad \mathbf{C}^T\widehat{\mathbf{h}} = j\omega\mathbf{M}_\varepsilon\widehat{\mathbf{e}}, \tag{11}$$

Here, $\mathbf{C}$ denotes the discrete curl operator, and $\mathbf{M}_\varepsilon$ and $\mathbf{M}_\mu$ are the discrete material matrices. For a Cartesian grid with n_p grid points the discrete field vectors have approximately $3n_p$ components, and the dimension of the matrices is approximately $3n_p \times 3n_p$. Eliminating $\widehat{\mathbf{h}}$ in equations (11) yields the discrete electromagnetic eigenvalue problem:

$$(\mathbf{C}^T\mathbf{M}_\mu^{-1}\mathbf{C} - \omega^2\mathbf{M}_\varepsilon)\widehat{\mathbf{e}} = 0. \tag{12}$$

It's a unique property of the FIT that the material matrices $\mathbf{M}_\varepsilon$ and $\mathbf{M}_\mu$ are diagonal and can be easily inverted. Thus, (12) can be transformed into the simple EVP:

$$(\mathbf{M}_\varepsilon^{-1}\mathbf{C}^T\mathbf{M}_\mu^{-1}\mathbf{C} - \omega^2\mathbf{I})\widehat{\mathbf{e}} = 0. \tag{13}$$

The periodic phase shift between the tangential fields at the front and the back plane is described by the Floquet condition: It maps the electric field from one boundary, $\widehat{\mathbf{e}}_1$, to those at the other one, $\widehat{\mathbf{e}}_2$, multiplied by the phase shift: $\widehat{\mathbf{e}}_1 = \widehat{\mathbf{e}}_2 \exp(j\varphi)$. With this relation, the tangential electric components at one side of the mesh are no longer independent degrees of freedom and can be eliminated from the formulation. This leads to a reduced vector $\widehat{\mathbf{e}}_{red}$ with a reduced dimension.

The phase shift — the parameter p of the EVP — is formally included into the matrix formulation using a sparse matrix $\mathbf{L}_\varphi(p)$ as described in [7] or [10]. Additionally, the permittivity matrix has to be slightly modified in its dimension as well as in its values at the boundary. This leads to the parametrized EVP:

$$\Big(\underbrace{\mathbf{M}_{\varepsilon,per}^{-1}\mathbf{L}_\varphi^H(p)\mathbf{C}^T\mathbf{M}_\mu^{-1}\mathbf{C}\mathbf{L}_\varphi(p)}_{=\mathbf{A}_{cc}(p)} - \omega^2\mathbf{I}\Big)\,\widehat{\mathbf{e}}_{red} = 0, \tag{14}$$

which can be tackled by our mode tracking algorithm. Note that the parameter dependency of this formulation is concentrated in the $\mathbf{L}_\varphi$ matrices, which makes it easy to compute the matrix derivative analytically.

The example shown in Fig. 2 is discretized using $n_p = 46.787$ grid points, resulting in approximately 140.000 degrees of freedom in the eigenvalue equation. The geometric modeling is performed within the CST software, and the mesh and matrix data are imported into Matlab [11], where the periodic boundaries and the mode tracking have been implemented. The problem size of this model is still quite small, and all computations can be performed on a standard computer. (CPU times are not reported here since the implementation has not been optimized so far.)

The simulation results are shown in Fig. 3. First some modes around a target frequency are calculated using Matlab's standard eigenvalue solver, and a mode in the middle of this part of the spectrum is chosen for the mode tracking algorithm. Additionally, the plot shows some more eigenvalues which are close to the chosen mode, and of course there exist a large number of further eigenvalues inside the spectrum. They do not affect the analysis of the targeted eigenmode and are not plotted to ensure the readability of the figure. The reference curves (in gray) in the figure are obtained by a multiple solution of the EVP for parameter values covering the phase shift between 0 and 180 degrees. The red curve is calculated from the mode tracking scheme as described above. As a first result we can state that both solutions agree very well although most of the results of the mode tracking scheme originate from Taylor expansions rather than from full EVP solutions.

