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Modeling the impact of imperfections in high-index-contrast photonic waveguides

M. Skorobogatiy*
École Polytechnique de Montréal, Génie physique, Montréal, Quebec, Canada H3C 3A7
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By formulating Maxwell's equations in perturbation-matched curvilinear coordinates, we have derived rigorous perturbation theory (PT) and coupled-mode theory expansions that are applicable in the case of generic nonuniform dielectric profile perturbations in high-index-contrast waveguides, including photonic band gap fibers, and two-dimensional (2D) and 3D waveguides. PT is particularly useful in the optimization stage of a component design process where fast evaluation of an optimized property with changing controlling variables is crucial. We demonstrate our method by studying radiation scattering due to common geometric variations in planar 2D photonic crystals waveguides.

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I. INTRODUCTION

Standard perturbation theory (PT) and coupled-mode theory (CMT) formulations are known to fail or exhibit a very slow convergence [1–6] when applied to the analysis of geometrical variations in the structure of high-index-contrast waveguides. In (CMT) framework applied to uniform waveguides (the waveguide profile remains unchanged along the direction of propagation), eigenvalues of the matrix of coupling elements approximate the values of the propagation constants of a uniform waveguide of perturbed cross section. When a large enough number of modes are included CMT, in principle, should converge to an exact solution for perturbations of any strength. Perturbation theory is a numerically more efficient method than coupled-mode theory, but it is mostly applicable to the analysis of small perturbations. For stronger perturbations, higher-order perturbation corrections must be included, converging, in the limit of higher orders, to an exact solution. To analyze nonuniform waveguides (waveguide profile is changing along the direction of propagation) within coupled-mode and perturbation theory frameworks one propagates the modal coefficients along the length of a waveguide using a first-order differential equation involving a matrix of coupling elements. Both uniform and nonuniform coupled-mode and perturbation theory expansions rely on the knowledge of correct coupling elements.

The conventional approach to the evaluation of the coupling elements proceeds by expansion of the solution for the fields in a perturbed waveguide into the modes of an unperturbed system, then computes a correction to the Hamiltonian of a problem due to the perturbation in question, and, finally, computes the required coupling elements. Unfortunately, this approach encounters difficulties when applied to the problem of finding perturbed electromagnetic modes in waveguides with shifted high-index-contrast dielectric boundaries. In particular, for a uniform geometric perturbation of a fiber profile with abrupt high-index-contrast dielectric interfaces, expansion of the perturbed modes into an increasing number of modes of an unperturbed system does not converge to a correct solution when the standard form of the coupling elements [7,8] is used. The mathematical reasons for such a failure are still not completely understood but probably lie either in the *incompleteness* of the basis of eigenmodes of an unperturbed waveguide in the domain of the eigenmodes of a perturbed waveguide or in the fact that the standard mode orthogonality conditions (Sec. IV A) do not constitute strict norms. We would like to point out that standard coupled-mode theory can still be used even in the problem of finding modes of a high-index-contrast waveguide with sharp dielectric interfaces. One can calculate such modes by using as an expansion basis eigenmodes of some reference waveguide with a "smooth" dielectric profile (empty metallic waveguide, for example). However, the convergence of such a method with respect to the number of basis modes is slow (linear). The perturbation formulation within this approach is also problematic, and even for small geometric variations of the waveguide profile matrix of the coupling element has to be recomputed anew. Other methods developed to deal with shifting metallic boundaries and dielectric interfaces originate primarily from the works on metallic waveguides and microwave circuits [9–14]. Dealing with nonuniform waveguides, these formulations usually employ an expansion basis of the "instantaneous modes." Such modes have to be recalculated at each different waveguide cross section, leading to potentially computationally demanding propagation schemes. When high-index waveguides exhibit only cylindrical features the multipole method and its derivatives could be used to analyze the eigenmodes and scattering in such waveguides [15–19]; however, these methods do not allow a perturbative formulation. Finally, time domain codes [20] are usually difficult to apply to the analysis of small variation and imperfections as one has to use meshes fine enough to resolve the imperfections, and model large propagation distances over which the effects of small variations become discernable. Similarly, frequency domain and mode matching methods [21–25] require large supercells and fine resolution to capture the impact of small perturbations.

In this paper we introduce a method of evaluating the coupling elements which is valid for any smooth geometrical waveguide profile variations and high-index contrast using the eigenmodes of an unperturbed waveguide (to which we

*Electronic address: maksim.skorobogatiy@polymtl.ca

refer as a reference waveguide) as an expansion basis. This paper presents a generalization of an earlier method developed to analyze imperfections in high-index-contrast fibers [1,30]. The main idea of our method is to introduce a coordinate transformation that maps a dielectric profile of a reference waveguide (whose eigenmodes are assumed to be known) onto a dielectric profile of a perturbed waveguide. Such mappings can be either defined analytically or computed numerically. Transforming Maxwell's equations into a curvilinear system where the dielectric profile is unperturbed we can use the eigenmodes of a reference waveguide as an expansion basis. These modes will be now coupled due to the curvature of space, which is, in turn, proportional to the strength of the perturbation in question. Another interpretation of the same methodology is to use the eigenmodes of a reference waveguide and to stretch them using a coordinate mapping in such a way as to make the discontinuities in their fields to coincide with the position of the perturbed dielectric interfaces and to finally use such stretched, perturbation fitted modes as an expansion basis. In further discussions we formulate geometrical waveguide profile variations in terms of a smooth mapping of an unperturbed dielectric profile onto a perturbed one. Given a perturbed dielectric profile $\epsilon(x,y,z)$ in a Euclidian system of coordinates (x,y,z) (where z is a general direction of propagation) we define a mapping $\mathbf{(}x(q^1,q^2,s),y(q^1,q^2,s),z(q^1,q^2,s)\mathbf{)}$ such that $\epsilon(q^1,q^2,s)$ corresponds to a dielectric profile of a reference waveguide in a curvilinear coordinate system associated with (q^1,q^2,s) (where s is a direction of propagation). We then perform a coordinate transformation from a Euclidian coordinate system (x,y,z) into a corresponding curvilinear coordinate system (q^1,q^2,s) by rewriting Maxwell's equations in such a curvilinear coordinate system. Finally, as the dielectric profile in a coordinate system (q^1,q^2,s) is that of a reference waveguide, we can use the basis set of its eigenmodes in (q^1,q^2,s) coordinates to calculate coupling matrix elements due to the geometrical variations of a waveguide profile.

