What optical fiber modes reveal: group velocity and effective index for external perturbations

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1. INTRODUCTION

Optical fibers represent one of the most successful photonic devices and guide light in a central core surrounded by a cladding. Particularly with respect to modal engineering, this cladding could be a homogeneous material, as in the case of step index and capillary fibers [1], or comprise complex structures, such as the periodic arrangements of holes or strands in microstructured fibers [2]. The guiding properties of both kinds of fibers are impacted by the constituent materials that comprise the core and cladding and react to changes of these materials. Due to the strong susceptibility of the core mode to changes of the refractive index, optical fibers represent one promising platform for bioanalytical or medical applications [3–6].

All of the mentioned applications demand optimizing the fiber structures via extensive numerical simulations, which can be time-consuming and may not be used for large-scale parameter sweeps. Here, the perturbation theory is known to be a suitable approach for such tasks, since it can significantly reduce the simulation time and complexity [9], thus providing a pathway toward design optimization. Optical perturbation theories based on the resonant states, also known as quasi-normal modes, are broadly used for optical resonators [10–12]. However, care has to be taken with respect to the normalization of unbound modes. These modes are leaky in the sense that they radiate part of their energy to the far field. Hence, their field distributions grow with distance to the resonator. In recent years, different approaches have been developed in order to normalize these modes correctly [13–16], resulting in accurate predictions for various refractive index sensors [9,17–19]. We have adapted the analytical normalization of Ref. [16] to fiber and leaky waveguide geometries [20], which allows for predicting changes of the effective index of bound and leaky fiber modes in the case of modifications of the refractive index with perturbation theory, as well as for describing the nonlinear pulse propagation of leaky modes [21]. Common to all of these perturbative approaches is that they deal exclusively with perturbations in the interior of the structure. This limitation is overcome for optical resonators in Ref. [22], where the resonance frequency shifts, and linewidth changes are predicted correctly for homogeneous and isotropic perturbations in the exterior.

More specifically, the infinite volume integral over perturbations in the exterior is replaced in Ref. [22] by an integral over the boundary of a finite volume. We adapt this approach to propagating modes in fiber geometries. An interesting fact is that for these modes, the wavelength is an input parameter to Maxwell’s equations similar to the refractive index, which, in turn, means that changes in wavelength can be treated as a perturbation. This allows for an exact prediction of the group velocity based on calculating the fiber modes and their field...
distributions at a single frequency, without having to repeatedly solve Maxwell’s equations for different wavelengths and approximating derivatives with respect to wavelengths by finite differences. Hence, we can predict the propagation constant for small changes in the wavelength, permittivity, and permeability (see Fig. 1), as long as the modification of Maxwell’s equations is homogeneous and isotropic in the exterior.

2. THEORY

In fiber geometries, the permittivity and permeability tensors, ε and μ, respectively, are translationally symmetric along one spatial direction, which we choose to be the z direction. Hence, we can apply the Fourier transformation

\[ \hat{f}(r_||; \beta) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dz f(r_||; z) e^{-i\beta z} , \]

with \( r_|| \) being the projection of \( r \) to the xy plane, and the hat denoting Fourier transformed quantities. Thus, Maxwell’s equations can be written in the frequency domain [time dependence exp(\(-i\omega t\)), Gaussian units] as

\[ \hat{\mathbf{M}}_{0}(r_||; \beta) \hat{F} = \hat{\mathbf{J}}(r_||) , \]

where

\[ \hat{\mathbf{M}}_{0}(r_||; \beta) = \left( \begin{array}{cc} k_0 \sigma & -\hat{\mathbf{V}}_{\beta} \times \\ -\hat{\mathbf{V}}_{\beta} \times & k_0 \mu \end{array} \right) , \quad \text{with} \quad \hat{\mathbf{V}}_{\beta} = \left( \frac{\partial_x}{i\beta}, \frac{\partial_y}{i\beta}, \frac{\partial_z}{i\beta} \right) . \]

