Waveguide Characteristics Near the Second Bragg Condition

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ABSTRACT
We show that in an optical waveguide with no material losses at wavelengths near the second-order Bragg condition, there exists two pairs of modes. One pair has identical propagation constants but have different attenuation coefficients, while a second pair with identical propagation constants (different from the first pair) has different attenuation coefficients. The four attenuation coefficients may have either a positive value, representing power leaking out of a waveguide mode or a negative value, representing power from an external source leaking into a mode. Moreover, a mode with a positive (negative) attenuation before the second Bragg condition, has a negative (positive) attenuation after the second Bragg condition. Radiation near the second-order Bragg condition of a periodic waveguide typically occurs at an angle perpendicular or nearly perpendicular to the propagation direction of the waveguide because the scattering centers have a period equal to or close to the period of the longitudinal propagation constant of the mode. In this paper, stable numerical solutions for the modes of periodic dielectric structures are developed using Floquet-Bloch theory. One primary focus in this paper illustrates a unique method of analyzing such modes using eigenvectors forming a Hilbert space, allowing for expansion of arbitrary vectors and their derivatives used for calculations such as that involving group velocities. The dimension of the vector space is determined by the number of space harmonics used in the solution of the Floquet-Bloch equations. The accuracy of the numerical solutions is affected by the number of space harmonics; as that number is increased, the number of waveguide partitions must be increased to maintain a given accuracy.

INDEX TERMS
Bragg gratings, semiconductor waveguides, semiconductor lasers, leaky wave antennas, distributed feedback devices, distributed Bragg reflectors, surface emitting lasers, antennas and propagation, nanotechnology, dielectric waveguide, periodic waveguides, second-order Bragg gratings.

I. INTRODUCTION
Periodic dielectric waveguides have electromagnetic characteristics that are considerably different from similarly constructed conventional waveguides. A mode propagating, say in the positive z direction, exp(iωt − γz), with periodicity along z, is identified by its complex propagation constant, γ = α + jβ, where β = 2π/λg, α is the attenuation, λg is the mode wavelength in the waveguide, and ω is the real angular frequency of the mode. The attenuation α is related to the loss (or gain) of mode power due to: 1) power coupled out of (or into) the periodic waveguide by leaky modes; 2) power transfer between co-directional and contra-directional propagating modes, depending on grating period [1]; and 3) material loss or gain. In this paper we assume that all material losses and gains are zero.

The Floquet-Bloch method provides a prescription for analyzing modes in periodic waveguides that extend to infinity in the direction of propagation. A key point in this paper, as discussed in Section III-F, is that computation of the modal attenuation coefficient, α, can only be determined by specifying boundary conditions at infinite lateral distances.
that are perpendicular to the propagation direction. Boundary conditions are set depending on the direction of the leaky mode. If the leaky mode propagates away from the central region of the waveguide the corresponding mode loses power, resulting in positive attenuation. On the other hand, there are leaky modes whose propagation direction is toward the waveguide, which results in negative attenuation (also called gain). By taking all combinations of inward propagating and outward propagating waves, there are four sets of boundary conditions yielding four modes for each waveguide mode. In this paper we assume for discussion purposes that the waveguide is single mode, although the mathematics presented apply to multi-mode waveguides.

Regardless of the boundary condition used to set the direction of leaky modes, the attenuation coefficient of dielectric waveguides without ohmic losses is zero at the exact second Bragg condition, that is, when the grating period is identical to the mode wavelength, the attenuation is zero. The derivative of the mode attenuation with respect to the grating period is infinite at the exact second Bragg condition. As a result, there is an infinitesimal small wavelength range where there is no leakage or attenuation.

The mathematical result of zero attenuation at the exact second Bragg condition is consistent with the analogy that a series of planar thin films of half-wavelength thicknesses of appropriate high and low indices provide anti-reflect coatings on optical surfaces. The mathematical reason that second-order gratings are successfully used as reflectors and outcouplers in optical waveguide devices is explained in Section IV and illustrated by Figs. 12 and 20. Physically, the exceedingly small variations in material compositions, layer thicknesses, grating depths and grating duty cycles along the propagation direction of periodic optical waveguides results in a variation of the extremely narrow range of wavelengths that correspond to the local exact Bragg condition. As a result, even with the precise fabrication techniques used today, the average effective attenuation is not zero, resulting in substantial reflection and outcoupling even at the exact Bragg condition.

In addition to leaky mode phenomena, periodic structures can exhibit significant power transfer between co-directional and contra-directional propagating modes (depending on grating period) resulting in major effects on the attenuation coefficient. In these cases, the power of each mode is transferred back and forth to the other mode and the two modes are said to be coupled.

The mathematical analysis of periodic structures has progressed on several fronts over the last half century. The early coupled-mode methods [2] applied to periodic structures gave relatively accurate results at wavelengths close to the first Bragg condition. The Floquet-Bloch method [3] discussed in this paper focus on characteristics of waveguide modes propagating in periodic structures at wavelengths near the second Bragg condition. In particular, the matrix resulting from boundary-condition settings is singular at a specific real frequency or wavelength and our algorithm using the Simpson method to calculate the real frequency is rigorous and numerically stable for hundreds of space harmonics.

A somewhat different focus is the understanding of scattering of light shining on planar structures with etched gratings on the surface or gratings embedded within the structure [4], [5]. The electromagnetic field is expanded in a Fourier series and a matrix is designed to account for all scattered light due to an incident plane-wave with a specific field polarization, and it results from the matching of Fourier components at boundaries. If the matrix is non-singular, the scattered fields may be determined. If the matrix is singular at the specified frequency, a resonant condition, the scattered fields cannot be determined at that frequency. However, because the scattering matrix is obtained by matching fields at all boundaries, the singularity of the matrix implies the existence of a waveguide mode [6], [7].

A scattering-matrix approach has also been used to address appearances of leaky waveguide modes in dielectric materials below a two-dimensional periodic pattern [8] and to analyze crystalline slabs with asymmetric and symmetric dielectric unit cells [9].

