Modal Theory for Twisted Waveguides

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ABSTRACT

Twisted waveguides are promising building blocks for broadband polarization rotation in integrated photonics. They may find applications in polarization-encoded telecommunications and quantum-optical systems. In our work, we develop a rigorous modal theory for such waveguides. To this end, we define an eigenmode of a twisted waveguide as a natural generalization of the eigenmode of a straight waveguide. Using covariant approach for expressing Maxwell's equations in helical reference frame, we obtain the eigenmode equation which appears to be nonlinear with respect to the eigenvalue, i.e. propagation constant. By analyzing the obtained equations we establish fundamental properties of the eigenmodes and prove their orthogonality. We develop a finite-difference full-vectorial scheme for solving the eigenmode equation and solve it using two approaches: with perturbation theory and using routines for nonlinear eigenvalue problems. By analyzing the obtained propagation constants and modal fields we explain the modal mechanism of polarization rotation in twisted waveguides and explain qualitatively polarization conversion efficiency dependence on twist length. Although photonic applications are of our primary concern, our results are general and apply to twisted waveguides of arbitrary architecture.

Keywords: Twisted waveguides, helical coordinates, nonlinear eigenvalue problem, finite-difference method, eigenmode expansion method, polarization conversion.

1. INTRODUCTION

State-of-the-art technologies in integrated photonic circuits fabrication give freedom to go beyond planar design and engineer features in all 3 dimensions. Particularly, these technologies allow creation of waveguides with variable cross-sections of virtually arbitrary shape. If the cross-section of such a waveguide is varied slowly along propagation direction, this waveguide can serve as an adiabatic mode converter. One of the promising architectures is a twisted waveguide, i.e., the waveguide with the core twisted along the propagation axis. It was shown numerically and experimentally, that photonic twisted waveguides can serve as broadband polarization rotators.[1,2]

In order to analyze light propagation in such waveguides, numerical methods such as Finite-Difference Time Domain (FDTD), Finite-Element Method (FEM), and Beam Propagation Method (BPM) are normally utilized. Applied to twisted waveguides, however, these methods suffer from a number of problems. Namely, FDTD and FEM methods require solving the 3D problem, which makes simulations quite memory- and CPU-demanding. On the other hand, BPM can be memory and CPU-efficient by sacrificing the precision, especially for high refractive index contrast platforms. Therefore, eigenmode expansion-based approaches are preferable.

Attempts of solving eigenmode equation for twisted waveguides were made by Lewin *et al.*[3,4] and by Yabe *et al.*[5,6] In these works authors found perturbative expressions to the propagation constants and modal fields in the particular case of rectangular waveguide with perfectly conducting walls. In another work by Ma *et al.*[7] authors develop a modal theory in helical reference frame, but in the weak-guidance limit.

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In present work we formulate and solve the eigenmode equation for a twisted waveguide with arbitrary cross-section and establish fundamental properties of its solutions paying special attention to polarimetric properties of the modes. Additionally, we combine the developed mode solver with eigenmode expansion method solver to analyze light propagation in twisted waveguides.

2. TWISTED COORDINATES

In order to study twisted waveguides we are going to use twisted coordinates discussed in a number of works.[8–10] In this section we outline some important properties of these coordinates.

Let us denote Cartesian and twisted bases by indices i' and i, respectively. The corresponding coordinates are $x^{i'} = \{x, y, z\}$ and $x^i = \{X, Y, Z\}$. Coordinate transformation is given by

$$\begin{cases} X = x\cos\alpha z + y\sin\alpha z \\ Y = -x\sin\alpha z + y\cos\alpha z \\ Z = z \end{cases}. \tag{1}$$

Accordingly, the inverse transformation is

$$\begin{cases} x = X\cos\alpha Z - Y\sin\alpha Z \\ y = X\sin\alpha Z + Y\cos\alpha Z \\ z = Z \end{cases}. \tag{2}$$

From tensor analysis it is known that a coordinate system at any given point P generates two sets of vectors $\mathbf{e}_{(i)}$ and $\mathbf{e}^{(i)}$ which form local tangent and cotangent bases, respectively.[11–13] The basis associated with the coordinate system is called a holonomic, or coordinate, basis. In present work we are going to express Maxwell's equations in basis associated with the twisted coordinates.

Basis vectors of the new coordinate system are related to the basis vectors of the initial Cartesian coordinate system as

$$\mathbf{e}_{(i)} = \Lambda^{i'}{}_{i}\mathbf{e}_{(i')}, \qquad \mathbf{e}^{(i)} = \Lambda^{i}{}_{i'}\mathbf{e}^{(i')}, \tag{3}$$

where transformation matrices $\Lambda^{i}{}_{i'}$ and $\Lambda^{i'}{}_{i}$ are

$$\Lambda^{i'}{}_{i} = \frac{\partial x^{i'}}{\partial x^{i}}, \qquad \Lambda^{i}{}_{i'} = \frac{\partial x^{i}}{\partial x^{i'}}. \tag{4}$$

In Eq. (3) and further in the text we use the Einstein summation convention for repeated indices. Explicitly, these matrices are*

$$\Lambda^{i}{}_{i'} = \begin{pmatrix} \cos\alpha z & \sin\alpha z & \alpha(y\cos\alpha z - x\sin\alpha z) \\ -\sin\alpha z & \cos\alpha z & -\alpha(x\cos\alpha z + y\sin\alpha z) \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \cos\alpha Z & \sin\alpha Z & \alpha Y \\ -\sin\alpha Z & \cos\alpha Z & -\alpha X \\ 0 & 0 & 1 \end{pmatrix} \tag{5}$$

and

$$\Lambda^{i'}{}_{i} = \begin{pmatrix} \cos\alpha z & -\sin\alpha z & -\alpha y \\ \sin\alpha z & \cos\alpha z & \alpha x \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \cos\alpha Z & -\sin\alpha Z & -\alpha(Y\cos\alpha Z + X\sin\alpha Z) \\ \sin\alpha Z & \cos\alpha Z & \alpha(X\cos\alpha Z - Y\sin\alpha Z) \\ 0 & 0 & 1 \end{pmatrix}. \tag{6}$$