Our paper is organized as following. We first describe some typical geometrical variations of two-dimensional (2D) waveguide profiles. Next, we discuss the properties of generic curvilinear coordinate transformations and formulate Maxwell's equations in a curvilinear coordinate system. We apply this formulation to develop the coupled-mode and perturbation theories using eigenstates of an unperturbed waveguide as an expansion basis. We conclude with analysis of several typical variations in 2D waveguides.

II. GEOMETRICAL VARIATIONS OF WAVEGUIDE PROFILES

We start by considering several common geometrical variations of waveguide profiles that can be either deliberately designed or arise during manufacturing as imperfections. Let (x,y,z) correspond to Euclidian coordinate system. In Fig. 1(a) an ideal 2D photonic crystal waveguide is presented. In what follows the operation frequency and all the waveguide dimensions are chosen for a reference waveguide to be single moded, with forward and backward propagating fundamental modes confined by the band gap of the reflector.

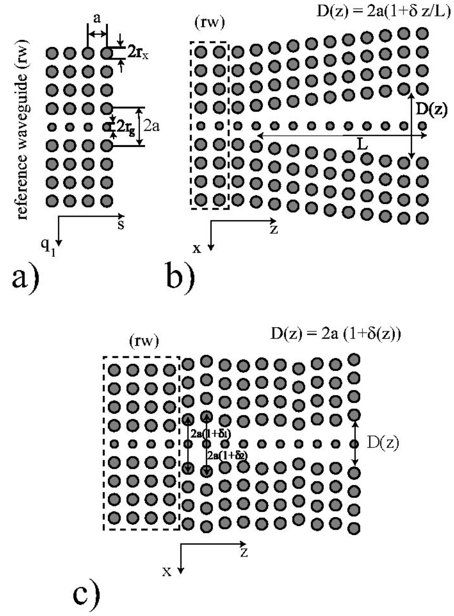

FIG. 1. (a) Dielectric profile of a reference 2D photonic crystal waveguide as formed in a square array of dielectric poles in air by a linear sequence of somewhat smaller dielectric poles. (b) Linear taper in a photonic crystal with "unzipping" photonic mirror. (c) Stochastic variations in a waveguide core size along the direction of propagation.

In Fig. 1(b) the photonic crystal taper with "unzipping" mirror is presented. When the core size is increased sufficiently, the fundamental mode becomes purely guided by the high index of the remaining corrugated waveguide. In Fig. 1(c) a waveguide with arbitrarily changing core size along the direction of propagation is presented. When such variations are small and random one can consider them to be a model of roughness.

We now define a dielectric profile mapping of a reference photonic crystal waveguide, Fig. 1(a), onto a waveguide with a changing core size, Fig. 1(c), by using the mapping $x=q_1+f_x(q_1)f_z(s), y=q_2, z=s$, where auxiliary functions $f_x(q_1)$ and $f_z(s)$ are chosen to be as in Fig. 2. As seen from this figure, in each of the unit cells along the waveguide length the functions $f_x(q_1)$ and $f_z(s)$ are defined in such a way as to translate the reflector rods along the x direction by an appropriate value of the core size change, while leaving the smaller rods

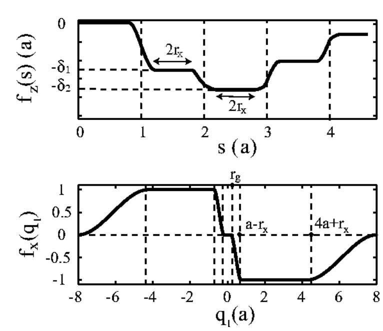

FIG. 2. Auxiliary functions for the coordinate mapping of a reference 2D photonic crystal waveguide [Fig. 1(a)] onto a waveguide of a changing core size [Fig. 1(c)].

of a defect waveguide intact. These auxiliary functions and their first derivatives have to be continuous everywhere. Although only the variations in the waveguide core size are considered in this paper, the CMT derived in this article is general. For other variations the corresponding coordinate mappings can be computed analytically or numerically from the original and final positions of the dielectric interfaces.

III. CURVILINEAR COORDINATE SYSTEMS

Following [26,27], we first introduce general properties of the curvilinear coordinate transformations. Let (x^1,x^2,x^3) be the coordinates in a Euclidian coordinate system. We introduce a smooth mapping (requiring continuity of the functions and all their partial derivatives in the computation domain) into a new coordinate system with coordinates (q^1,q^2,q^3) as $\mathbf{(}x^1(q^1,q^2,q^3),x^2(q^1,q^2,q^3),x^3(q^1,q^2,q^3)\mathbf{)}$. A new coordinate system can be characterized by its covariant basis vectors $\vec{a}_i$ defined in the original Euclidian system as $\vec{a}_i=(\partial x^1/\partial q^i,\partial x^2/\partial q^i,\partial x^3/\partial q^i)$. Now, define the reciprocal (contravariant) vector $\vec{a}^i$ as $\vec{a}^i=(1/\sqrt{g})\vec{a}_j\times\vec{a}_k$, $(k,j)\neq i$, where the metric g_{ij} is defined as $g_{ij}=(\partial x^k/\partial q^i)(\partial x^k/\partial q^j)$, and $g=\det(g_{ij})$. Vectors $\vec{a}_i$ and their reciprocal $\vec{a}^i$ satisfy the orthogonality conditions $\vec{a}^i\cdot\vec{a}_j=\delta_{i,j}$, $\vec{a}_i\cdot\vec{a}_j=g_{ij}$, and $\vec{a}^i\cdot\vec{a}^j=g^{ij}$, where g^{ij} is an inverse of the metric g_{ij}. In general, a vector may be represented by its covariant components $\vec{E}=e_i\vec{a}^i$ or by its contravariant components $\vec{E}=e^i\vec{a}_i$. These components might have unusual dimensions because the underlying vectors $\vec{a}_i$ and $\vec{a}^i$ are not properly normalized in a Euclidian coordinate system. Components having the usual dimensions are defined by $E_i=e_i/\sqrt{g^{ii}}$, $E^i=e^i/\sqrt{g_{ii}}$, and $\vec{E}=e_i\vec{a}^i=E_i\vec{i}^i$ and $\vec{E}=e^i\vec{a}_i=E^i\vec{i}_i$, where $\vec{i}_i$ and $\vec{i}^i$ are unitary vectors. Normalized covariant and contravariant components are connected by $E_i=G_{ij}E^j$ and $E^i=G^{ij}E_j$ where $G_{ij}=(\sqrt{g^{ii}/g_{jj}})g_{ij}$ and $G^{ij}=(\sqrt{g_{ii}/g^{jj}})g^{ij}$. For orthogonal coordinate systems the metric matrixes are diagonal and for the regular orthogonal and polar coordinate systems they are $g^{0xx}=1$, $g^{0yy}=1$, $g^{0zz}=1$, $g^0=1$ and $g^{0\rho\rho}=1$, $g^{0\theta\theta}=1/\rho^2$, $g^{0zz}=1$, $g^0=\rho^2$, correspondingly.