Although this work has a narrow focus on the wavelength range near the second Bragg condition where the mode leaks normal or near normal to the propagation direction, leaky modes at high-order Bragg conditions leak at different angles [10], [11]. The leaky mode radiation direction is determined by interaction of the space harmonics in the Floquet-Bloch expansion. Assuming the periodic structure can be modeled with a set of scattering centers such as shown Fig. 2, the field phases of the scattering centers fix the radiation direction. When phases are identical, such as the phases at the second Bragg condition, the main radiation lobe is in the normal direction. At higher-order Bragg conditions, the equivalent scattering-center spacing increases producing a radiation pattern with grating lobes. There is a broadside beam, but grating lobes appear at an angle \( \theta \), relative to the normal of the array axis, which satisfies \( \sin \theta = \pm \lambda / \Lambda \). For example, a forth-order Bragg condition, \( \Lambda = 2 \lambda \), has two grating lobes at \( \theta = \pm \pi / 6 \). Nevertheless, unlike an antenna array that may radiate at broadside, a periodic dielectric waveguide does not radiate at the exact second Bragg condition because the amplitude of the -1 space harmonic producing the leaky wave vanishes at the exact second Bragg condition.

Complex coupling coefficients occur if the waveguide periodicity is a result of both index and loss (or gain) periodicity [2]. Coupled mode theory (CMT) can address coupling between a guided wave and radiating partial waves [12]. Distributed feedback (DFB) grating-coupled surface-emitting (GSE) lasers were characterized from an expanded CMT to active second-order gratings [13]. Modeling of second-order structures was used to design GSE lasers [14]. A Greens function method was proposed to obtain the complex coupling coefficient of gain or loss in second- and high-order gratings [15]. The Greens function method was also used to analyze and design DFB lasers with second-order gratings [16]. A volume current method (VCM) was used to calculate...
the radiation scattered from gratings by using a Greens function to calculate the radiation fields [17]. Both the CMT and the VCM methods are perturbation techniques with accurate results if the periodic perturbation is weak.

On the other hand, Floquet-Bloch theory (FBT) provides a near exact solution, depending on the number of space harmonics utilized and can be used to analyze characteristics of gratings of all orders. Although analytic formulas for first-order gratings based on CMT provide accurate answers for shallow gratings, exact numerical techniques are required for deep gratings or for gratings located at an interface with a large index step [1]. Floquet’s theorem states that the envelope of the propagating wave is periodic with a period identical to the grating period. This theorem was used by Bloch to analyze electron behavior in crystals using Schrodinger’s wave equation.

The boundary element method (BEM) with Floquet components was developed to evaluate the dispersion relationship and the transmission, reflection and radiation efficiencies over a finite length of a second-order grating [18], [19]. Reflected and transmitted powers of finite-length distributed Bragg reflectors (DBRs) were computed using the Floquet-Bloch theory and the least square residual method [20].

A fiber-to-chip grating coupler in a silicon-on-insulator (SOI) rib waveguide emitting at an angle of −13.4° from the vertical had a coupling efficiency of −2.2 dB operating with a fourth-order grating [21]. Another fiber-to-chip grating coupler with only upward radiation was demonstrated using a third-order grating [22]. A crossed-grating out-coupler was used to emit light of two different wavelengths from a semiconductor laser [23]. A thin liner layer along with a high index cover layer over a simple grating can theoretically reduce the length of an out-coupler grating by an order of magnitude [24]. The Fourier eigenmode expansion method with Floquet theory (Ref. [25]) was applied to analyze the structures in Refs. [21] and [22]. Highly efficient radiation from second-order silicon photonic waveguides with tightly confined modes has been analyzed and demonstrated [26].

The method developed in this paper analyzes characteristics of waveguides commonly used in the integration of semiconductor lasers and optical devices [24]. Dielectric waveguides containing one or more special layers whose dielectric constant varies with z (the propagation direction) are typically fabricated with additional parallel multiple uniform layers as shown in Fig. 1. As a result, the shape of the mode propagating in the z direction is dependent upon both x and z. In this paper, the characteristics of waveguide modes in a multi-layer structure, with special layers whose dielectric constant varies along the propagation direction, will be developed. All layers, except the grating layers, are uniform and isotropic.

II. GRATINGS

A coordinate system is chosen such that the grating layers are referenced at the transverse location x = 0 such as illustrated in Fig. 1 for a simple grating formed in Layer 3. The propagation direction z has an origin at the center of the tooth so that the dielectric constant is symmetric about the tooth center. The periodic grating of Layer 3 has two regions with two different dielectric materials. The dielectric constant of the lth layer is given by \( \kappa_l \). Although the dielectric materials of the grating may be formed with arbitrary materials, it is typically formed with the dielectric materials of the neighboring layers. For example, the central tooth region usually would have a dielectric constant \( \kappa_t = \kappa_2 \) and the fill region would have a relative dielectric constant \( \kappa_f = \kappa_2 \).

In the grating layer the dielectric constant is independent of y and x but it is periodic with respect to z, the propagation direction, and may be expanded in a spatial Fourier series (The grating layer in Fig. 1 has \( l = 3 \)).

\[
\kappa_l(z) = \sum_{m=-\infty}^{\infty} \mathcal{K}_m^l e^{-jmKz},
\]

(1)

where the \( K = 2\pi/\Lambda \) is the grating wave number and \( \mathcal{K}_m^l \), is the Fourier coefficient

\[
\mathcal{K}_m^l = \frac{1}{\Lambda} \int_{-\Lambda/2}^{\Lambda/2} \kappa_l(z) e^{jmKz} \, dz.
\]

(2)

A non-grating layer has only the \( m = 0 \) Fourier coefficient.

When the grating layer thickness, \( t_h \), is small compared to the width of the transverse field, the periodic layer will have only a slight influence (perturbation) on the shapes of the transverse fields. A first-order analysis of the electromagnetic fields can be obtained by replacing the periodic layer with a material whose dielectric constant is the average value

\[
\mathcal{K}_0^l = \frac{1}{\Lambda} \left[ t_w \kappa_t + (\Lambda - t_w) \kappa_f \right],
\]

(3)

which is the 0th Fourier coefficient. If the duty cycle, \( d_c \), is defined as \( t_w/\Lambda \), the average dielectric constant becomes \( \mathcal{K}_0^l = d_c \kappa_t + (1-d_c) \kappa_f \). In the absence of material dispersion, all Fourier coefficients are independent of the grating period, \( \Lambda \), and the free-space wavelength, \( \lambda \).