Let us denote basis vectors of Cartesian reference frame as $\mathbf{e}_{(i')} = \{\hat{\mathbf{x}}, \hat{\mathbf{y}}, \hat{\mathbf{z}}\} \equiv \{\hat{x}^{j'}, \hat{y}^{j'}, \hat{z}^{j'}\}$, where the subscript in brackets designates the basis vector number. Analogously, let us denote the basis vectors of the twisted

*In the transformation matrices, upper index corresponds to the row number and lower index corresponds to the column number.

reference frame as $\mathbf{e}_{(i)} = \{\hat{\mathbf{X}}, \hat{\mathbf{Y}}, \hat{\mathbf{Z}}\}$ and $\mathbf{e}^{(i)} = \{\hat{\xi}, \hat{\eta}, \hat{\zeta}\}$ for tangent and cotangent bases, respectively. They read as

$$\mathbf{e}_{(1)} \equiv \hat{\mathbf{X}} = \Lambda^{i'}{}_1 \mathbf{e}_{(i')} = \cos\alpha z \hat{\mathbf{x}} + \sin\alpha z \hat{\mathbf{y}}, \tag{7a}$$
$$\mathbf{e}_{(2)} \equiv \hat{\mathbf{Y}} = \Lambda^{i'}{}_2 \mathbf{e}_{(i')} = -\sin\alpha z \hat{\mathbf{x}} + \cos\alpha z \hat{\mathbf{y}}, \tag{7b}$$
$$\mathbf{e}_{(3)} \equiv \hat{\mathbf{Z}} = \Lambda^{i'}{}_3 \mathbf{e}_{(i')} = -\alpha y \hat{\mathbf{x}} + \alpha x \hat{\mathbf{y}} + \hat{\mathbf{z}} \tag{7c}$$

and

$$\mathbf{e}^{(1)} \equiv \hat{\xi} = \Lambda^1{}_{i'} \mathbf{e}^{(i')} = \cos\alpha Z \hat{\mathbf{x}} + \sin\alpha Z \hat{\mathbf{y}} + \alpha Y \hat{\mathbf{z}}, \tag{8}$$
$$\mathbf{e}^{(2)} \equiv \hat{\eta} = \Lambda^2{}_{i'} \mathbf{e}^{(i')} = -\sin\alpha Z \hat{\mathbf{x}} + \cos\alpha Z \hat{\mathbf{y}} - \alpha X \hat{\mathbf{z}}, \tag{9}$$
$$\mathbf{e}^{(3)} \equiv \hat{\zeta} = \Lambda^3{}_{i'} \mathbf{e}^{(i')} = \hat{\mathbf{z}}. \tag{10}$$

Now, when we know forward and inverse transformation matrices (or Jacobians), we can determine co- and contravariant metric tensors. Remembering that the metric tensor in Cartesian coordinates is trivial as $g_{i'k'} = \delta_{i'k'}$ we find

$$g_{ik} = \Lambda_i^{i'} \Lambda_k^{k'} g_{i'k'} = \begin{pmatrix} 1 & 0 & \alpha y \\ 0 & 1 & -\alpha x \\ \alpha y & -\alpha x & 1+\alpha^2(x^2+y^2) \end{pmatrix} = \begin{pmatrix} 1 & 0 & -\alpha Y \\ 0 & 1 & \alpha X \\ -\alpha Y & \alpha X & 1+\alpha^2(X^2+Y^2) \end{pmatrix}, \tag{11}$$

$$g^{ik} = \Lambda_{i'}^{i} \Lambda_{k'}^{k} g^{i'k'} = \begin{pmatrix} 1+\alpha^2 y^2 & -\alpha^2 xy & -\alpha y \\ -\alpha^2 xy & 1+\alpha^2 x^2 & \alpha x \\ -\alpha y & \alpha x & 1 \end{pmatrix} = \begin{pmatrix} 1+\alpha^2 Y^2 & -\alpha^2 XY & \alpha Y \\ -\alpha^2 XY & 1+\alpha^2 X^2 & -\alpha X \\ \alpha Y & -\alpha X & 1 \end{pmatrix}. \tag{12}$$

Notably, the determinant of the Jacobian and, hence, metric tensor is unity: $\det\left[\Lambda_i^{i'}\right] = 1$ and $\det[g_{ik}] = 1$.

3. MAXWELL'S EQUATIONS IN TENSOR FORM

Maxwell's equations for harmonic fields with an angular frequency ω in arbitrary reference system with the use of tensor notation can be written as follows:[12,13]

$$\varepsilon^{ijk}\nabla_j H_k = \mathrm{i}\omega n^2 \varepsilon_0 E^i, \tag{13a}$$
$$\varepsilon^{ijk}\nabla_j E_k = -\mathrm{i}\omega \mu_0 H^i, \tag{13b}$$
$$\nabla_i n^2 E^i = 0, \tag{13c}$$
$$\nabla_i H^i = 0, \tag{13d}$$

where ∇_k is covariant derivative, ε^{ijk} is the fully antisymmetric Levi-Civita tensor, vectors with upper and lower indices are *contravariant* and *covariant* vectors, respectively, $n = n(x^i)$ is the refractive index, ε_0 and μ_0 is the permittivity and permeability of vacuum, respectively.

Redefining the magnetic field as

$$H^i = \sqrt{\frac{\varepsilon_0}{\mu_0}} \tilde{H}^i \tag{14}$$

and by substituting (14) to (13) the Maxwell equations are recast to

$$\varepsilon^{ijk}\nabla_j \tilde{H}_k = \mathrm{i}k_0 n^2 E^i, \tag{15a}$$
$$\varepsilon^{ijk}\nabla_j E_k = -\mathrm{i}k_0 \tilde{H}^i, \tag{15b}$$
$$\nabla_i n^2 E^i = 0, \tag{15c}$$
$$\nabla_i \tilde{H}^i = 0, \tag{15d}$$

where $k_0 = \frac{\omega}{c}$ is the free space wavenumber. Further we drop the tilde keeping in mind that the magnetic field is rescaled.