![Fig. 1](image-url). Real part of the propagation constant \( \beta \) as a function of wavenumber \( k_0 \) for an unperturbed photonic crystal fiber (see schematic on the right) with permittivity \( \varepsilon \) and permeability \( \mu \) (green dashed–dotted line) and for a perturbed fiber with permittivity \( \varepsilon' \) and permeability \( \mu' \) (red solid line). Via our first-order perturbation theory, we can predict the change of the propagation constant \( \Delta \beta \) not only for small modifications \( \Delta \varepsilon \) and \( \Delta \mu \) of the permittivity and permeability, respectively, but also for wavenumber changes \( \Delta k_0 \). The radius of the inclusions in the photonic crystal fiber is 0.5 \( \mu \)m, and the pitch is 2.3 \( \mu \)m. The unperturbed fiber in the dispersion plot has a background refractive index of 1.47, while the perturbed fiber has a background refractive index of 1.44. The index of the inclusions (holes) is one.

Here, \( \hat{\mathbf{E}} \) is the electric field, \( \hat{\mathbf{H}} \) is the magnetic field, \( k_0 = \omega / c \) is the wavenumber, while \( \varepsilon = \varepsilon(r_||) \) and \( \mu = \mu(r_||) \) denote the permittivity and permeability tensors, respectively. Furthermore, \( \hat{\mathbf{J}} = -4\pi \hat{\mathbf{J}} / c \) is the source of the fields, where \( \hat{\mathbf{J}} \) is the electric current. Resonant states are solutions of Maxwell’s equations in the absence of source terms that satisfy outgoing boundary conditions in the transversal directions with complex propagation constants \( \beta_m \):

\[ \hat{\mathbf{M}}_0(r_||; \beta_m) \hat{F}_m = 0 . \]

We now introduce a perturbation in our system as a change in permittivity \( \varepsilon \rightarrow \varepsilon + \Delta \varepsilon \) or permeability \( \mu \rightarrow \mu + \Delta \mu \) or a change in wavenumber \( k_0 \rightarrow k_0 + \Delta k_0 \) that can be converted to a change in wavelength. We also introduce a factor \( \Lambda \) to turn the perturbation on and off. The new perturbed operator \( \hat{\mathbf{M}} \) can be written as

\[ \hat{\mathbf{M}} = \hat{\mathbf{M}}_0 + \Lambda \Delta \hat{\mathbf{M}} , \]

where

\[ \Delta \hat{\mathbf{M}} = \Delta \hat{\mathbf{M}}_{k_0} + \Delta \hat{\mathbf{M}}_x + \Delta \hat{\mathbf{M}}_{\mu} , \]

with

\[ \Delta \hat{\mathbf{M}}_{k_0} = \left( \begin{array}{cc} \Delta k_0 \varepsilon & 0 \\ 0 & \Delta k_0 \mu \end{array} \right) , \]
\[ \Delta \hat{\mathbf{M}}_x = \left( \begin{array}{cc} k_0 \Delta \varepsilon & 0 \\ 0 & 0 \end{array} \right) , \]
\[ \Delta \hat{\mathbf{M}}_{\mu} = \left( \begin{array}{cc} 0 & 0 \\ 0 & k_0 \Delta \mu \end{array} \right) . \]

Henceforth, we consider the subscript \( \nu \) for the resonant states of the perturbed system, which satisfy

\[ \hat{\mathbf{M}}(r_||; \beta_m) \hat{F}_\nu = 0 . \]

For every solution \( \hat{\mathbf{F}}_m \) of Eq. (5) with propagation constant \( \beta_m \), there exists a reciprocal conjugate solution \( \hat{\mathbf{F}}_R^R \) with propagation constant \( -\beta_m \). We now use the forward and reciprocal conjugate, i.e., backward propagating modes as in Ref. [20], to get

\[ \hat{\mathbf{F}}_\nu \cdot \hat{\mathbf{M}}_{0}(r_||; \beta_m) \hat{\mathbf{F}}^R_\nu \hat{\mathbf{F}}^R = 0 . \]