The Fourier expansion of the relative dielectric constant in (1) can be used to extract information regarding the interaction with an electromagnetic mode that impinges on a region
with an embedded grating such as that in Fig. 1. For example, if the grating period, \( \Lambda \), is near the half-wavelength of a propagating mode, \((\lambda/2)/n_e\), where \( n_e \) is the effective index of the mode, then back scatter from the multiple waveguide discontinuities are in-phase, and results in first-order in-plane reflection. In general, back scatter can be accomplished with a multitude of grating periods such as for \( m \)-th-order Bragg scattering,

\[
\Lambda = \frac{\lambda_e}{2} m, \tag{4}
\]

where \( \lambda_e = \lambda/n_e \) is the effective wavelength of the mode in the waveguide. When \( \Lambda \) is approximately satisfied, the space harmonic, \( m \) in \( (1) \), strongly interacts with the incident mode.

If the distance between the scattering centers, illustrated in Fig. 2, is \( \lambda_e/2 \) then there is a phase difference of \( \pi \) radians between each neighboring center; this is similar to an end-fire antenna array and produces back scattering. When the distance between scattering centers is \( \lambda_e \), the second Bragg condition, then neighboring elements are in phase, analogous to a broadband array and produces scattering/radiation at 90° to the array axis. At a spacing of \( 3 \lambda_e/2 \), the third Bragg condition, neighboring elements are again \( \pi \) radians out of phase, resulting in radiation from the waveguide and waveguide mode reflection.

The strength of the Fourier coefficients for the various spatial harmonics determines the amount of interaction of a mode with a grating, assuming wavelengths in the vicinity of condition \( (4) \) is satisfied. For the rectangular grating shown in Fig. 1, the Fourier coefficients for layer \( l = 3 \) are given as

\[
\mathcal{K}_m^l = (\kappa_l - \kappa_f) \begin{cases} 
    d_c; & \text{if } m = 0, \\
    \sin m\pi d_c/m\pi; & \text{if } m \neq 0.
\end{cases} \tag{5}
\]

When the duty cycle \( d_c = 1/2 \), the coefficients \( \mathcal{K}_m^l = 0 \) when \( m \) is an even integer so it appears there would be little or no interaction with a propagating mode whose effective wavelength, \( \lambda_e \) satisfies the Bragg condition. Similarly, when the duty cycle \( d_c = 1/3, \mathcal{K}_m^l = 0 \) when \( m \) is a multiple of 3. However, when \( d_c = 1/2 \), the Fourier coefficients \( \mathcal{K}_m^l \) have maximum values. The magnitude of the Fourier coefficients decreases slowly, (as \( 1/|m| \)), because of the abrupt changes in the dielectric constant at the tooth edges.

A first-order Bragg reflector has the largest Fourier coefficient when the duty cycle is approximately \( 1/2 \), whereas a second-order Bragg reflector has the largest Fourier coefficient for approximately a \( 1/4 \) duty cycle, which is half the size of the coefficient of the first-order Bragg reflector. The value of the coefficient \( \mathcal{K}_m^l \) is calculated by multiplying the factors in the table with the relative dielectric constant difference \( \kappa_l - \kappa_f \). The calculations for duty cycles of \( 2/3 \) and \( 3/4 \) can be obtained using the coefficients in Table 1 by interchanging \( \kappa_l \) and \( \kappa_f \).

### III. FLOQUET-BLOCH WAVES

Early studies of periodic waveguides were focused on the problems in antenna design and analysis, such as wave guiding, scattering and radiation patterns \([27],[28],[29],[30]\). In a dielectric slab waveguide without loss or gain, in any layer, there is no power loss for a bounded propagating mode. Waveguide power loss can occur if there are waveguide discontinuities. Since a grating tooth is a discontinuity, a periodic sequence of teeth produces significant scattering.

Wave phenomena such as that of electromagnetic propagation in periodic waveguides can be described by the superposition of all forward and backward waves which are excited by the periodic structure. According to Floquet’s theorem, the fields can be characterized mathematically in terms of the phase difference between the propagating fields and the fields are discrete and are equal to the multiple of the unit reciprocal grating period, \( K = 2\pi/\Lambda \).

In general, the field distribution of a wave propagating in the positive \( z \) direction in a waveguide that is periodic along the propagation direction \( z \) can be expressed in terms of Floquet-Bloch analysis as

\[
\Psi(x, z) = R(x, z) e^{-\gamma z}, \tag{6}
\]

where \( R(x, z) = R(x, z + \Lambda) \) is a periodic function along \( z \) and \( \gamma = \alpha + j\beta \) is the complex propagation constant. The attenuation coefficient \( \alpha \) may have a positive or a negative value, however, the forward wave requires \( \beta > 0 \).

The Fourier series for \( R(x, z) \) is written as

\[
R(x, z) = \sum_{n=\infty}^{\infty} \psi_n(x) e^{-j\gamma_n z}, \tag{7}
\]

which produces the field solution

\[
\Psi(x, z) = \sum_{n=\infty}^{\infty} \psi_n(x) e^{-j\gamma_n z}, \tag{8}
\]

where \( \gamma_n = \gamma + jnK \).

In general, the space harmonics \( \psi_n(x) \) and \( \psi_n^* \) are not orthogonal, i.e.,

\[
\langle \psi_m | \psi_n \rangle = \int_{-\infty}^{\infty} \psi_m^*(x) \psi_n(x) dx \neq 0. \tag{9}
\]
Thus, the propagating wave consists of a set of space harmonics called partial waves that all travel with the same group velocity so the longitudinal shape will remain intact as it propagates. However, there may be an exchange of power from one partial wave to another because of their non-orthogonality. When there exists multiple modes, interaction between two modes can occur when $\beta_p + \beta_q = rK$, where $p$, $q$, and $r$ are integers. The subscripts $p$ and $q$ pertain to different guided modes in a periodic waveguide.

A. TE MODES

In practice, dielectric waveguides with a periodic region embedded are constructed from uniform, isotropic materials. This construction will produce two independent sets of waveguide modes, TE and TM. While modes of either the TE set or the TM set may interact as they propagate, TE and TM modes will not interact because their polarization is orthogonal. When there exists multiple modes, interaction between two modes can occur when $\beta_p + \beta_q = rK$, where $p$, $q$, and $r$ are integers. The subscripts $p$ and $q$ pertain to different guided modes in a periodic waveguide.