Using the metric tensor g_{ik} for raising and lowering indices as

$$v_i = g_{ik} v^k,\ v^i = g^{ik} v_k, \tag{16}$$

we will rewrite the equations with respect to contravariant electric E^i and covariant magnetic field H_i:

$$\varepsilon^{ijk} \nabla_j H_k = \mathrm{i} k_0 n^2 E^i, \tag{17a}$$
$$\varepsilon^{ijk} g_{kl} \nabla_j E^l = -\mathrm{i} k_0 g^{ik} H_k, \tag{17b}$$
$$\nabla_i n^2 E^i = 0, \tag{17c}$$
$$g^{ik} \nabla_i H_k = 0. \tag{17d}$$

Here we account for that the covariant derivative satisfies $\nabla_i g_{jk} = 0$.

The covariant derivative of contra- and covariant vectors is respectively[12]

$$\nabla_k v^i = \partial_k v^i + \Gamma^i_{sk} v^s,\ \nabla_k u_i = \partial_k u_i - \Gamma^s_{ik} u_s, \tag{18}$$

where Γ^i_{sk} is the metric connection, or Christoffel symbols, expressed as [†]

$$\Gamma^i_{kl} = \frac{1}{2} g^{is} (\partial_k g_{ls} + \partial_l g_{sk} - \partial_s g_{kl}). \tag{19}$$

It is important that although we are going to use curvilinear coordinates the manifold we are working in is still flat Euclidean space with zero torsion and curvature. The flatness of Euclidean space leads to symmetries in Christoffel symbols which, in their turn, allow to replace covariant derivatives in Maxwell's equations by partial derivatives:[12]

$$\varepsilon^{ijk} \partial_j H_k = \mathrm{i} k_0 n^2 E^i, \tag{20a}$$
$$\varepsilon^{ijk} g_{kl} \partial_j E^l = -\mathrm{i} k_0 g^{ik} H_k, \tag{20b}$$
$$\partial_i n^2 E^i = 0, \tag{20c}$$
$$g^{ik} \partial_i H_k = 0. \tag{20d}$$

To obtain the wave equation with respect to E^i we multiply Eq. (17b) by $\varepsilon^{prs} g_{is} \nabla_r$ and replace $\varepsilon^{prs} \nabla_r H_s$ by $\mathrm{i} k_0 n^2 E^p$ using Eq. (17a)

$$\varepsilon^{prs} \varepsilon^{ijk} g_{is} g_{kl} \nabla_r \nabla_j E^l - k_0^2 n^2 E^p = 0. \tag{21}$$

Performing contractions and taking into account symmetries of covariant derivative of the flat Euclidean space we finally get

$$g^{kl} \nabla_k \nabla_l E^i - g^{ik} \nabla_k (\nabla_l E^l) + k_0^2 n^2 E^i = 0. \tag{22}$$

3.1 Reciprocity theorem

To later prove orthogonality of modes we refer to the Lorentz reciprocity theorem. Let us express it in tensor notations. Here we follow the derivation by Snyder and Love.[14]

Consider a vector

$$F^i = \varepsilon^{ijk} (E_j \bar{H}^*_k + \bar{E}^*_j H_k), \tag{23}$$

[†]In nonholonomic bases, expression for connection also includes object of nonholonomity.[11] We everywhere assume that the basis is holonomic i.e. defined by the coordinate system.

where * denotes complex conjugate. The unbarred fields satisfy Maxwell's equations (17), and the barred fields satisfy the conjugated forms of these equations with the corresponding refractive index function $\bar{n}^*$. Let us calculate the divergence of the vector F^i and use Maxwell's curl equations (17)

$$\begin{aligned}\nabla_i F^i &= \varepsilon^{ijk}\nabla_i(E_j\bar{H}^*_k + \bar{E}^*_j H_k)\\ &= \cancel{-\mathrm{i}k_0 H^k \bar{H}^*_k} + \mathrm{i}k_0(\bar{n}^*)^2\bar{E}^{j*}E_j + \cancel{\mathrm{i}k_0\bar{H}^{k*}H_k} - \mathrm{i}k_0 n^2 E^j\bar{E}^*_j\\ &= \mathrm{i}k_0\left((\bar{n}^*)^2 - n^2\right)E^j\bar{E}^*_j. \quad (24)\end{aligned}$$

The two-dimensional form of the divergence theorem for F^i is

$$\int\limits_A \nabla_i F^i dA = \frac{\partial}{\partial z}\int\limits_A F_i\hat{z}^i dA + \oint_{\delta A} F_i\hat{n}^i dl, \quad (25)$$

where A is an arbitrary cross-sectional area in xy-plane, $\hat{z}^i$ is the unit vector parallel to the z-axis, the contour δA is the boundary of A, and $\hat{n}^i$ is the unit outward normal on δA in the plane of A. If A is chosen to be infinite, the integral over the boundary δA vanishes for the bound mode fields as they exponentially decay outside the waveguide core and can be dropped in (25). Thus, we obtain the reciprocity theorem in its conjugated form

$$\int\limits_{A_\infty} \nabla_i F^i dA = \frac{\partial}{\partial z}\int\limits_{A_\infty} F^i\hat{z}_i dA = \frac{\partial}{\partial Z}\int\limits_{A_\infty} F^i\hat{z}_i dA. \quad (26)$$

We can freely switch from $\frac{\partial}{\partial z}$ to $\frac{\partial}{\partial Z}$ and vice-versa, since the integral in (26) does not depend neither on x, y nor on X, Y.

4. EIGENMODES OF A TWISTED WAVEGUIDE

4.1 Definition of an Eigenmode

Let us consider a twisted waveguide of an arbitrary cross-section $n(X, Y)$ with constant twist rate α and infinite length. Such a system is invariant in Z in twisted coordinates. Therefore it is intuitive to define an eigenmode for this system in a way analogous to the straight waveguide case, but using twisted coordinates.