IV. COUPLED-MODE THEORY FOR MAXWELL'S EQUATIONS IN CURVILINEAR COORDINATES

In the following, we summarize coupled-mode theory for Maxwell's equations in curvilinear coordinates to treat radiation propagation in generic nonuniform waveguides. The Hamiltonian formulation of Maxwell's equations in regular Euclidian coordinates is detailed in [2,3,13], while the Hamiltonian formulation and coupled-mode theory in curvilinear perturbation-matched coordinates for the case of uniform and nonuniform fibers of arbitrary cross sections is detailed in [3,4,30].

The form of Maxwell's equations in curvilinear coordinates can be found in a variety of references [26–29]. Assuming the standard time dependence of the electromagnetic fields $\mathbf{F}(q_1,q_2,q_3,t)=\mathbf{F}(q_1,q_2,q_3)\exp(-i\omega t)$ [$\mathbf{F}=(E_{q_1}/\sqrt{g^{11}}; E_{q_2}/\sqrt{g^{22}}; E_{q_3}/\sqrt{g^{33}}; H_{q_1}/\sqrt{g^{11}}; H_{q_2}/\sqrt{g^{22}}; H_{q_3}/\sqrt{g^{33}})$ denotes a 6 component column vector of the electromagnetic fields] these expressions are compactly presented in terms of the normalized covariant components of the fields, and in the absence of free electric currents they are

$$-i\omega\epsilon(q^1,q^2,q^3)D^{ij}\frac{E_j}{\sqrt{g^{jj}}}=e^{ijk}\frac{\partial\dfrac{H_k}{\sqrt{g^{kk}}}}{\partial q^j},$$

$$i\omega\mu(q^1,q^2,q^3)D^{ij}\frac{H_j}{\sqrt{g^{jj}}}=e^{ijk}\frac{\partial\dfrac{E_k}{\sqrt{g^{kk}}}}{\partial q^j}, \tag{1}$$

where $D^{ij}=\sqrt{g}g^{ij}$ and e^{ijk} is a Levi-Cività symbol.

A. Modal orthogonality relations and normalization

In the following we assume that reference waveguide is either uniform (planar waveguide, fiber) or strictly periodic (photonic crystal waveguide, fiber grating) along the direction of propagation $q^3=s$. This implies that both ϵ_0 and μ_0 (marking parameters related to reference waveguide with a subscript zero) either do not depend on s or they are periodic functions of s. We assume that eigenmodes and eigenvalues of a reference waveguide are found in a coordinate system with a diagonal (non-necessarily unitary) space metric corresponding to orthogonal coordinate system. Several orthogonality relations between the eigen modes of a reference waveguide are possible.

A norm operator $\hat{B}$ and its matrix representation [13] can be introduced as

$$\hat{B}=\begin{pmatrix}0&0&0&0&1&0\\0&0&0&-1&0&0\\0&0&0&0&0&0\\0&-1&0&0&0&0\\1&0&0&0&0&0\\0&0&0&0&0&0\end{pmatrix}, \tag{2}$$

relating the transverse components of the eigenfields. Depending upon the symmetry of a reference waveguide several orthogonality relations are possible.

If reference waveguide profile is uniform along s, then the eigenfields have an additional symmetry $\mathbf{F}(q^1,q^2,s)=\mathbf{F}_\beta(q^1,q^2)\exp(i\beta s)$.

(i) If ϵ_0 and μ_0 are strictly real, we introduce Dirac notation as $|\beta\rangle=\mathbf{F}_\beta(q^1,q^2)$ and $\langle\beta|=\mathbf{F}^+_\beta(q^1,q^2)$ and a product operator $\langle\beta_i|\hat{O}|\beta_j\rangle=\int_{cros}dq^1dq^2\mathbf{F}^+_{\beta_i}(q^1,q^2)O\mathbf{F}_{\beta_j}(q^1,q^2)$, where O is a 6×6 operator matrix and integration is performed over the waveguide cross section. Then, for any two eigenmodes labeled by their propagation constants β_i, β_j the eigenmodes can be normalized as $\langle\beta_i|\hat{B}|\beta_j\rangle=\delta_{\beta_i^*,\beta_j}\eta_{\beta_j}$ and $|\eta_{\beta_j}|=1$.

(ii) If ϵ_0 or μ_0 has a complex part, we introduce Dirac notation as $|\beta\rangle=\mathbf{F}_\beta(q^1,q^2)$ and $\langle\beta|=\mathbf{F}_\beta(q^1,q^2)$, (no complex conjugation) and a product operator $\langle\beta_i|\hat{O}|\beta_j\rangle=\int_{cros}dq^1dq^2\mathbf{F}^T_{\beta_i}(q^1,q^2)O\mathbf{F}_{\beta_j}(q^1,q^2)$, where integration is performed over the waveguide cross section. Then for any two eigenmodes labeled by their propagation constants β_i, β_j the eigenmodes can be normalized as $\langle\beta_i|\hat{B}|\beta_j\rangle=\delta_{\beta_i,\beta_j}\eta_{\beta_j}$ and $|\eta_{\beta_j}|=1$.