Floquet-Bloch modes.

The propagation characteristics of TE-type waves. The TE waves (electric field has an eigenvector method originally developed by Peng and a large intermediate layer separating the main waveguide for a periodic waveguide with a large grating tooth height similar accuracy, stability and convergence issues, especially for a periodic waveguide with a large grating tooth height and a large intermediate layer separating the main waveguide and the grating region. In the section below, an algebraic eigenvector method originally developed by Peng et al. [3] will be extended for analysis and understanding of Floquet-Bloch modes. This section will be concerned with the propagation characteristics of TE-type waves. The TE waves (electric field has only an $E_y$ component) propagating in the positive $z$ direction is governed by three components of Maxwell’s equations

$$-\frac{\partial E_y}{\partial z} = -j\omega \mu_0 H_z,$$  
$$\frac{\partial E_y}{\partial x} = -j\omega \mu_0 H_z,$$  
$$\frac{\partial H_z}{\partial z} - \frac{\partial H_z}{\partial x} = j\omega \varepsilon_0 \kappa(x, z) E_y.$$  

Substituting the first two equations into the third gives the wave equation representing the field component $E_y$.

The Helmholtz equation for the isotropic grating layer can be written as

$$\frac{\partial^2 \Psi^2}{\partial x^2} + \frac{\partial^2 \Psi}{\partial z^2} + k^2 \kappa(x, z) \Psi = 0,$$  

where $k$ is the free-space wavenumber. The resulting field solutions are

$$E_y = \Psi(x, z),$$  
$$H_z = \frac{1}{j\omega \mu_0} \frac{\partial \Psi}{\partial z},$$  
$$H_z = -\frac{1}{j\omega \varepsilon_0} \frac{\partial \Psi}{\partial x}.$$  

The periodic relative dielectric constant is separated into two parts, $\kappa_0(x)$, representing the average value of $\kappa(x, z)$ along the $z$ direction, and $\kappa'(x, z)$, representing the periodic variation of $\kappa(x, z)$. Accordingly, the average value of $\kappa'(x, z)$ (along $z$) is 0 and $\kappa'(x, z) \equiv 0$ if $x$ is not a point of a grating layer.

The coefficient of the Floquet multiplier, $R(x, z)$, for forward propagation satisfies the differential equation

$$\frac{\partial^2 R}{\partial x^2} + \frac{\partial^2 R}{\partial z^2} - 2\gamma \frac{\partial R}{\partial z} + [k^2 \kappa_0(x) + \gamma^2] R + k^2 \kappa'(x, z) R = 0.$$  

Assuming the dielectric constants, $\kappa'(x, z)$, are even functions of $z$, $\kappa'(x, z) = \kappa'(x, -z)$, or odd functions of $z$, $\kappa'(x, z) = -\kappa'(x, -z)$, and reactive, other solutions similar to (6), can be obtained in terms of $\gamma$ and $R(x, z)$ as

$$\tilde{R}(x, z) e^{-\gamma z} = \left\{ \begin{array}{ll} R^*(x, -z) e^{\gamma z}; & \kappa'(x, z) = \kappa'(x, -z), \\
-R^*(x, -z) e^{\gamma z}; & \kappa'(x, z) = -\kappa'(x, -z), \end{array} \right.$$  

where $\tilde{R}(x, z) = \pm R^*(x, -z)$ satisfies (17) with $\gamma = -\alpha + j\beta$, a forward wave with an attenuation coefficient of opposite sign. When $\kappa'$ is an even function of $z$, the two field solutions are conjugates of one another at $z = 0$. However, when $\alpha = 0$, such as at the second Bragg condition, the solutions merge, making $\tilde{R}(x, z) = \pm R^*(x, -z)$.

A set of differential equations for the space harmonics in the $l$th layer can be obtained by substituting (8) into the Helmholtz equation, (13) and using the expansion, (1)

$$\frac{d^2 \psi^l_n(x)}{dx^2} + \gamma_n^2 \psi^l_n(x) + k^2 \sum_{m=-\infty}^{\infty} \kappa^l_{n-m} \psi^l_m(x) = 0.$$  

The summation in (19) represents the discrete convolution of the space harmonics with Fourier coefficients of the relative dielectric constant.

If the largest coefficient, $\kappa^l_{0}$, of the $l$th layer is removed from the summation in (19), one gets

$$\frac{d^2 \psi^l_n(x)}{dx^2} + \left( \gamma_n^2 + k^2 \kappa^l_{0} \right) \psi^l_n(x) + k^2 \sum_{m=-\infty}^{\infty} \kappa^l_{n-m} \psi^l_m(x) = 0.$$  

The summation which omits the $m = n$ term, acts as a perturbation on the set of uncoupled differential equations; it represents the convolution of the space harmonics with the Fourier components of $\kappa'$.

In Fig. 1, the grating tooth is rectangular, rendering $\kappa_l$ and $\kappa^l_{n-m}$ independent of $x$. When the grating tooth is not rectangular, then $\kappa_l$ and the corresponding $\kappa^l_{n-m}$ Fourier coefficient have transverse $x$ dependence, which results in a set of differential equations with non-constant (with respect to $x$) coefficients. (While differential equations with constant coefficients have well-known solutions, solutions of differential equations with variable coefficients may not have simple closed-form answers and one must rely on the use of numerical methods.)

The fill regions of the grating may consist of multiple material compositions. For example, Fig. 3 illustrates a single grating period that consists of a tooth region and several fill...
regions. Furthermore, the dielectric constant in the grating layer is also independent of the transverse $x$ dimension.