Within the twisted reference frame there are four possible ways to define an eigenmode depending on combination of contra- and covariant electric and magnetic vectors we choose i.e., contravariant magnetic and electric vectors, covariant magnetic and electric vectors, contravariant electric and covariant magnetic vectors, covariant electric and contravariant magnetic vectors. Any choice allows to separate Z variable and formulate a two-dimensional eigenvalue problem. We note also that remaining components can be always obtained by contracting with the metric tensor g_{ik} or g^{ik}.

Here we define the eigenmode with contravariant electric and covariant magnetic vectors as follows

$$E^i(X, Y, Z) = e^i(X, Y)\mathrm{e}^{-\mathrm{i}\beta Z}, \quad (27a)$$

$$H_i(X, Y, Z) = h_i(X, Y)\mathrm{e}^{-\mathrm{i}\beta Z}. \quad (27b)$$

4.2 Eigenmode Equation

With this definition Maxwell's curl equations in twisted coordinates take the form

$$\partial_Y h_\zeta + \mathrm{i}\beta h_\eta = \mathrm{i}k_0 n^2 e_X, \quad (28a)$$

$$-\partial_X h_\zeta - \mathrm{i}\beta h_\xi = \mathrm{i}k_0 n^2 e_Y, \quad (28b)$$

$$-\partial_X h_\eta - \partial_Y h_\xi = \mathrm{i}k_0 n^2 e_Z, \quad (28c)$$

$$\partial_Y e_Z + \mathrm{i}\beta e_Y + \alpha\left(-e_X + (X\partial_Y - Y\partial_X)e_Y + \mathrm{i}\beta X e_Z\right) + \alpha^2 X\left(X\partial_Y - Y\partial_X\right)e_Z = -\mathrm{i}k_0 h_\xi, \quad (28d)$$

$$\partial_X e_Z - \mathrm{i}\beta e_X + \alpha\left(-e_Y - (X\partial_Y - Y\partial_X)e_X + \mathrm{i}\beta Y e_Z\right) + \alpha^2 Y\left(X\partial_Y - Y\partial_X\right)e_Z = -\mathrm{i}k_0 h_\eta, \quad (28e)$$

$$\begin{aligned}&\partial_X e_Y - \partial_Y e_X + \alpha\left(2e_Z - \mathrm{i}\beta(X e_X + Y e_Y)\right)\\ &\quad + \alpha^2\left(-X^2\partial_Y e_X + Y^2\partial_X e_Y + XY(\partial_X e_X - \partial_Y e_Y) - X e_X + Y e_Y\right) = -\mathrm{i}k_0 h_\zeta, \quad (28f)\end{aligned}$$

while divergence equations read as

$$
\begin{aligned}
&\partial_X e_X + \partial_Y e_Y - \mathrm{i}\beta e_Z + \partial_X \ln n^2 e_X + \partial_Y \ln n^2 e_Y = 0, && \text{(29a)}\\
&\partial_X h_\xi + \partial_Y h_\eta - \mathrm{i}\beta h_\zeta \\
&+ \alpha \left(X(-\partial_Y h_\zeta + \mathrm{i}\beta h_\eta) + Y(\partial_X h_\zeta - \mathrm{i}\beta h_\xi) \right) \\
&+ \alpha^2 \big((X^2\partial_Y - XY\partial_X - Y)h_\eta + (Y^2\partial_X - XY\partial_Y - X)h_\xi \big) = 0. && \text{(29b)}
\end{aligned}
$$

Equation (29a) readily allows to express e_Z component in terms of e_X and e_Y. This motivates our choice of contravariant electric field since we are going to formulate eigenmode equation in terms of electric field. Expressing wave equation (22) in twisted coordinates and substituting e_Z from (29a) we obtain a differential equation

$$
\mathcal{L}(\beta, \alpha) \left| e \right\rangle = 0 \tag{30}
$$

with respect to the two-component column-vector $|e\rangle$

$$
|e\rangle = \begin{pmatrix} e_X \\ e_Y \end{pmatrix} \tag{31}
$$

and the differential operator $\mathcal{L}(\beta, \alpha)$ of the form

$$
\mathcal{L}(\beta, \alpha) = \mathcal{A} - \beta^2 + 2\mathrm{i}\alpha(\beta^{-1}\mathcal{B} + \beta\mathcal{C}) + \alpha^2\mathcal{D}, \tag{32}
$$

where $\mathcal{A}, \mathcal{B}, \mathcal{C}, \mathcal{D}$ are operators depending only on $X, Y, \partial_X, \partial_Y$, and $n(X, Y)$[‡]

$$
\mathcal{A} = \begin{pmatrix} \partial_X^2 + \partial_Y^2 + k_0^2 n^2 + \partial_X^2(\ln n^2) + \partial_X \ln n^2 \partial_X & \partial_Y \ln n^2 \partial_X + \partial_X \partial_Y (\ln n^2) \\ \partial_X \ln n^2 \partial_Y + \partial_X \partial_Y (\ln n^2) & \partial_X^2 + \partial_Y^2 + k_0^2 n^2 + \partial_Y^2(\ln n^2) + \partial_Y \ln n^2 \partial_Y \end{pmatrix}, \tag{33a}
$$

$$
\mathcal{B} = \begin{pmatrix} \partial_X \partial_Y + \partial_X \ln n^2 \partial_Y & \partial_Y^2 + \partial_Y \ln n^2 \partial_Y \\ -\partial_X^2 - \partial_X \ln n^2 \partial_X & -\partial_X \partial_Y - \partial_Y \ln n^2 \partial_X \end{pmatrix}, \tag{33b}
$$

$$
\mathcal{C} = \begin{pmatrix} X\partial_Y - Y\partial_X - Y\partial_X \ln n & 1 + Y\partial_Y \ln n \\ -1 + X\partial_X \ln n & X\partial_Y - Y\partial_X + X\partial_Y \ln n \end{pmatrix}, \tag{33c}
$$

$$
\mathcal{D} = \begin{pmatrix} -1 - X\partial_X - Y\partial_Y + (X\partial_Y - Y\partial_X)^2 & 2(X\partial_Y - Y\partial_X) \\ -2(X\partial_Y - Y\partial_X) & -1 - X\partial_X - Y\partial_Y + (X\partial_Y - Y\partial_X)^2 \end{pmatrix}. \tag{33d}
$$