If unperturbed waveguide profile is periodic along s with period Λ, then according to the Bloch-Floquet theorem the eigenfields still retain a symmetry $\mathbf{F}(q^1,q^2,s)=\mathbf{F}_\beta(q^1,q^2,s)\exp(i\beta s)$, where $\mathbf{F}_\beta(q^1,q^2,s)=\mathbf{F}_\beta(q^1,q^2,s+\Lambda)$. If ϵ_0 and μ_0 are strictly real, we introduce Dirac notation as $|\beta\rangle=\mathbf{F}_\beta(q^1,q^2,s)$ and $\langle\beta|=\mathbf{F}^+_\beta(q^1,q^2,s)$, as well as a product operator $\langle\beta_i|\hat{O}|\beta_j\rangle=\int_{cell}dq^1dq^2ds\mathbf{F}^+_{\beta_i}(q^1,q^2,s)O\mathbf{F}_{\beta_j}(q^1,q^2,s)$, where O is a 6×6 operator matrix and integration is performed over the whole unit cell of a periodic waveguide. Then for any two eigenmodes labeled by their propagation constants β_i, β_j the eigenmodes can be normalized as $\langle\beta_i|\hat{B}|\beta_j\rangle=\delta_{\beta_i^*,\beta_j}\eta_{\beta_j}$ and $|\beta_j|=1$. Moreover, a corollary of the Bloch-Floquet theorem states that the eigenmodes at β and $\beta+2\pi l/\Lambda$ are equivalent for any integer l, and thus $|\beta+2\pi l/\Lambda\rangle=\exp(-2\pi i l/\Lambda z)|\beta\rangle$. This implies that it suffices to choose all the eigenvalues β in the first Brillouin zone $\mathrm{Re}(\beta)\in(-\pi/\Lambda,\pi/\Lambda]$, and for such modes the definition of the norm can be furthermore relaxed to be $\langle\beta_i|\hat{B}|\beta_j\rangle=\int_{cell}dq^1dq^2ds\mathbf{F}^+_{\beta_i}(q^1,q^2,s)B\mathbf{F}_{\beta_j}(q^1,q^2,s)=\Lambda\int_{cros}dq^1dq^2\mathbf{F}^+_{\beta_i}(q^1,q^2,s)B\mathbf{F}_{\beta_j}(q^1,q^2,s)$, where the integral over a reference waveguide cross section is invariant for any cross section (any s) in the first Brilloun zone. Thus, the definition of the norm in the case of real ϵ_0 and μ_0 for periodic and uniform waveguides can be chosen to be the same.

B. Expansion basis

We now construct an expansion basis to treat radiation propagation in a perturbed waveguide using the eigenfields of a reference waveguide in the perturbation matched curvilinear coordinate system. Equivalently, in the Euclidian coordinate system associated with a perturbed waveguide we construct an expansion basis from the eigenfields of an unperturbed waveguide by spatially stretching them in such a way as to match the regions of discontinuity in their field components with the position of the perturbed dielectric interfaces. Finally, we find expansion coefficients by satisfying Maxwell's equations. In the following, we first define an expansion basis and then demonstrate how perturbation theory and a coupled mode theory can be formulated in such a basis.

Let (x,y,z) to define a Euclidian coordinate system associated with a perturbed waveguide and (q^1,q^2,s) be a coordinate system corresponding to an unperturbed waveguide, where s is a direction of propagation, with corresponding smooth coordinate transformation relating the two coordinate systems being $\mathbf{(}x(q^1,q^2,s),y(q^1,q^2,s),z(q^1,q^2,s)\mathbf{)}$. Using the transverse eigenfields of a reference waveguide expressed in the coordinates (q^1,q^2,s) we form an expansion basis in the Euclidian coordinate system (x,y,z) as follows:

$$|\Psi_\beta\rangle=\begin{pmatrix}\dfrac{E^0_{q^1}(q^1(x,y,z),q^2(x,y,z),s(x,y,z))}{\sqrt{g^{0q^1q^1}}}\vec{i}^{q^1}+\dfrac{E^0_{q^2}(q^1(x,y,z),q^2(x,y,z),s(x,y,z))}{\sqrt{g^{0q^2q^2}}}\vec{i}^{q^2}\\ \dfrac{H^0_{q^1}(q^1(x,y,z),q^2(x,y,z),s(x,y,z))}{\sqrt{g^{0q^1q^1}}}\vec{i}^{q^1}+\dfrac{H^0_{q^2}(q^1(x,y,z),q^2(x,y,z),s(x,y,z))}{\sqrt{g^{0q^2q^2}}}\vec{i}^{q^2}\end{pmatrix}_\beta. \tag{3}$$

There are several important properties that basis vector fields (3) possess. First, if the coordinate transformation is orthogonal $(\vec{i}^{q\{1,2,3\}}=\vec{i}_{q\{1,2,3\}})$, then one can show that any two basis fields of Eq. (3) are orthogonal in the sense of the orthogonality condition discussed in Sec. IV A. Moreover, in the case of nonorthogonal smooth transformations, basis fields (3) will be almost orthogonal with an amount of nonorthogonality proportional to the strength of perturbation. Second, the regions of discontinuity in the field components of the basis fields (3), by construction, coincide with the positions of the perturbed dielectric interfaces.