As the tooth and fill regions increase in number, the variation of $\kappa(z)$ tends to a continuous function, with respect to $z$. Further, the continuously varying dielectric constant is also independent of the transverse direction $x$. Accordingly, the expansion coefficients, $\mathcal{K}_{n-m}(x)$, in (19) are independent of $x$. For example, if $\kappa_{\text{max}}$ and $\kappa_{\text{min}}$ are the maximum and minimum values of $\kappa(z)$ in the grating period $\Lambda$, then a sinusoidal grating might have a functional dependence

$$\kappa(z) = \left(\frac{\kappa_{\text{max}} - \kappa_{\text{min}}}{2}\right) \cos \frac{\kappa_{\text{max}} + \kappa_{\text{min}}}{2}. $$

This analysis constrains dielectric variation in the grating layers to the propagation direction, i.e., the dielectric constant varies only with $z$. To allow for arbitrarily shaped profiles, the grating layer must be partitioned into multiple layers with rectangular shaped teeth that approximate the arbitrary profile. Fig. 4 illustrates both rectangular and non-rectangular tooth shapes. In Fig. 4, the triangular-shaped tooth is represented by a sequence of rectangular-shaped regions which may be increased or decreased in number depending on a desired approximation of the actual shape [3]. Although, modal characteristics of arbitrarily-shaped grating profiles have been developed, [19], [20], [31], [32], [33] the partitioning of the arbitrary shapes into a series of rectangular regions can similarly provide solutions to any desired accuracy. Although the material used to form layers in devices have dielectric constants that are uniform and isotropic, devices with non-uniform, anisotropic materials may be used. When non-uniformity is an issue, the rectangular regions may also be partitioned to approximate the non-uniformity.

Outside grating regions, solutions of the Helmholtz equation can be reduced to that of solving a second-order differential equation in all layers without a grating. However, to find solutions for waveguide modes it is necessary to match solutions outside grating regions to field solutions within grating regions.

### B. FIELD SOLUTIONS IN A PERIODIC LAYER

A main contribution of this work is identifying and using the eigenvectors of the eigenvalue problem stated in (25). The vectors allow computation of derivatives required for finding the propagation constant via Newton’s method, group velocities and other parameters requiring the necessary derivatives.

One technique of solving for the fields in the grating is to assume that only a finite number of space harmonics in (19) play a significant role in the determination of the mode. Assuming that the smallest indexed space harmonic is $\psi_L$, while the largest is $\psi_H$ (the total number of space harmonics is $M = H - L + 1$), then the infinite set of differential equations reduces to a finite set of $M$ second-order differential equations that may be written in vector form:

$$\frac{d^2\Psi}{dx^2} = -\left(\Gamma^2 + k^2\mathcal{K}\right)\Psi \equiv -P\Psi,$$  \hspace{1cm} (21)

where $\Gamma$ is a diagonal matrix of $\gamma_n$’s, and $\mathcal{K}$ is a Toeplitz matrix whose entries are obtained from the set of Fourier coefficients $\{\mathcal{K}_n\}$ in (1). The resulting matrix $P$ has elements

$$p_{mn} = (\gamma + jn\mathcal{K})^2\delta_{mn} + k^2\mathcal{K}_{m-n},$$  \hspace{1cm} (22)

where $\delta_{mn}$ is the Kronecker delta. The vector $\Psi$ is

$$\Psi = \begin{pmatrix} \psi_L \\ \psi_{L+1} \\ \vdots \\ \psi_H \end{pmatrix},$$  \hspace{1cm} (23)

and has entries made from the individual space harmonics. It should be noted that the set of $M$ second-order equations may be reduced to a set of $2M$ first-order equations. The set of $2M$ equations will produce a set of $2M$ $x$-dependent solutions.

When the matrix $P$ is independent of $x$, the solution of the vector differential equation, (21), can be written in terms of a vector of constants, $v$, and a transverse propagation constants, $h$, as

$$\Psi = ve^{jhx},$$  \hspace{1cm} (24)

and the substitution of $\Psi$ into (21) gives

$$Pv = h^2v \equiv \sigma v.$$  \hspace{1cm} (25)

The solution of (19) reduces to the algebraic eigenvalue problem where $\sigma_n = h_n^2$ is the $n$th eigenvalue of $P$ and $v_n$ is the corresponding eigenvector. There are two exponential functions in the solution vector, composed of $\exp(jhx)$ and $\exp(-jhx)$ or a combination of the two exponential functions. The number of different pairs of lateral propagation constants, $(h_n = \pm \sqrt{\sigma_n})$, corresponds to the dimension of the $P$ matrix and is equal to $M$, the number of space harmonics that will be used to form the solution. The set of eigenvectors
The $m$th vector $v_m$ with the corresponding eigenvalue $\sigma_m$, is called a right-hand eigenvector. There is a left-hand eigenvector $u_m$ that has the same eigenvalue and satisfies

$$u_m^H P = \sigma_m u_m^H,$$

(26)

where $u_m^H$ is the transpose of the complex conjugate of $u_m$. The vectors in the set $S_v$ form a Hilbert space and are orthogonal to vectors in $S_v$, [34] i.e., if the eigenvalues $\sigma_m \neq \sigma_n$, then the inner product $u_m^H \cdot v_n = 0$. (In case degeneracy sets in, the Gram-Schmidt [35] process can be employed.) Orthogonality allows for simple expansion of eigenfunctions of an arbitrary vector and the corresponding coefficients are optimum in a mean-square sense for any vector in a subspace. (Expansions of eigenfunctions are commonly used for various applications. Perturbation analysis of energy eigenvalues and their corresponding wave functions can be accomplished using eigenvector expansions [36].) For example, assume the vector $e_i = \text{col}(0, \ldots, 1, \ldots, 0)$, where the non-zero element appears in the $i$th row, then

$$e_i = \sum_{j=1}^H E_{ij} v_j,$$

(27)

and the expansion coefficients become $E_{ij} = u_i^H \cdot e_i$, and provided the vectors have been normalized, $u_i^H \cdot v_j = \delta_{ij}$.

### C. Vector Expansions for Symmetric Gratings

In the special case when the dielectric constant is symmetric about $z = 0$, $\kappa(x, -z) = \kappa(x, z)$, then the complex matrix $P$ is symmetric, and it follows that $u_m^H = v_n^T$, the transpose of $v_n$. The expansions of the eigenvectors about the point $\gamma = \gamma_0$, in terms of the eigenvectors obtained from (25) will be developed for gratings that are symmetric about $z = 0$. The expansions will be used in the evaluation of the derivatives of $\psi$ and $\sigma$ with respect to $\gamma$, required when using Newton’s method as discussed in references [37] and [38].