Equation (30) is nonlinear with respect to the eigenvalue β. Eigenvalue problem associated with this operator is a nonlinear eigenvalue problem (NLEVP). NLEVPs are encountered in a variety of physical and engineering applications such as vibrational acoustics, fluid dynamics, photonic crystals with dispersive permittivity. An extensive collection of NLEVPs can be found in.[15] There is a plenty of numerical approaches existing and being developed for solving NLEVPs. The review of those can be found, e.g., in the survey by Güttel and Tisseur.[16]

4.3 Approaches of Solving the NLEVP

If the twist is slow, i.e, $\alpha \ll k_0$, the terms in operator $\mathcal{L}$ (32) related to twist can be considered as a small perturbation to the unperturbed (i.e, untwisted) operator $\mathcal{L}_0 = \mathcal{L}(\beta, 0)$. Then, eigenvalues and eigenvectors can be obtained in terms of perturbation series in α using the perturbation theory, namely,

$$
\beta = \beta^{(0)} + \alpha\beta^{(1)} + \alpha^2\beta^{(2)} + \dots, \tag{34a}
$$

$$
|e\rangle = |e^{(0)}\rangle + \alpha\, |e^{(1)}\rangle + \alpha^2\, |e^{(2)}\rangle + \dots, \tag{34b}
$$

[‡]In expression for $\mathcal{D}$ we dropped terms proportional to $\ln n$ for brevity. Nevertheless, in the calculations we have taken them into account.

where $\beta^{(n)}$ and $|e^{(n)}\rangle$ are n-th order corrections to the eigenvalues and eigenvectors, respectively. For $n = 0$ we have unperturbed, i.e., untwisted eigenvalues and eigenvectors. It was shown by Lewin,[3] that due to the fact that change in propagation constant must be insensitive to the sign of the twist, expansion (34a) only contains terms of even order. This means that in the first order perturbation theory eigenvalues and eigenvectors are equal to those of untwisted waveguide. More specifically, e_X, e_Y components of the twisted mode in this case are equal to e_x, e_y components of the untwisted mode. Normally, the modes of the straight rectangular waveguide are quasi-TE and TM modes, i.e., linearly polarized modes. Taking into account the relation between basis vectors of the twisted and Cartesian systems, we can see that to the lowest order perturbation, the modal fields of twisted rectangular waveguide have the helical shape with the twist rate as the twisted waveguide, i.e., α. In other words, in the adiabatic regime, polarization of the mode is twisted synchronously with the waveguide core. This justifies utilization of twisted waveguides as adiabatic polarization rotators.

The perturbation theory for NLEVPs with generally non-Hermitian operators was developed by Mensah *et al.*[17] The authors provide a link to a repository with the implementation of their perturbation approach along with other methods for solving NLEVPs in python programming language.

To obtain numerically exact solutions to the NLEVP (30) one can apply nonlinear optimization method such as Newton method. Newton method requires careful choice of the initial guess. Solutions obtained within the perturbation theory can serve as a good initial guess.

5. EIGENMODE EXPANSION METHOD FOR TWISTED WAVEGUIDES

To analyze light propagation in twisted waveguide we adopted the Eigenmode Expansion (EME) Method and generalized it to twisted waveguides. EME is a semi-analytical method based on the fact, that any solution to Maxwell's equations in a waveguide can be expressed as a superposition of the waveguide modes. The particular solutions are obtained by finding modal amplitudes resulting from certain excitation at the waveguide end facets. The process of finding the amplitudes uses continuity properties of the transverse fields at the waveguide end facets[18] and orthogonality of the waveguide modes.

In order to generalize the EME method to twisted waveguides, one need firstly to establish orthogonality properties of their eigenmodes, which we do in two following sections.

5.1 Fields of Backward-Propagating Modes

In order to establish orthogonality properties of eigenmodes we firstly find the relations between the fields of forward and backward propagating modes. To obtain backward-propagating modes one need to simultaneously flip the z-axis and sense of twist. In the equations (28) this results in change of β to $-\beta$ and α to $-\alpha$. It is straightforward to show that the fields

$$\bar{e}^i = \{e_X, e_Y, -e_Z\}, \qquad \bar{h}_i = \{-h_\xi, -h_\eta, h_\zeta\} \tag{35}$$

are the solutions for the transformed equations, where $e^i = \{e_X, e_Y, e_Z\}$ and $h_i = \{h_\xi, h_\eta, h_\zeta\}$, are the corresponding forward-propagating modal fields. Analogous relations hold for covariant electric and contravariant magnetic fields

$$\bar{e}_i = \{e_\xi, e_\eta, -e_\zeta\}, \qquad \bar{h}^i = \{-h_X, -h_Y, h_Z\}. \tag{36}$$

5.2 Orthogonality of Eigenmodes

Let us now establish orthogonality relations for the modes of twisted waveguides. To this end, we substitute two eigenmodes into the reciprocity theorem (26) so $E^i = E^i_\mu$, $\bar{E}^i = E^i_\nu$ with latin indices designating components and greek indices designating mode numbers. For the modes of nonabsorbing waveguides left side of Eq. (26) vanishes due to Eq. (24), since the refractive index is real, so $n^* = n$

$$\mathrm{i}k_0 \int\limits_{A_\infty} \left((n^*)^2 - n^2\right) E^j_\mu E^*_{j,\nu} dA = 0. \tag{37}$$

Substituting to the right hand side modal ansatz (27) we get

$$(\beta_\nu - \beta_\mu) \int\limits_{A_\infty} \varepsilon^{ijk}(e_{j,\mu}h^*_{k,\nu} + e^*_{j,\nu}h_{k,\mu})\hat{z}_i dA = 0. \tag{38}$$