C. Coupled-mode theory

Maxwell's equations in curvilinear coordinates (1), while seemingly complicated, involve an unperturbed dielectric profile $\epsilon(q^1,q^2,s)$. We look for a solution of Maxwell's equations (1) in terms of the basis fields (3) which in the (q^1,q^2,s) coordinate system are the eigenfields of a reference waveguide entering with corresponding coefficients $C^\beta(s)$ coordinates varying along the direction of propagation. Thus, in the covariant coordinates for both uniform and periodic waveguides we look for a solution in the form

$$\begin{pmatrix} \dfrac{E_{q^1}(q^1,q^2,s)}{\sqrt{g^{q^1q^1}}} \\ \dfrac{E_{q^2}(q^1,q^2,s)}{\sqrt{g^{q^2q^2}}} \\ \dfrac{H_{q^1}(q^1,q^2,s)}{\sqrt{g^{q^1q^1}}} \\ \dfrac{H_{q^2}(q^1,q^2,s)}{\sqrt{g^{q^2q^2}}} \end{pmatrix} = \sum_{\beta_j} C^{\beta_j}(s) \begin{pmatrix} \dfrac{E^0_{q^1}(q^1,q^2,s)}{\sqrt{g^{0q^1q^1}}} \\ \dfrac{E^0_{q^2}(q^1,q^2,s)}{\sqrt{g^{0q^2q^2}}} \\ \dfrac{H^0_{q^1}(q^1,q^2,s)}{\sqrt{g^{0q^1q^1}}} \\ \dfrac{H^0_{q^2}(q^1,q^2,s)}{\sqrt{g^{0q^2q^2}}} \end{pmatrix}_{\beta_j} . \qquad (4)$$

Note that for a uniform reference waveguide, the expansion fields (3) are functions of (q^1,q^2) only, and for both uniform and periodic reference waveguides basis fields are stripped of the phase factor $\exp(i\beta z)$. Substituting expansion (4) into Eq. (1), expressing s components of the fields through the transverse components, using the orthogonality relations of Sec. IV A, and manipulating the resultant expressions we arrive at the following equation:

$$B\frac{\partial \vec{C}(s)}{\partial s} = i[B\mathcal{B}_0 + \Delta M(s)]\vec{C}(s), \qquad (5)$$

where $B_{\beta_i,\beta_j} = \langle \beta_i | \hat{B} | \beta_j \rangle$ is a constant normalization matrix, $\mathcal{B}_0$ is a diagonal matrix of eigenvalues of an unperturbed reference waveguide, and $\Delta M(s)$ is a matrix of coupling elements given by

$$\Delta M_{\beta_i,\beta_j}(s) = \omega \int_{cros} dq^1 dq^2 \begin{pmatrix} \dfrac{E^0_{q^1}(q^1,q^2,s)}{\sqrt{g^{0q^1q^1}}} \\ \dfrac{E^0_{q^2}(q^2,q^2,s)}{\sqrt{g^{0q^2q^2}}} \\ \dfrac{E^0_{s}(q^1,q^2,s)}{\sqrt{g^{0ss}}} \\ \dfrac{H^0_{q^1}(q^1,q^2,s)}{\sqrt{g^{0q^1q^1}}} \\ \dfrac{H^0_{q^2}(q^1,q^2,s)}{\sqrt{g^{0q^2q^2}}} \\ \dfrac{H^0_{s}(q^1,q^2,s)}{\sqrt{g^{0ss}}} \end{pmatrix}^{\dagger,T}_{\beta_i} \begin{pmatrix} d\epsilon_{q^1q^1} & d\epsilon_{q^1q^2} & d\epsilon_{q^1s} & 0 & 0 & 0 \\ d\epsilon_{q^2q^1} & d\epsilon_{q^2q^2} & d\epsilon_{q^2s} & 0 & 0 & 0 \\ d\epsilon_{sq^1} & d\epsilon_{sq^2} & d\epsilon_{ss} & 0 & 0 & 0 \\ 0 & 0 & 0 & d\mu_{q^1q^1} & d\mu_{q^1q^2} & d\mu_{q^1s} \\ 0 & 0 & 0 & d\mu_{q^2q^1} & d\mu_{q^2q^2} & d\mu_{q^2s} \\ 0 & 0 & 0 & d\mu_{sq^1} & d\mu_{sq^2} & d\mu_{ss} \end{pmatrix} \begin{pmatrix} \dfrac{E^0_{q^1}(q^1,q^2,s)}{\sqrt{g^{0q^1q^1}}} \\ \dfrac{E^0_{q^2}(q^2,q^2,s)}{\sqrt{g^{0q^2q^2}}} \\ \dfrac{E^0_{s}(q^1,q^2,s)}{\sqrt{g^{0ss}}} \\ \dfrac{H^0_{q^1}(q^1,q^2,s)}{\sqrt{g^{0q^1q^1}}} \\ \dfrac{H^0_{q^2}(q^1,q^2,s)}{\sqrt{g^{0q^2q^2}}} \\ \dfrac{H^0_{s}(q^1,q^2,s)}{\sqrt{g^{0ss}}} \end{pmatrix}_{\beta_j}, \qquad (6)$$

where integration is performed over an unperturbed waveguide profile. Complex conjugation of the field on the left of the matrix of coupling elements can be used when ϵ_0 and μ_0 are real and the reference waveguide is either uniform or periodic. The unconjugated product can only be used with a uniform reference waveguide while an arbitrary (real or complex) ϵ_0 and μ_0 as described in Sec. IV A. Assuming that the eigenfields of an unperturbed waveguide were found in a diagonal metric, nonzero elements of 6×6 matrix $\Delta\hat{M}(s)$ are

$$d\epsilon_{q^1q^1} = \epsilon D^{q^1q^1} - \epsilon_0 D_0^{q^1q^1} - \epsilon\frac{(D^{q^1s})^2}{D_{ss}}, \quad d\mu_{q^1q^1} = \mu D^{q^1q^1} - \mu_0 D_0^{q^1q^1} - \mu\frac{(D^{q^1s})^2}{D_{ss}},$$

$$d\epsilon_{q^1q^2} = d\epsilon_{q^2q^1} = \epsilon\left(D^{q^1q^2} - \frac{D^{q^1s}D^{q^2s}}{D_{ss}}\right), \quad d\mu_{q^1q^2} = d\mu_{q^2q^1} = \mu\left(D^{q^1q^2} - \frac{D^{q^1s}D^{q^2s}}{D_{ss}}\right),$$

$$d\epsilon_{q^1s} = d\epsilon_{sq^1} = \epsilon_0\frac{D^{q^1s}D_0^{ss}}{D_{ss}}, \quad d\mu_{q^1s} = d\mu_{sq^1} = \mu_0\frac{D^{q^1s}D_0^{ss}}{D_{ss}},$$