Integrating over a circular surface \( S \) of radius \( R \) in the xy plane that encloses all regions of spatial inhomogeneities and applying vector identities, we obtain

\[ R \int d\phi (\hat{\mathbf{E}}_\nu \cdot \hat{\mathbf{H}}^R_{\nu x z} - \hat{\mathbf{E}}_{\nu x z} \cdot \hat{\mathbf{H}}^R_\nu - \hat{\mathbf{E}}^R_{\nu x z} \cdot \hat{\mathbf{H}}_\nu + \hat{\mathbf{E}}^R_{\nu x z} \cdot \hat{\mathbf{H}}^R_\nu) \rho = R \int d\phi (\hat{\mathbf{E}}_\nu \cdot \hat{\mathbf{H}}^R_{\nu x z} - \hat{\mathbf{E}}_{\nu x z} \cdot \hat{\mathbf{H}}_\nu - \hat{\mathbf{E}}^R_{\nu x z} \cdot \hat{\mathbf{H}}_\nu + \hat{\mathbf{E}}^R_{\nu x z} \cdot \hat{\mathbf{H}}_\nu) \rho \]

\[ + \int dA (\hat{\mathbf{F}}^R_m \cdot \hat{\mathbf{D}}_{\nu x z} - \hat{\mathbf{F}}_{\nu x z} \cdot \hat{\mathbf{D}}^R_m - \hat{\mathbf{F}}^R_{\nu x z} \cdot \hat{\mathbf{D}}_{\nu x z} + \hat{\mathbf{F}}_{\nu x z} \cdot \hat{\mathbf{D}}^R_{\nu x z}) \]

\[ + \int dA (\hat{\mathbf{F}}^R_m \cdot \hat{\mathbf{D}}_{\nu x z} - \hat{\mathbf{F}}_{\nu x z} \cdot \hat{\mathbf{D}}^R_m - \hat{\mathbf{F}}^R_{\nu x z} \cdot \hat{\mathbf{D}}_{\nu x z} + \hat{\mathbf{F}}_{\nu x z} \cdot \hat{\mathbf{D}}^R_{\nu x z}) = 0 , \]

(11)
where we have introduced cylindrical coordinates \( \rho \) and \( \phi \) for the sake of convenience.

Similar to perturbation theories in quantum mechanics [23] and the first-order external perturbation theory in Ref. [22], we write the propagation constant \( \beta \) and fields of the perturbed system as a power series, i.e.,

\[
\beta_c = \beta_m + \Delta \beta^{(1)} + O(\lambda^2) + \cdots,
\]

and

\[
\hat F_v = \hat F_m + \Delta \hat F^{(1)} + O(\lambda^2) + \cdots.
\]

Substituting these expansions in Eq. (11) and equating the zero-order terms with respect to \( \Lambda \), we obtain

\[
R \int d\phi (E_\phi H^R_z - E_z H^R_\phi - E_\phi H^R_z + E_R^R H^R_\phi)_{\rho=R} = 0.
\]

For the sake of convenience, we exclude the hat and subscript \( m \). Using the symmetries of the system [20], the reciprocal conjugate (backward propagating) modes can be converted to forward propagating modes by multiplying a factor of \(-1\) to the in-plane components of the magnetic field and the \( z \) component of the electric field. The other components remain unchanged. Hence, Eq. (14) is trivially fulfilled. We now equate the first-order terms for \( \Delta \) to get

\[
R \int d\phi (E_\phi H^{(1)}_z + E_z H^{(1)}_\phi - E_\phi H^{(1)}_z - E_z H^{(1)}_\phi)_{\rho=R}
+ 2i \beta^{(1)} \int_S dA (E_\rho H_\phi - E_\phi H_\rho) - i \int_S dA \hat F_m \cdot \Delta \hat M F_m = 0.
\]

We evaluate the first-order correction terms in Eq. (15) in order to obtain the first-order correction term of the propagation constant. The details of deriving the first-order correction terms for the fields are described in Appendix A.