Since

$$\hat{z}_i = \Lambda_i^{i'}\delta_{i'}^{3'} = \Lambda_i^{3'} = \delta_i^3, \tag{39}$$

integrand of equation (38) expands as

$$\varepsilon^{312}(e_{1,\mu}h^*_{2,\nu} + e^*_{1,\nu}h_{2,\mu}) + \varepsilon^{321}(e_{2,\mu}h^*_{1,\nu} + e^*_{2,\nu}h_{2,\mu}) = e_{\xi,\mu}h^*_{\eta,\nu} + e^*_{\xi,\nu}h_{\eta,\mu} - e_{\eta,\mu}h^*_{\xi,\nu} - e^*_{\eta,\nu}h_{\xi,\mu}, \tag{40}$$

therefore, only terms with $e_{\xi,\eta}, h_{\xi,\eta}$ take part in (38). Keeping this and relations (35) and (36) in mind, we change μ to $-\mu$ in Eq. (38) to obtain

$$(\beta_\nu + \beta_\mu) \int\limits_{A_\infty} \varepsilon^{ijk}(e_{j,\mu}h^*_{k,\nu} - e^*_{j,\nu}h_{k,\mu})\hat{z}_i dA = 0. \tag{41}$$

Summing and subtracting Eqs. (38) and (41) we obtain the orthogonality condition for the modes of a twisted waveguide

$$\int\limits_{A_\infty} \varepsilon^{ijk}e_{j,\mu}h^*_{k,\nu}z_i dA = \int\limits_{A_\infty} \varepsilon^{ijk}e^*_{j,\nu}h_{k,\mu}\hat{z}_i dA = 0;\ \mu \neq \nu. \tag{42}$$

5.3 Modal Amplitudes

Once we found the eigenmodes of a twisted waveguide and proved that they form an orthogonal set, we are able to find particular expansion coefficients, i.e., the modal amplitudes. Practical case of light coupling to the twisted waveguide via a butt-coupled straight waveguide is of our interest. Let us assume for definiteness that the straight waveguide is placed in the left half-space $z < 0$ while the twisted one is placed in the right half-space $z > 0$. In order to find the expansion coefficients we expand field in $z < 0$ and $z > 0$ regions in terms of the modes of the straight and twisted waveguides, respectively. This procedure involves calculation of overlap integrals between the modes of the straight and twisted waveguide according to the procedure described in.[18] This procedure extrapolates to the twisted waveguides without changes due to the previously established properties of the modes of twisted waveguides.

6. RESULTS

6.1 Finite-Difference Mode Solver for Twisted Waveguides

For solving NLEVP of equation (30) we adapted the code from the aforementioned repository by Mensah *et al.*. We have published our fork of the repository online[§] We implemented a finite-difference scheme in python to represent operators $\mathcal{A}, \mathcal{B}, \mathcal{C}, \mathcal{D}$ of Eq. (33) in terms of sparse matrices. Our finite-difference scheme is inspired by the Yee-grid-based scheme proposed by Zhu and Brown.[19] For verification of our results we performed BPM simulations in VPIphotonics Device Designer simulation package.[20]

6.2 Modal Indices and Fields

As a test example we take the waveguide similar to the one studied by Hou *et al.*[2] The core material is SU-8 with refractive index $n_{\text{co}} = 1.5552$ at the telecom wavelength $\lambda = 1.55\ \mu$m. The surrounding medium is air with $n_{\text{cl}} = 1$. The dimensions of the core are $4 \times 2\ \mu\text{m}^2$. The twist angle is constant 90° while twist length is variable.

In Figure 1 effective indices as a function of twist length of the six lowest-order guided modes are depicted.

§https://bitbucket.org/jokesfor300/pyholtz/src/master/

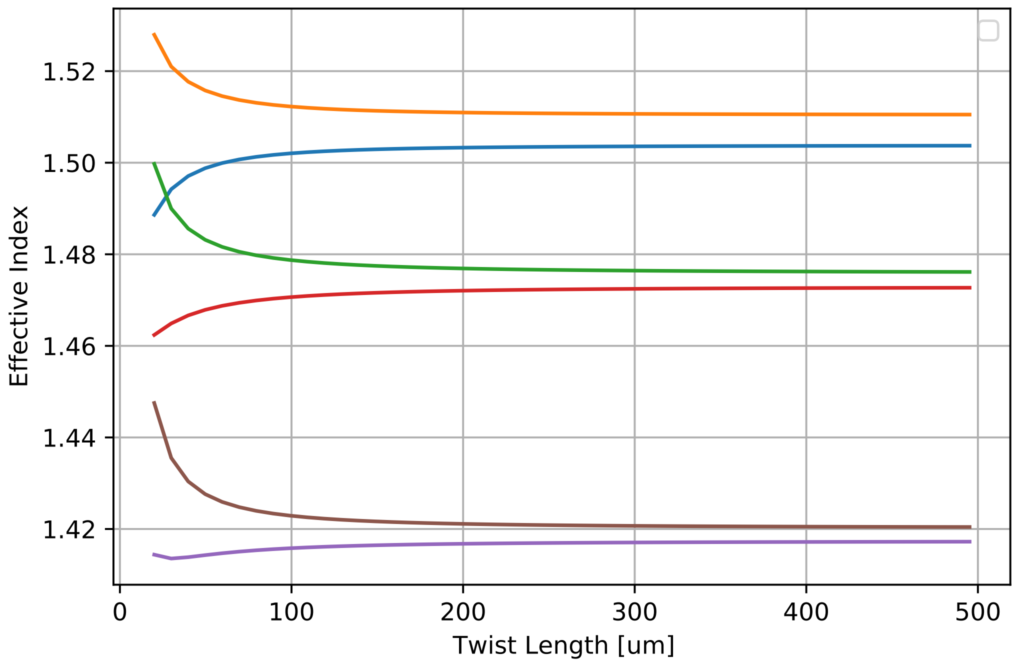

Figure 1. Effective indices $n_{\text{eff}} = \frac{\beta}{k_0}$ of the lowest-order modes of the twisted waveguide as a function of twist length. The waveguide parameters are defined in the text.

We can see that the twist leads to divergence of the eigenvalues of the quasi-TE and -TM modes of the like order. In the case of very strong twist, eigenvalues of the modes of different order can even cross. This is quite a curious effect since at the crossing point the modes degenerate. Thorough analysis of this effect is the matter of our further research.