$$d\epsilon_{q^2q^2} = \epsilon D^{q^2q^2} - \epsilon_0 D_0^{q^2q^2} - \epsilon\frac{(D^{q^2s})^2}{D_{ss}}, \quad d\mu_{q^2q^2} = \mu D^{q^2q^2} - \mu_0 D_0^{q^2q^2} - \mu\frac{(D^{q^2s})^2}{D_{ss}},$$

$$d\epsilon_{q^2s} = d\epsilon_{sq^2} = \epsilon_0 \frac{D^{q^2s}D_0^{ss}}{D_{ss}}, \quad d\mu_{q^2s} = d\mu_{sq^2} = \mu_0 \frac{D^{q^2s}D_0^{ss}}{D_{ss}},$$

$$d\epsilon_{ss} = \epsilon_0 D_0^{ss}\left(1 - \frac{\epsilon_0 D_0^{ss}}{\epsilon D^{ss}}\right), \quad d\mu_{ss} = \mu_0 D_0^{ss}\left(1 - \frac{\mu_0 D_0^{ss}}{\mu D^{ss}}\right), \tag{7}$$

where ϵ and μ describe the profile of a perturbed waveguide (the case $\epsilon=\epsilon_0$ and $\mu=\mu_0$ corresponds to shifting material boundaries) and $D^{ij}=\sqrt{g}g^{ij}$. Note that the matrix of coupling elements $\Delta M(s)$ is symmetric or Hermitian depending upon the choice of normalization. Equation (5) presents a system of first-order linear coupled differential equations with respect to a vector of expansion coefficients $C^{\beta}(s)$. The boundary conditions such as the modal content of an incoming and an outgoing radiation define a boundary value problem that can be further solved numerically.

The presented coupled-mode theory describes completely radiation scattering in arbitrary index-contrast waveguides with shifting dielectric boundaries and changing dielectric profile. Moreover, Eq. (5) allows perturbative expansion. As the metric of a slightly perturbed coordinate system is only slightly different from the metric of an unperturbed coordinate system, that will naturally introduce a small parameter for small geometrical perturbations of waveguide profiles. For application of this theory to analysis of variations in high-index-contrast fibers see [3,4,30].

V. VARIATIONS IN 2D PHOTONIC CRYSTAL WAVEGUIDES

In further examples we study propagation of TE polarized radiation (the electric field is directed out of the xz plane) in a line defect waveguide made of a periodic sequence of high-index cylinders of radii $r_g=0.2a$ embedded in a square lattice of $r_x=0.3a$ dielectric rods of the reflector [13]. The parameter a defines the periodicity of a photonic crystal waveguide in the direction of propagation. All the dielectric rods have index $n=3.37$. Perfectly conducting boundary conditions were imposed in the x direction $\pm 8a$ from the waveguide center line. The frequency $\omega=0.25\times 2\pi c/a$ is chosen so that the waveguide formed solely by a sequence of the dielectric rods of radii $r_g=0.2a$ is guiding and is single moded, while a reference photonic crystal waveguide is also single moded guiding in the band gap of the reflector. We use asymptotically exact CAMFR [31] code to compute an expansion basis constructed of the guided and evanescent eigenmodes of an unperturbed photonic crystal waveguide defined by the first unit cell in the Fig. 1(a). A total of four guided modes with real β's (where backward and forward modes with the same absolute values of their propagation constants are counted ones) and up to 58 evanescent modes with complex propagation constants were used in the expansion basis to study convergence of the CMT. The advantage of our coupled-mode theory is the use at all points along the propagation direction of a single expansion basis precalculated in advance. This can be of great advantage for computationally demanding simulations of long structures.

A. Eigenmodes of a perturbed uniform waveguide

We first study convergence of a CMT when perturbed waveguide remains uniform along the direction of propagation [Fig. 3(a)]. For such variations, a perturbed waveguide still exhibits eigenmodes labeled by a new set of propagation constants. Presented in Fig. 3(b) is convergence of a fundamental mode propagation constant for a weakly $\delta=0.1$ and a strongly $\delta=1.0$ perturbed reference waveguide in a CMT framework. For $\delta=0.1$ (top plot), inclusion of a single forward propagating fundamental mode results in errors of only several percent, suggesting the validity of a perturbation theory regime for a variation of this magnitude. For $\delta=1.0$ (bottom plot), the variation is large and more than 30 modes are needed to reduce the errors to several percent. In both cases propagation constants calculated by CMT are compared to the propagation constants calculated by the asymptotically exact CAMFR code.

B. Scattering from abrupt variations in a waveguide core

We next study convergence of the transmitted and reflected powers from an abrupt variation in a waveguide core size. In Fig. 4(a) a single-cell defect of strength $\delta=1.0$ is presented. Scattered powers into the forward and backward propagating fundamental modes as calculated by CMT are shown in Fig. 4(b). For a strong variation of $\delta=1.0$, 30 modes are needed for convergence, while convergence is faster than linear when additional modes are added. As in the case of uniform variations, for small perturbations $\delta<0.1$ scattering coefficients can be calculated accurately with only a few modes using perturbation theory.

C. Scattering from tapers

In Fig. 5(a) a schematic of a taper between a line defect waveguide in a square lattice of dielectric rods in air and a waveguide formed by a 1D sequence of dielectric rods is presented. To the left and to the right of the taper the photonic crystal is that of a reference waveguide. Many nuances of transmission of a fundamental mode through such a taper for TE polarization have been previously studied in the instantaneous mode framework [13]. We believe that the method of instantaneous modes can be more efficient when larger variations (nonadiabatic tapers) are considered, and therefore convergence with a fixed basis is slow. However, for smaller variations (adiabatic tapers) convergence with a fixed basis is