A zoom of an interesting section of the dispersion diagram is shown in the bottom right corner of Fig. 3. As mentioned previously, the algorithm detects an intersection as well as a touching point and properly tracks the eigenvalue through these challenging domains. Note that such a tracking is not available from the reference solution: The standard strategy to multiply solve the EVP fails to distinguish between these intersection or touching points, although the parameter step width is very small and a correlation factor between two solutions is used. The reason is that even when the two solutions of the EVP are close to each other and the changes in the eigenvalue are quite small, the changes in the eigenvector become very high at intersection and touching points, as well as their derivatives. As a consequence, the eigenvector

correlation between two solutions can become very unstable and unable to identify the correlation between the modes.

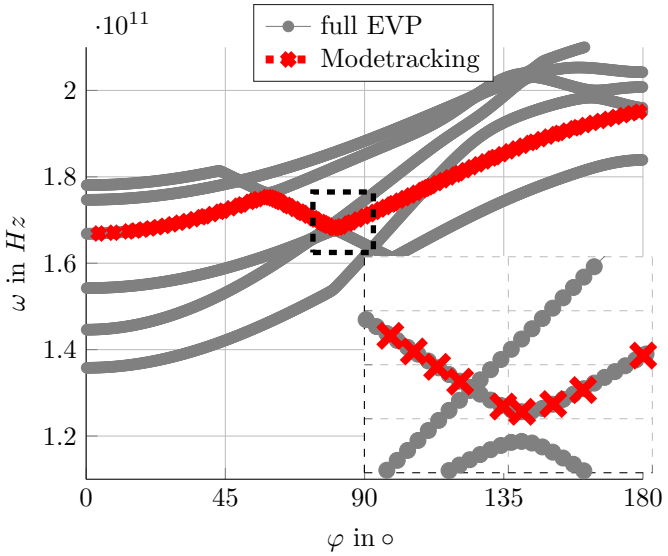

Fig. 3. Mode tracking of a chosen mode of the periodic structure within the spectrum with a zoom on the black marked section of interest.

The correlation factor ρ introduced in the previous section, however, does not show this weakness, since it does not rely on two nearby vector solutions calculated separately, but on the solution at one point and the approximation of this solution which is obtained from the previous one. This method is very robust in detecting the proper eigenmode.

B. Dielectric Filter

The second example is a dielectric filter which has been reported in many publications so far and may serve as a quasi-standard application for the simulation of highly-resonant microwave devices. Here we do not calculate the transfer behavior related to the two input/output ports, but only the relevant eigenmodes which are dominated by two dielectric rings with high permittivity. More details of the structure and all geometric dimensions are given in [12].

This example, as shown in Fig. 4, is modeled using the finite element method (FEM) on a tetrahedral mesh and first-order edge-elements $\mathbf{w}_i$. The parameter considered here is the permittivity of the ceramic resonator rings. To obtain a more challenging situation of the parameter dependency of the eigenmodes, including an intersection point, the investigated range was shifted from the original value $\varepsilon_r = 38$ to an interval around $\varepsilon_r = 57$.

The theory behind the finite element discretization is not repeated here and can be found, e.g., in [13]. The FEM model has $n_e = 130.872$ non-zero edge-elements, and the resulting EVP is a generalized one, reading:

$$\left(\mathbf{A} - \omega^2 \mathbf{B}\right)\ (E_i) = 0, \tag{15}$$

where the electric field $\mathbf{E}(\mathbf{r}) = \sum_i E_i \mathbf{w}_i(\mathbf{r})$ is represented by the degrees of freedom (E_i) with $i = 1 \ldots n_e$. The matrix $\mathbf{A}$ denotes the stiffness matrix and $\mathbf{B}$ the so-called mass matrix, respectively, with entries as reported in [13]. The main difference to the FIT formulation is that in FEM the matrix $\mathbf{B}$ holding the permittivity information is not a diagonal matrix and thus can not be efficiently inverted. Therefore the extended mode tracking variant for GEVP has to be used here.