The first-order correction term then yields

\[
\beta_m^{(1)} = \frac{\int dA \hat F_m \cdot \Delta \hat M F_m + \Delta \varepsilon L^\varepsilon + \Delta \mu L^\mu + \Delta k_0^\lambda L^k_0}{S_0 + L_0},
\]

where \( \Delta \varepsilon \) and \( \Delta \mu \) are homogeneous and isotropic modifications of the permittivity and permeability in the surroundings, respectively. Furthermore, \( L^\varepsilon, L^\mu, \) and \( L^k_0 \) are defined as

\[
L^\varepsilon = \beta I_0 + I_1 - I_E,
\]

\[
L^\mu = \beta I_0 + I_1 - I_H,
\]

\[
L^k_0 = L^\varepsilon + L^\mu,
\]

with \( I_0, I_1, I_E, \) and \( I_H \) as line integrals in the exterior:

\[
I_0 = \int_0^{k_0^\lambda \pi^2} d\phi \left( E_z \frac{\partial H_z}{\partial \phi} - H_z \frac{\partial E_z}{\partial \phi} \right)_{\rho=R}.
\]
yielding a constant value (green solid line) irrespective of the radius of integration. Note that the same radius of integration is applied to all quantities in Eq. (16), including its denominator.

We now apply the first-order perturbation theory for an external ε perturbation to a step index fiber. The chosen fiber has a teflon amorphous fluoropolymer (AF) core with an index of \( n = 1.29 \) [24] and a radius of \( r = 5 \) µm. We choose this fiber for its low index solid core that can be placed in high index liquids for refractive index sensing and other applications [25,26]. The unperturbed background index is \( n_{bg} = 1.60 \). The schematic of this fiber can be seen in the inset of Fig. 3(a). In Figs. 3(a) and 3(b), we compare first-order perturbation theory (blue solid lines) and exact solutions (red circles) for the real and imaginary parts of the effective index, respectively, as a function of the background index for the fundamental core mode. The propagation constant is related to the effective index as \( \beta = k_0n_{eff} \). We see that there is a good agreement between the exact solution and first-order perturbation theory for small index changes of the background material. The considered wavelength is 1 µm.

We now investigate a second example of a liquid surrounding a light-cage structure [28]. The schematic of the light cage is shown in the inset of Fig. 4(b). Since the light-cage structure is placed in the liquid, the background index is the same as the core index, which leads to higher field intensities interacting with the change in background index. The radius of the twelve strands of the light-cage structure is \( r = 1 \) µm, and the material of the strands is a polymer, as in Ref. [29]. We display the real and imaginary part of the effective index in Figs. 4(a) and 4(b), respectively, for exact numerical solutions and first-order perturbation theory. We see that there is a very good agreement for the real part of the effective index in Fig. 4(a) due to its linear behavior as a function of the background index. Particularly, the slope of the numerical calculations is predicted correctly. The imaginary part also shows a good agreement as long as the perturbation is not too high. The unperturbed background index, indicated by the arrow in Fig. 4, is \( n_{bg} = 1.32 \) (water [30]).

4. WAVENUMBER PERTURBATION

Now let us consider only a \( k_0 \) perturbation, which essentially translates to a change in wavelength treated as a perturbation. We first investigate the case of a simple capillary fiber of radius \( r = 5 \) µm. The unperturbed wavelength is 1 µm. Figures 5(a) and 5(b) display the real and imaginary parts of the effective index, respectively, as a function of wavelength, for the exact solution and first-order perturbation. We see that there is a very good agreement between the two for both the real and imaginary parts, especially for small perturbations in wavelength. In fact, our perturbation theory can be used to calculate the exact value of the group velocity in fiber geometries as a single post processing step, in contrast to conventional numerical approaches.
that our theory is extremely valuable for calculating parameters and we have demonstrated good agreement between the propagation constants using exact solutions and first-order perturbation theory for small perturbations using different example fibers. We have also treated wavelength as a perturbation and shown that our theory is extremely valuable for calculating parameters such as group velocity as a simple post processing step. The results achieved will allow for speeding up simulations in order to determine modal properties, which is essential for areas such as dispersion engineering within, e.g., supercontinuum generation or refractive index sensing with respect to bioanalytical applications.

5. CONCLUSION

Precise knowledge of modal properties is essential for many photonic applications including bioanalytics, mode coupling, or ultrafast nonlinear frequency conversion. Here, we have derived a first-order perturbation theory for material perturbations of permittivity and permeability in the external surroundings. We have demonstrated good agreement between the propagation constants using exact solutions and first-order perturbation theory for small perturbations using different example fibers.