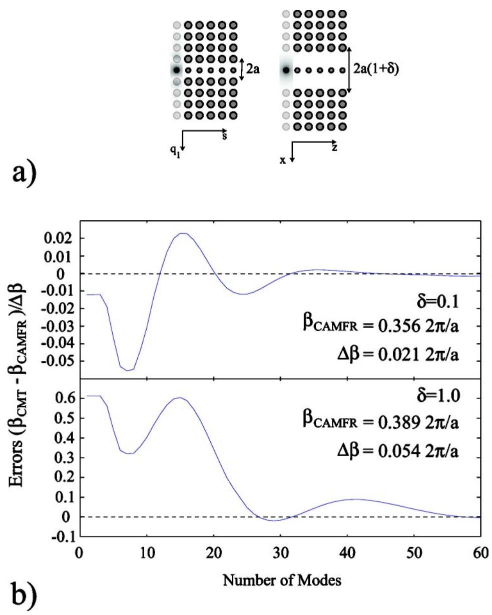

FIG. 3. (a) Schematics of a reference waveguide (left) and a perturbed uniform waveguide (right) of a larger core. Electric energy distributions in the fundamental modes are presented in the corresponding first unit cells. (b) Convergence of the fundamental mode propagation constant for a weakly $\delta=0.1$ and a strongly $\delta=1.0$ perturbed reference waveguide in a CMT framework.

efficient, while it becomes costly to recompute the instantaneous expansion basis at different cross sections, thus rendering a method employing a fixed basis to be more efficient than a method employing instantaneous modes (for a detailed discussion see [9]).

Here we investigate the magnitude of the backscattering into the backward propagating fundamental mode as a function of the taper length. In Fig. 5(b) we plot the reflected power from the "unzipping" taper of strength $\delta=0.25$ at $\omega=0.25\times 2\pi c/a$ as a function of the taper length L. The expected $1/L^2$ decrease of the reflected power for the large taper lengths $20<L<100$ is clearly observed. It was found that 16 expansion modes were enough to reduce the error in the scattering coefficients below 2%.

D. Scattering from random variations in a waveguide core size

We now calculate the strength of backscattering from small stochastic variations in a waveguide core size. The computational domain is defined by taking a reference waveguide and changing the waveguide core size (shifting the lower and upper reflector parts) in each unit cell i by $2a\delta_i$, where $2a$ is a core size of a reference waveguide [Fig. 6(a)]. The random variable δ_i is considered to be distributed according to the Gaussian distribution with variance δ. For each $\delta=0.0025$, 0.005, 0.01, 0.02 and $\omega=0.25\times 2\pi c/a$, backreflected power from a waveguide with stochastic core size variations is presented as a function of propagation distance L. Each δ curve represents an average over 30 realizations of stochastic variations [Fig. 6(b)]. First, we observe that power in the backscattered fundamental mode scales linearly with the length of propagation L, defining average scattering losses of 9.4×10^{-5} dB/a, 2.6×10^{-4} dB/a, 1.3×10^{-3} dB/a, and 4.6×10^{-3} dB/a for the corresponding δ's. One also observes δ^2 scaling of losses with perturbation strength. It was found that six expansion modes were enough to reduce the errors in the scattering coefficients below 1% for all δ's.

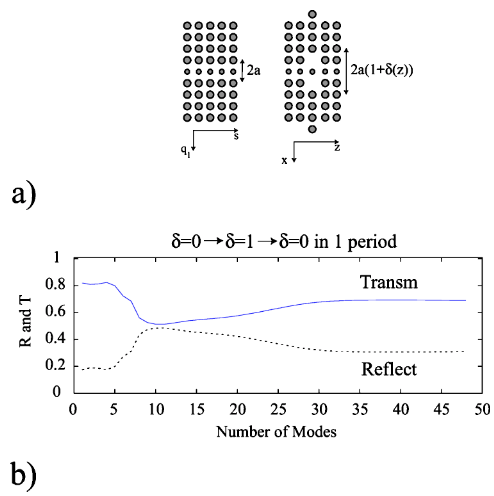

FIG. 4. (a) Schematics of a reference waveguide (left) and a single-cell defect in a reference waveguide (right). (b) Convergence of the transmitted and reflected powers into the forward and backward propagating fundamental modes as calculated by CMT and $\delta=1.0$ perturbation.

E. Compensation of geometrical variations by changing dielectric profile

Finally, we demonstrate how PT expansions can be useful to design dielectric profiles that compensate for the undes-

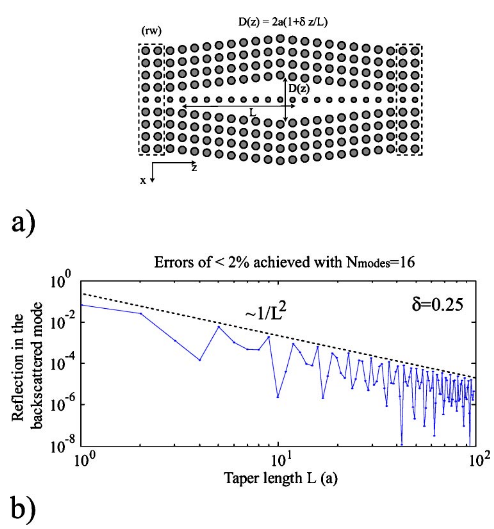

FIG. 5. (a) Taper of an "unzipping" reflector around an index guiding waveguide. To the left and to the right of the taper the photonic crystal waveguide is infinite and is described by the first unit cell of the schematic. (b) Reflected power from the taper at $\omega=0.25\times 2\pi c/a$ as a function of taper length L. Observe a $1/L^2$ decrease of the reflected power with taper length.

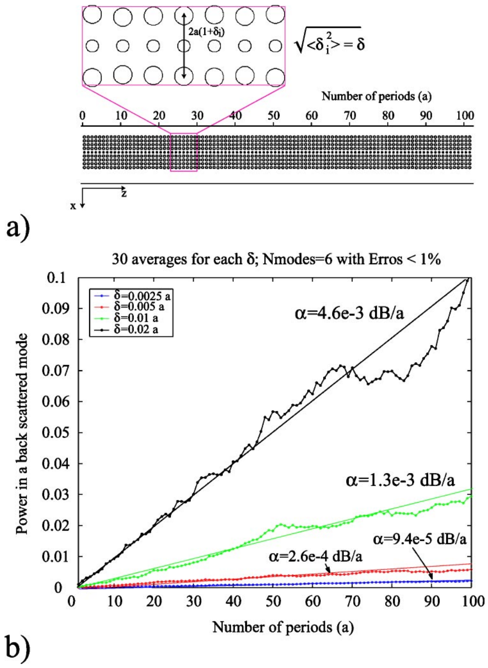

FIG. 6. (a) Schematic of a computational domain to study backscattering losses due to waveguide core size variations. Variations in the core size are assumed to be uncorrelated from one unit cell to another and distributed according to the Gaussian distribution with variance δ. (b) For each δ, backreflected power from a waveguide with "roughness" is presented as a function of propagation distance L. Each δ curve represents an average over 30 realizations of "roughness."