Figure 2 shows the electric field of the fundamental quasi-TE mode for different twist rates. In the absence of twist (see Figure 2(a)) almost all mode power is stored in X polarization. When the twist rate is rather small (see Figure 2(b)), the field patterns still closely resemble the unperturbed ones. In this regime, as we will see later, the waveguide works as an adiabatic polarization converter. In the regime of rapid twist (see Figure 2(c)) e_Y component becomes comparable with e_X component. This indicates the breakdown of adiabaticity of polarization rotation. Namely, the polarization rotation ceases being synchronous with the waveguide core twist.

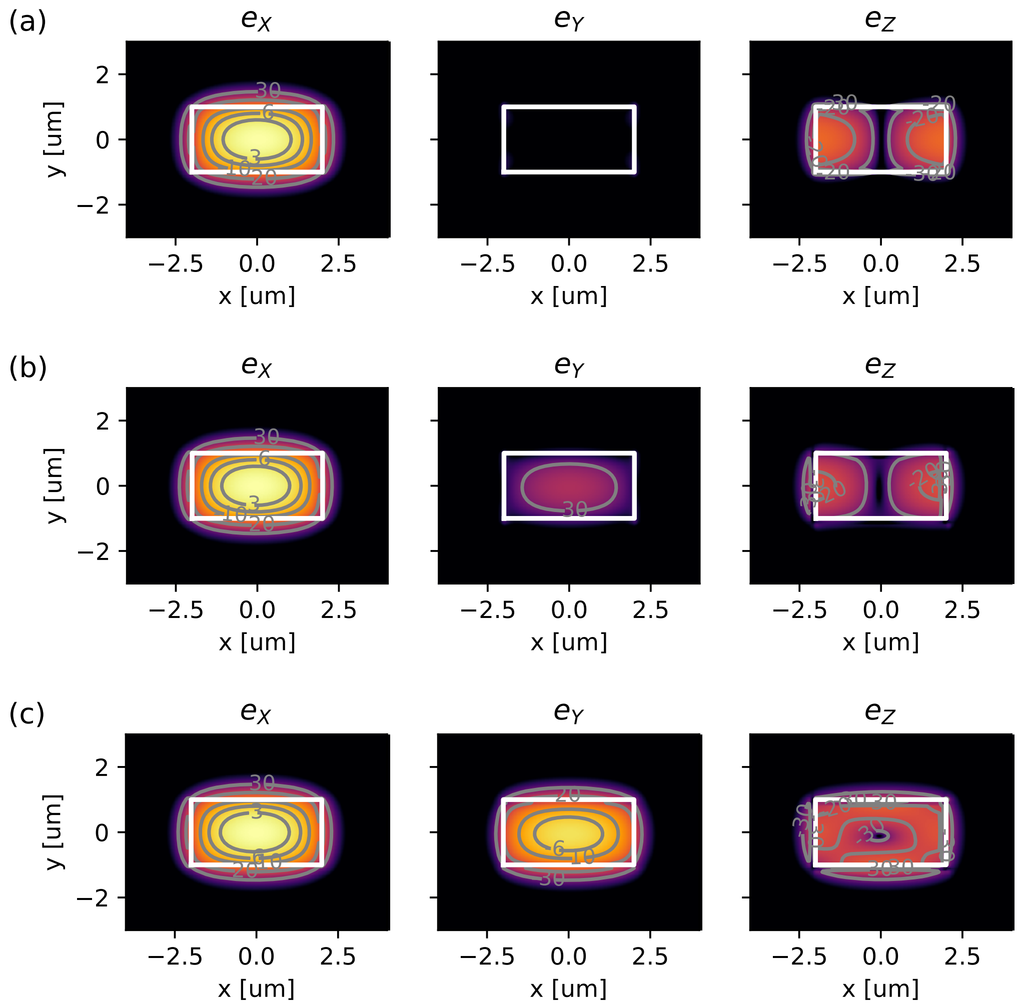

Figure 2. Modal electric field of the fundamental quasi-TE mode for (a) untwisted, (b) and (c) twisted waveguide with twist length $L = 1000$ μm and $L = 60$ μm

6.3 Polarization Conversion

We have tested the ability of the developed twisted EME (tEME) method to correctly predict polarization conversion by twisted waveguide. We have launched the fundamental quasi-TE mode of the straight (untwisted) waveguide into twisted waveguide. The results are shown in Figures 3 and 4. Figure 3 demonstrates the slice of the simulated fields within the plane $y = 0$ in the straight waveguide region and within the curved surface $Y = 0$ in the twisted waveguide region.

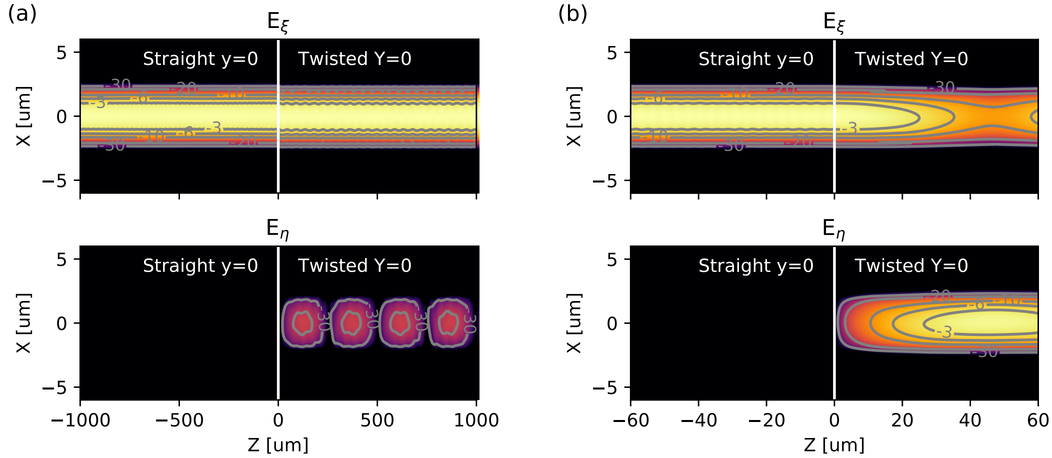

Figure 3. Simulated propagation in twisted waveguide with the twist length (a) 1000 μm, (b) 60 μm. Waveguide parameters are defined in the text.