We now predict the values of the group velocity using the first-order perturbation and compare it with the numerical solutions for a silica–air photonic crystal fiber in Fig. 6. The background index is $n_{bg} = 1.44$ (silica), and the strands have $n = 1$ (air). The pitch is kept constant at 2.3 μm. We see in Figs. 6(a) and 6(b) that there is an excellent agreement of the group velocity for different strand radii and wavelengths. The group velocity is plotted in units of $c$, the speed of light. Hence, perturbation theory constitutes an efficient tool for predicting the group velocity of complicated fiber systems.

APPENDIX A: FIRST-ORDER CORRECTION TERMS FOR THE FIELDS

In order to derive the first-order correction of the fields, let us consider Eq. (13). In this equation, we can write

$$\beta_m(\Lambda) = \beta_m + \Delta \beta_m(\Lambda) + O(\Lambda^2) + \cdots$$

and

$$\beta = \beta_m(\Lambda)$$

we get

$$\frac{\partial \beta}{\partial \Lambda} \bigg|_{\Lambda = 0} = \frac{\Delta \mu k_0^2 + \epsilon \Delta \epsilon k_0^2 + 2\mu k_0 \Delta \epsilon}{2 \epsilon k_0} = \frac{\gamma}{2 \epsilon k_0},$$

$$\frac{\partial \beta}{\partial \rho} \bigg|_{\Lambda = 0} = \frac{-\beta_m}{\epsilon k_0}.$$
Next, we express $E_{m\phi}^{(1)}$ in dependence of the $z$ components [32]:

$$E_{m\phi}^{(1)} = \frac{i\beta}{x^2 \rho} \frac{\partial E_z}{\partial \phi} - \frac{i(k_0 + \Lambda \Delta k_0)(\mu + \Lambda \Delta \mu)}{x^2} \frac{\partial H_z}{\partial \rho}. \quad (A9)$$

By applying Eq. (27) to the above equation, we obtain the first-order correction term for the electric field as

$$E_{m\phi}^{(1)} = \frac{i x^m \beta^2 m^2 \beta^{(2)} m - i \beta m \gamma}{x^m} \frac{\partial E_m}{\partial \phi} + \left( \frac{i \beta m \gamma - 2i \beta^2 m \beta^{(1)} m}{2 x^m} \right) \frac{\partial^2 E_m}{\partial \phi^2} + \left( \frac{i k_0 \mu \gamma - 2i k_0 \mu \beta^{(1)} m}{2 x^m} \right) \frac{\partial \beta E_m}{\partial \rho} + \left( \frac{2ik_0 \mu \beta^{(1)} m - i k_0 \mu \gamma}{2 x^m} \right) \frac{\partial^2 E_m}{\partial \rho^2}. \quad (A10)$$

For $H_{m\phi}^{(1)}$, we use the relation

$$H_{m\phi}^{(1)} = \frac{i \beta}{x^2 \rho} \frac{\partial H_z}{\partial \phi} + \frac{i(k_0 + \Lambda \Delta k_0)(\epsilon + \Lambda \Delta \epsilon)}{x^2} \frac{\partial E_z}{\partial \rho}. \quad (A11)$$

which yields

$$H_{m\phi}^{(1)} = \frac{i x^m \beta^2 m^2 \beta^{(2)} m - i \beta m \gamma}{x^m} \frac{\partial H_m}{\partial \phi} + \left( \frac{i \beta m \gamma - 2i \beta^2 m \beta^{(1)} m}{2 x^m} \right) \frac{\partial^2 H_m}{\partial \phi^2} + \left( \frac{2ik_0 \beta^{(1)} m - ik_0 \Delta \beta}{2 x^m} \right) \frac{\partial E_m}{\partial \rho} + \left( \frac{ik_0 \beta \gamma}{2 x^m} \right) \frac{\partial^2 E_m}{\partial \rho^2}. \quad (A12)$$

Substituting the above correction terms to Eq. (15) of the main text and using the relations in Eqs. (35) and (37) at $\Lambda = 0$ for the remaining $\phi$ components in the first line of Eq. (15), we obtain Eq. (16).

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