The propagation constant, $\gamma$, of a Floquet-Bloch mode is determined from the solution of a set of transcendental equations that form a matrix $G(\gamma, k)$, given in (60). Typically, an iterative approach to finding a solution for $\gamma$ is obtained by varying the determinant of $G(\gamma, k)$ to zero. An iteration that uses Newton’s method requires calculating the derivative of $G(\gamma, k)$ with respect to $\gamma$, so that the derivatives of the eigenvalues and eigenvectors in (25) must be calculated in the vicinity of $\gamma = \gamma_0$. Retaining only the first three terms, the expansion of (25) about $\gamma = \gamma_0$ for the $n$th eigenvalue/vector, gives

$$\left( p_n^{(0)} + p_n^{(1)} \delta \gamma + \frac{1}{2} p_n^{(2)} \delta \gamma^2 \right)$$

$$\left( v_n^{(0)} + v_n^{(1)} \delta \gamma + \frac{1}{2} v_n^{(2)} \delta \gamma^2 \right),$$

(28)

where the derivatives $\partial^j / \partial \gamma^j$ are evaluated at $\gamma = \gamma_0$. A first-order solution of the eigenvector is $v_n = v_n^{(0)} + v_n^{(1)} \delta \gamma$, and the corresponding normalization $v_n^{(0)}\cdot v_n = 1$ requires $v_n^{(0)} \cdot v_n^{(1)} = 0$. Hence, the vector $v_n^{(1)}$ is orthogonal to $v_n^{(0)}$, i.e., $v_n^{(1)} \cdot v_n = 0$.

The first-order results allow for the calculation of $\sigma_n^{(1)}$, and $v_n^{(2)}$, given by

$$\sigma_n^{(1)} = \tilde{\rho}_{mn},$$

(29)

$$\nu_n^{(1)} = \sum_{m \neq n} \frac{\tilde{\rho}_{mn}^{(1)}}{\sigma_n - \sigma_m} v_m^{(0)},$$

(30)

where the matrix elements $\tilde{\rho}_{mn}^{(1)} = u_m^{(0)} H^T P^{(1)} u_n^{(0)}$. The second-order coefficients are

$$\sigma_n^{(2)} = \tilde{\rho}_{mn}^{(2)} + 2 \sum_{k \neq n} \frac{\tilde{\rho}_{mn}^{(1)} \tilde{\rho}_{nk}^{(1)}}{\sigma_n - \sigma_k},$$

(31)

$$\nu_n^{(2)} = \sum_{j \neq n} \left( \frac{\tilde{\rho}_{mn}^{(1)} \tilde{\rho}_{kn}^{(1)}}{\sigma_n - \sigma_k} - \frac{\tilde{\rho}_{mn}^{(1)} \tilde{\rho}_{kn}^{(1)} \tilde{\rho}_{mn}^{(2)}}{\sigma_n - \sigma_j} \right) \frac{v_m^{(0)} v_j^{(0)}}{\sigma_n - \sigma_j}.$$

(32)

### D. Grating Fields

Since the set of vector equations are derived from the second-order differential equation, the general solution will be written as the sum of $2M = 2(H - L + 1)$ independent solutions as

$$\psi_v = (A_v \cos h_v x + B_v \sin h_v x / h_v) \psi_v, \quad v = L, \ldots, H.$$  (33)

The coefficient of $\psi_v$ is the expansion variable that depends only on the index $v$ so that a general vector, $\psi$ in the space $S_v$ will be a linear combination of the base vectors as in (27),

$$\psi = \sum_{v=L}^{H} (A_v \cos h_v x + B_v \sin h_v x / h_v) \psi_v.$$  (34)

The complete set of base eigenvectors and their derivatives can be written as matrices,

$$V = (v_L v_{L+1} \ldots v_H); \quad V^{(1)} = (v_L^{(1)} v_{L+1}^{(1)} \ldots v_H^{(1)}).$$  (35)

For multiple grating layers, say the $l$th layer, the matrices are denoted as $V^l$ and $V^l_{\gamma}$. As opposed to non-grating layers that have a single transverse wave number associated with a space harmonic, in a grating layer a single transverse wave number $h_v$ does not define a space harmonic, as a space harmonic is obtained from a specific combination of the set of eigenvalues, $\{h_v^c\}$. Indeed, rows of $V$ are associated with the individual space harmonics, viz.,

$$\psi_n = \sum_v V_{nv} (A_v \cos h_v x + B_v \sin h_v x / h_v),$$  (36)
where the expansion coefficients are $A_n\cos h_n x + B_n \sin h_n x / h_n$. The coefficients $A_n$, $B_n$ are determined from the process of the matching the individual space harmonics across all layers of the waveguide while the matrix $V$ is formed from the vectors in the set $\mathcal{S}_d$. Coupling between the space harmonics comes from the off-diagonal elements of the Toeplitz matrix whose entries are the Fourier coefficients of the dielectric expansion in the grating region. It is interesting to note the evolution of $V$ as the duty cycle changes. For duty cycles of zero and unity, $V$ is a diagonal unit matrix with proper vector order and normalization. For other duty cycles $\nu_c$ cannot represent a space harmonic because it has more than one non-zero elements. Table 1 shows that the 50 percent duty cycle produces the largest, in magnitude, of off-diagonal terms and produces the strongest coupling of all vectors in $\mathcal{S}_d$.

E. TRANSVERSE GRATINGS WAVENUMBERS

Before addressing field calculations outside the grating, it is important to estimate the behavior of transverse wave numbers, $h_n$, because the nature of the space harmonics play a major role in forecasting numerical accuracy of the complex propagation constant $\gamma = \alpha + j\beta$ where $\alpha$ can be correlated with the transmission, reflection and radiation characteristics of a finite-length grating fabricated on a waveguide. Also, the number of space harmonics used for the solution affects accuracy.

An estimate of the transverse grating wavenumber can be obtained by dropping off-diagonal terms of the Toeplitz matrix $\mathcal{K}$, leaving only the diagonal terms, which are all identical, having a value of $\mathcal{K}_d^l_0$, given in (3). In a typical structure, the main sub-waveguide region, containing a majority of the mode power, is separated by a cladding layer whose dielectric constant is $\kappa_c$. The grating is then etched onto the cladding layer, often taking about 10 to 50 percent of cladding thickness for the grating. A strong grating can be next to the main sub-waveguide with no cladding or even etched into the main waveguide. The dielectric constants of layers forming the main sub-waveguide are generally larger than the dielectric constant of the cladding layer. The resulting geometry produces modes whose effective indices are larger than the refractive index of the cladding. Thus, the grating tooth material is the same as that of the cladding, whereas the fill material is typically air or some combination of dielectric materials. For a 50 percent duty cycle, the average value $\bar{k}_l = \mathcal{K}_d^l_0 = (\kappa_c + 1)/2$. The eigenvalues $\sigma_l = h_n^2$ of $P$ are solutions of the algebraic equation

$$ f(h^2) = \prod_{n=L}^H (y^2 + k^2 \bar{k}_l - h^2) = 0. \tag{37} $$

For space harmonic $n$, the corresponding eigenvalue, $h_n^2$, of the $l$th grating layer satisfies

$$ h_n^2 = (\alpha + jk n_c + jnK)^2 + k^2 \bar{k}_l. \tag{38} $$

The free-space wavenumber $k$ and the effective index of refraction of the propagating mode $n_c$ have replaced the propagation constant $\beta$.