It is seen, that in accordance with our considerations, when the twist is rather slow (twist length $L = 1000$ μm, Figure 3(a)), the adiabatic regime is observed: almost all power remains in E_ξ component, which means that the polarization twists synchronously with the waveguide core. On the other hand, when the twist is non-adiabatic (twist length $L = 60$ μm, Figure 3(b)), significant part of the power migrates to E_η component, which means that the polarization is no more aligned with the waveguide core and, consequently, polarization conversion is far from perfect.

In the Figure 3(a) one can observe small oscillations in E_η component. They arise from interference of multiple excited twisted waveguide modes. We claim, that this interference is responsible for non-monotonic behavior of polarization conversion efficiency with respect to twist length, observed in[2] and Figure 5.

Figure 4 additionally shows the transverse electric field at the output facet.

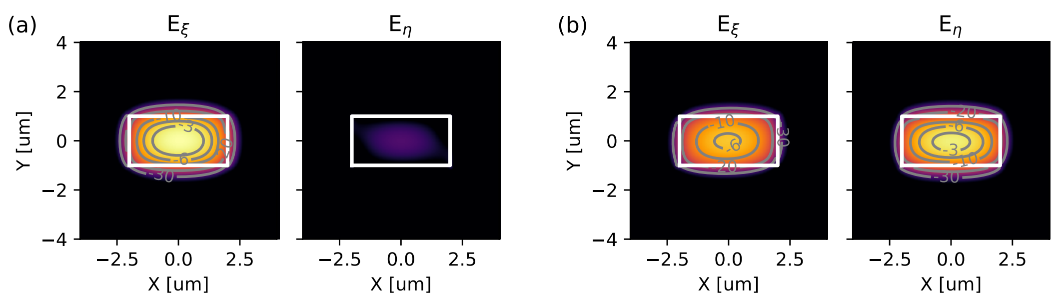

Figure 4. Transverse electric field at the output facet of twisted waveguide with the twist length (a) 1000 μm, (b) 60 μm. Waveguide parameters are defined in the text.

To quantitatively analyze polarization conversion efficiency (PCE) we use a similar definition to the one used by Hou *et al.*

$$\eta = \frac{\int_{z=L} |E_y|^2 dA}{\int_{z=L} |E_x|^2 dA}, \tag{43}$$

where E_y and E_x are taken at the output facet of the twisted waveguide. We compared the results obtained within our modal approach with BPM simulations and found excellent agreement. The results of PCE calculation are shown in Figure 5. One can see that starting from twist length of approximately 250 μm PCE oscillates around 90-100 %. This corresponds to adiabatic polarization conversion. The oscillations occur due to interference of different excited twisted waveguide modes.

Our results agree well with the results for the similar waveguide studied by Hou *et al.*[?] These results prove viability of the developed approach.

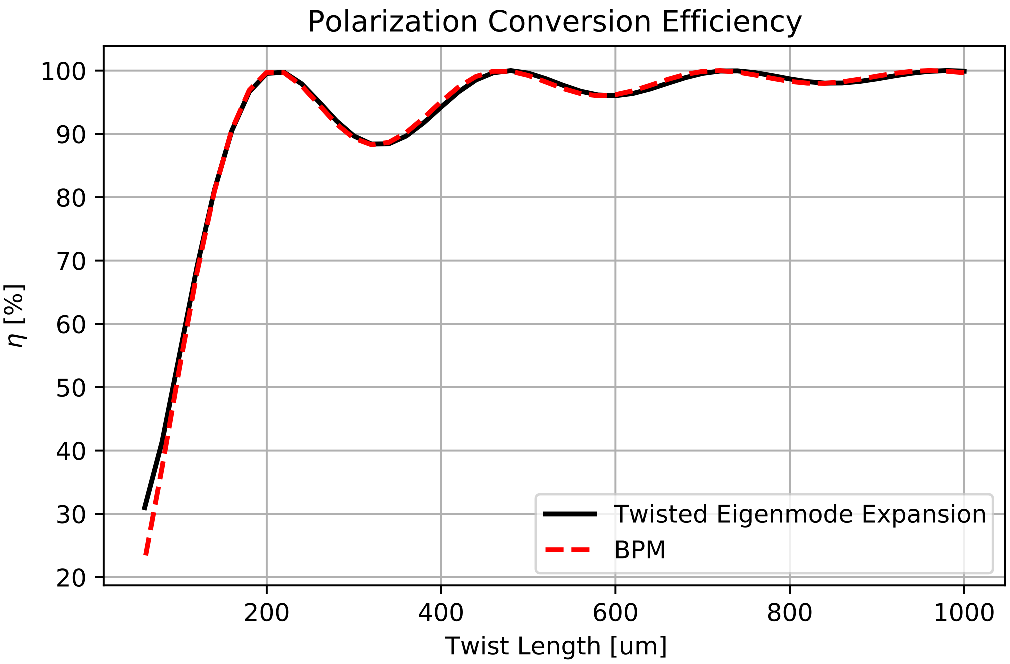

Figure 5. Polarization conversion efficiency of the studied twisted waveguide as a function of twist length. Waveguide parameters are defined in the text.

7. SUMMARY

To conclude, we have rigorously defined an eigenmode of a twisted waveguide as a natural generalization of the eigenmode of a straight waveguide. Using covariant approach, we have obtained the eigenmode equation which is nonlinear with respect to eigenvalue, or propagation constant. For solving the eigenmode equation we have combined the NLEVP solver with a Yee-grid-based finite-difference full-vectorial scheme, which we developed specifically. By analyzing the obtained propagation constants and modal fields we have explained the modal mechanism of polarization rotation. We want to stress, that although optics applications are of our primary concern in this work, our results are general and apply to twisted waveguides of arbitrary nature. We believe that our results can facilitate further investigations of more advanced on-chip devices that use twisted waveguide as a basis element, e.g., couplers and Möbius rings. Such devices can possess unique polarimetric features and may find applications in polarization-encoded telecommunications as well as quantum information technologies.

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