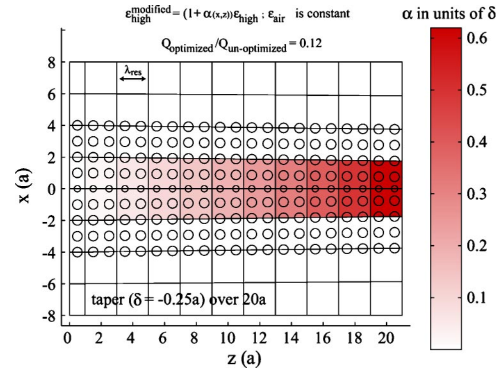

FIG. 7. Designing dielectric profile to negate the effects of variations in a waveguide geometry. Presented is an undesired taper of strength $\delta = -0.25$ over the length of 20 unit cells. The square mesh corresponds to the nonoverlapping regions where dielectric is modified, thus modeling the finite resolution and positioning accuracy of the index changing tool. The values of the dielectric constant in various square regions were chosen to make the propagation constant of a perturbed waveguide match closely the propagation constant of an unperturbed reference waveguide along the whole length of a taper. Only the material of high refractive index is modified, $\epsilon_{high}^{modified} = [1+\alpha(x,z)]\epsilon_{high}$. The required change in the dielectric constant $\alpha(x,z)$ is presented in shades. In general, we observe that $\alpha \sim \delta$, consistent with the predictions of perturbation theory.

ired weak variations in a waveguide geometry. One way of changing the dielectric constant of an underlying material could be via an interaction with femtosecond laser radiation. The material interaction with femtosecond radiation is currently actively investigated for writing bulk and planar waveguides in various materials. With such a process the index change is proportional to the exposure time to the radiation, while spatial resolution λ_{res} is determined by the laser spot size in focus. Thus, given the spatial resolution ("spot size") of the focused laser beam and positioning resolution of a setup we investigate at what spatial points and with what intensities the laser beam has to be applied to reduce the effects of undesired variations.

Particularly, in the case of a weak slow variation (taper, for example), the local propagation constant of a fundamental mode $\beta(z)$ at a point z along the waveguide can be approximated by the first-order perturbation correction $\beta(z) = \beta_0 + \langle\beta_0|\Delta M_{\beta_0,\beta_0}(z)|\beta_0\rangle / \langle\beta_0|\hat{B}|\beta_0\rangle$, where β_0 corresponds to the fundamental mode of a reference waveguide, while $\Delta M_{\beta_0,\beta_0}(z)$ and $\hat{B}$ are defined in Sec. IV. As the matrix of coupling elements (6) $M_{\beta_0,\beta_0}(z)$ depends simultaneously on the geometry of variation and underlying dielectric profile, by modifying such a dielectric profile one can, in principle, compensate for the effects of undesired variations in waveguide geometry. To construct optimization problem we can define an objective function as follows:

$$Q = \int_0^L dz|\beta(z) - \beta_0|^2 = \int_0^L dz \left| \frac{\langle\beta_0|\Delta M_{\beta_0,\beta_0}(z,\epsilon)|\beta_0\rangle}{\langle\beta_0|\hat{B}|\beta_0\rangle} \right|^2 . \tag{8}$$

By minimizing the objective function Q via changing the dielectric profile we force the local propagation constant to be that of an unperturbed reference waveguide, thus negating the effect of an undesired taper. We introduce possible changes in the dielectric profile as $\epsilon = \epsilon_0 + \sum_i c_i \phi(x-x_i, z-z_i)$, where ϵ_0 corresponds to the dielectric profile of a reference waveguide, while the spot function $\phi(x-x_i, z-z_i)$ is a localized function defining the intensity distribution of a laser spot focused at a point (x_i, z_i). For a set of focusing points (x_i, z_i) defined by the positioning resolution of the device, the unknown coefficients c_i are then chosen to minimize the value of the objective function Q. In general, such a formulation leads to a nonlinear optimization problem that can be approached by a variety of well-established numerical methods. Finally, the modified dielectric profile is reconstructed using optimal c_i's, and the success of optimization is judged by the ratio of $Q_{optimal}/Q_{unoptimized}$.

In Fig. 7 we present the results of optimization of the dielectric profile to negate the effects of an undesired taper of strength $\delta = -0.25$ over the length of $L = 20$ unit cells. The waveguide on the left of the taper is assumed to be infinite and described by the leftmost unit cell of the taper. The spot function $\phi(x-x_i, z-z_i)$ is chosen to be unity defined on a square of size $\lambda_{res} = 2a$. It is also assumed that only the high-index dielectric can be modified, $\epsilon_{high}^{modified} = [1+\alpha(x,z)]\epsilon_{high}$. The focus points (x_i, z_i) were chosen to create a square mesh of nonoverlapping laser spots. The intensities in various spots were optimized to reduce the objective function (8). With such a chosen realistic spot size and positioning scheme we managed to reduce the objective function by a factor of 10. In Fig. 7 we plot in shades the required change in the high-index dielectric in each of the focusing points. As expected, the largest change in the dielectric profile happens in the region of the largest geometric variation. As a rule, for slow weak variations we find that the absolute change α in the dielectric profile needed to compensate for the geometric variation and the absolute strength of such a geometric variation δ are proportional to each other, $\alpha \sim \delta$, which is consistent with the predictions of perturbation theory.

VI. CONCLUSION

In this work, we presented a general form of the coupled-mode and perturbation theories to treat geometric variations of generic waveguide profiles with an arbitrary dielectric index contrast. Applications to various aspects of light propagation in deformed 2D photonic crystal waveguides were demonstrated. We conclude that semianalytical CMT and PT can offer substantial computational advantages over time domain and frequency domain methods when analyzing the impact of small imperfections or weak variations over large propagation distances.

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