To investigate the solution obtained for various eigenvalues, the solution of $h^2$ for different space harmonics can easily be observed. For example, when $n = 0$,

$$ h_0^2 = k^2 \bar{k}_l + \alpha^2 - k^2 n_c^2 + j2\alpha k n_c. \tag{39} $$

Because $k^2 n_c^2 > k^2 \bar{k}_l$, $h_0^2$ lies in the second or third quadrant, depending on the value of $\alpha$, which is generally small compared to other terms in the expression. Splitting $h_n^l$ into its real and imaginary parts, $h_n^l = h_n^l' + jh_n^l''$, produces $|h_n^l''| \gg |h_n^l'|$, so that the corresponding field associated with $h$ will be predominately evanescent. On the other hand, near the second Bragg condition, when the grating wave number $K \approx k n_c$, the eigenvalue for the $n = -1$ space harmonic becomes

$$ h_{-1}^2 = k^2 \bar{k}_l + \alpha^2, \tag{40} $$

so that $h_{-1}^2 \approx k \sqrt{\kappa_l}$ indicating the fields are oscillatory rather than evanescent, corresponding to light radiating away from (or into) the waveguide.

Employing a large number of space harmonics will of course, increase the accuracy yielded by the model. On the other hand, using a large number of space harmonics makes the model vulnerable to numerical inaccuracies associated with machine precision. (The numerical accuracy can be addressed by splitting thick layers to a number of thin layers.) As $n$ becomes large,

$$ h_n^2 \rightarrow -n^2 K^2 + 2\alpha + k^2 \bar{k}_l + j2k n_c. \tag{41} $$

which clearly indicates the fields are evanescent. The expression in (36) represents the field when the space harmonics are coupled (the off-diagonal terms of the Toeplitz matrix $\mathcal{K}$ are not assumed to be zero). However, the approximate solution may be written as

$$ \psi_n^l(x) \approx A_n^l \cosh h_n^{l''} x + B_n^l \sinh h_n^{l''} x / h_n^{l''}, \tag{42} $$

where $h_n^l$ in (41) is replaced by the dominant imaginary part $jh_n^{l''}$. When the layer thickness $d_l$ makes the numerical value of $\exp(-2h_n^{l''} d_l)$ below machine precision, calculations become ill-conditioned, causing numerical instability. Numerical stability requires splitting thick layers to several smaller layers.

At wave lengths near the second Bragg condition, the discussion above points to the fact that all of the space harmonics, save $n = -1$, have electromagnetic fields in the grating region that are predominately evanescent.

F. FIELD SOLUTIONS EXTERNAL TO GRATINGS LAYERS

Exterior to the grating region, space harmonics are uncoupled because the dielectric constant is independent of $z$, and in the $l$th layer (19) becomes

$$ \frac{d^2 \psi_n^l(x)}{dx^2} + (\gamma_n^2 + k^2 \kappa_l) \psi_n^l(x) = 0. \tag{43} $$
The field in the \( l \)th layer may be written in terms of the transverse wave number,

\[
h_n^l = k^2 l + (\gamma + jnK)^2, \tag{44}\]

as

\[
\psi_n(x) = A_n^l \cos h_n^l(x - x_l) + B_n^l \sin h_n^l(x - x_l)/h_n^l, \tag{45}\]

Layer-interface points \( x_l \) are illustrated in Fig. 1. In the two semi-infinite regions the solutions will be written specifically as

\[
\psi_n^1(x) = A_n^1 e^{-h_n^l(x-x_1)}, \tag{46}\]

\[
\psi_n^N(x) = A_n^N e^{h_n^l(x-x_{N-1})}, \tag{47}\]

\[
h_n^l = -\left[ k^2 l + (\gamma + jnK)^2 \right]; \quad l = 1, N. \tag{48}\]

The definition of the transverse wave numbers are different for internal layers and the outer semi-infinite layers. To allow for the possibility of fast waves or leaky modes, allowances must be made for power propagation away from the guided structure, leaking out, or for power propagation toward the guided structure, leaking in, as illustrated in Fig. 5.

A mode is leaky if one of its space harmonics is in the fast-wave region. In the superstrate, Layer 1, the \(-1\) space harmonic will leak when the propagation constant satisfies

\[
| \beta - K | < k\sqrt{k_1}, \tag{49}\]

and the mode will leak in the substrate, Layer \( N \), when \( \beta \) satisfies

\[
| \beta - K | < k\sqrt{k_N}. \tag{50}\]

The direction of power flow of the leaky space harmonic depends on the imaginary part of the lateral wave numbers \( h_1^1 \) and \( h_N^N \). For example, when \( h_1^1 > 0 \) power flows in the positive \( x \) direction, away from the central waveguide region. When \( h_1^1 < 0 \), power flows in the negative \( x \) direction, toward the central waveguide region. Similarly, when \( h_N^N > 0 \), power flows out of the central waveguide region through the substrate and power flows into the central waveguide region by way of the substrate when \( h_{N-1}^N > 0 \). In the computation of \( h_1^1 \) and \( h_N^N \), from (48), their imaginary parts will be positive when the branch cut is along the negative imaginary axis, and their imaginary parts will be negative when the branch cut is along the positive imaginary axis.

At the exact second Bragg condition, the transverse wave numbers are imaginary, \( h_1^1, h_{N-1}^N = 0 \), however, their amplitudes, \( A_1^1, A_{N-1}^N = 0 \). Accordingly, there is no power leaking out of the mode or power leaking into the mode at the exact second Bragg condition.