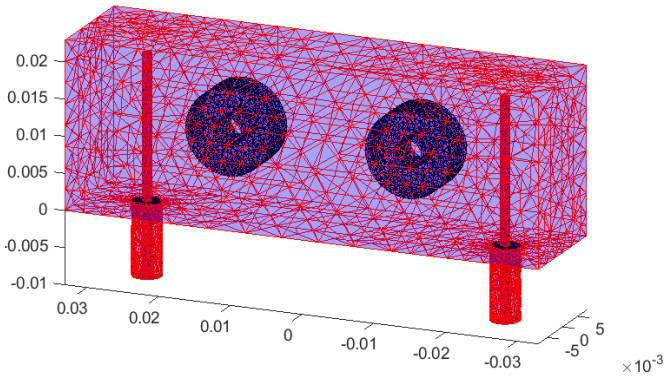

Fig. 4. Simulation setup of the dielectric filter, with different permittivity for the inner rings.

The derivatives of the matrix $\mathbf{A}$ and $\mathbf{B}$ are calculated numerically using a finite different (FD) approach. This results in a slightly increased computational effort compared to the case of matrix derivatives which are available analytically. Note, however, that the way these matrix derivatives are calculated does not play an important role in our mode tracking algorithm. Also, the algorithm is not limited to a specific kind of discretization technique.

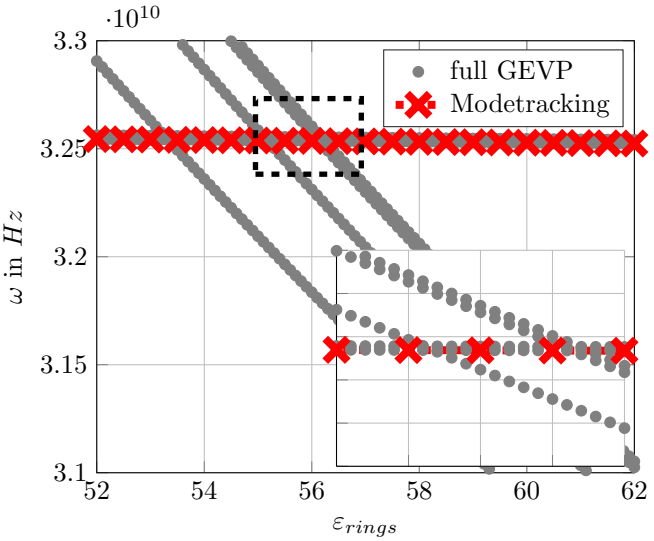

Fig. 5. Mode tracking of a chosen mode of the dielectric filter within the spectrum with a zoom on the black marked section of interest.

The results of the mode tracking algorithm for the dielectric filter are shown in Fig. 5. A mode with some candidates for intersection or touching points inside the parameter range is chosen for the analysis. As for the previous example, only a

small part of the eigenvalue spectrum is plotted for readability. Again, on the right bottom of Fig. 5 a zoom of the black dashed section is depicted. In contrast to the first example, the modes in the dielectric filter interact only weakly with each other due to the more separated geometric distribution of the corresponding fields. Thus, the eigenvector changes do not become as large as in the first example in the intersection points, and a larger step width can be chosen by the algorithm. Again, the intersection points are handled properly by the algorithm also in this case.

V. Conclusion and Outlook

A mode tracking algorithm for parametrized eigenvalue problems in computational electromagnetics has been presented. It can be used for simple as well as generalized EVP and thus be applied to discrete models from different discretization methods such as the finite integration technique or the finite element method.

A significant advantage of the new algorithm is its ability to handle intersection and touching points within eigenvalue curves without any additional post-processing, which is often necessary for comparable approaches. Furthermore, the presented algorithm is not limited to periodic structures with varying phase shift or changes in the permittivity, and it has been successfully tested with other parameter dependent problems like geometric variations. The presented formulas for generalized eigenvalue problems open the path to tackle also nonlinear EVP using a linearization as described in Sect. II-C. A next step could be to find a formulation for polynomial EVP without using linearization.

Finally, the method should also be easily extendable to mode tracking in EVP which depend on more than one parameter.

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