To avoid the complexities of material dispersion, calculations are made by varying the grating period for a fixed free space wavelength. The wavelength of the waveguide mode, \( \lambda_e \), will vary with grating period, duty cycle and grating depth. Below the second Bragg condition, \( \Lambda < \lambda_e \), at the second Bragg condition \( \Lambda = \lambda_e \), and above the second Bragg condition \( \Lambda > \lambda_e \). Assuming the phase of the traveling wave at the 1st scattering center in Fig. 2 is 0, the phase at the second scattering center will be retarded by an amount, say, \( \exp(-j\varphi) \); the phase at the 3rd scattering center will be retarded by \( \exp(-j2\varphi) \). Assuming the scattering centers represent a phased array, the far-field will peak at an angle of \(-\varphi\) relative to the \( x \) axis, the normal to the array axis. In Fig. 5, the red leaky waves occur below the second Bragg condition whereas the blue leaky waves occur above the second Bragg condition.

Figs. 5 (a), (b), (c) and (d) represent different modes near the second Bragg condition. In (a) the mode radiates power for grating periods below the second Bragg condition but gains power above the second Bragg condition, whereas (b) shows the opposite behavior. In (c) the mode radiates in the superstrate while it receives power from the substrate, before the second Bragg condition; after the second Bragg condition, the mode receives power from the substrate and radiates power out the superstrate. In (d), the mode exhibits the opposite behavior as that of the mode in (c). In particular, the fields in (a) and (b) satisfy \( R_{II}(x, z) = R_{II}(x, -z) \), and the fields in (c) and (d) satisfy \( R_{IV}(x, z) = R_{IV}(x, -z) \).
is 0.61\(\lambda\) which is less than the grating period at the second Bragg condition when \(\Lambda \equiv \Lambda_B \approx 0.631072\lambda\). The fields \(|R(x, z)|^2\) in (b) and (d) can be obtained from the fields in (a) and (c) because of dielectric symmetry about \(z = 0\), the tooth center.

Leaky waves in the superstrate and substrate have different radiation angles governed by the mode’s wave length relative to the second Bragg condition. In particular, the radiation direction for the \(-1\) space harmonic in the superstrate, Layer 1, is determined from \(\Im h_{1,l}\), for the \(x\) component, and \(\beta - K_x\), for the \(z\) component. Leak-in modes have a negative attenuation coefficient and amplify the power of the propagating mode. These modes are physically unrealizable unless there are sources at \(x = \pm \infty\) and the sources produce waves with proper phase and angles of incidence on the central waveguide region. On the other hand, a leak-out mode such as that illustrated in Fig. 5 (a), at grating periods below the second Bragg, does not require external sources so that modes switch at the second Bragg condition as in Fig. 5 (b). Fig. 7 illustrates the attenuation and propagation characteristics for the structure listed in Table 2 for the various modes as a function of grating period. At the second Bragg condition the attenuation of one mode goes continuously from a positive value to a negative value while a second mode transforms continuously from a negative value to a positive value. On the other hand, the propagation constant \(\beta\) is continuous across

The inverse functions \(\Lambda(\alpha)\) and \(\Lambda(\beta)\) derived from Fig. 7 have inflection points at the second Bragg condition, representing smooth transitions across the second Bragg condition;
hence, a smooth transition between 00 and 11. For structures composed of lossless materials, the attenuation coefficient is zero at the second Bragg condition so that in one sense, leak in and leak out modes are equal at the second Bragg. Indeed, at the second Bragg condition, there are eight Floquet-Bloch modes four in the forward direction and four in backward direction, all with $\alpha = 0$.

Fig. 9 shows the calculated points starting at positions below and above the second Bragg condition. Calculations stop when the real part of the lateral wavenumbers, $|\Re\{h_{1}^{1}\}|$ and $|\Re\{h_{N}^{N}\}|$ are below machine precision (64 bit floating numbers). The second Bragg condition occurs at $\Lambda \approx 0.631072$ when the number of space harmonics is greater than $\sim 35$. (For calculations with five space harmonics the second Bragg condition occurs at $\Lambda \approx 0.63111$; the second Bragg condition moves toward the asymptotic value of 0.631072 when the number of space harmonics exceeds $\sim 13$.

Modes having power leak out can be obtained by making the branch cut, used for square-root calculations of $h_{1}^{1}$ and $h_{N}^{N}$, $(n = -1$ for leaky space harmonics at the second Bragg condition) along the negative imaginary axis. Thus, all square-root calculations will be in the first and second quadrants, making $h_{n}^{n+1}$, $h_{n}^{nN} > 0$. In this case, propagation is away from the waveguide. Similarly, if the branch cut is taken along the positive imaginary axis, propagation in the clad regions will be toward the central waveguide region. In particular, at $z = 0$, (18) implies $\bar{R}(x, 0) = R^*(x, 0)$ (for the symmetric grating) so that the modes leak along $x$ in opposite directions.

The coefficient $A_{n}^{l}$ represents the field at the base of each layer while $B_{n}^{l}$ represents flux or field derivative with respect
to $x$. The tangential field components at the layer interfaces are $E_y$ and $H_z$, and (14) and (16) indicate the continuity of $E_y$ and $H_z$ can be accomplished by matching $\psi_n^l(x)$, and its derivative $d\psi_n^l(x)/dx$ between layers. The matrix that transfers the field and its derivative across a layer accomplishes the matching condition, and results in field coefficients as

$$
\begin{pmatrix}
A_{n-1}^l \\
B_{n-1}^l
\end{pmatrix} = 
\begin{pmatrix}
\cos h_n^ldl & \sin h_n^ldl/h_n^l \\
-h_n^l \sin h_n^ldl & \cos h_n^ldl
\end{pmatrix} 
\begin{pmatrix}
A_n^l \\
B_n^l
\end{pmatrix}.
$$

(52)

By repeated application of (52) the field and its derivative can be transferred from the substrate layer, $N$, to the grating layer. To simplify the expressions, the transfer matrix is written as

$$
T_n^l = \begin{pmatrix}
A_n^l & B_n^l \\
C_n^l & D_n^l
\end{pmatrix} = 
\begin{pmatrix}
\cos h_n^ldl & \sin h_n^ldl/h_n^l \\
-h_n^l \sin h_n^ldl & \cos h_n^ldl
\end{pmatrix},
$$

(53)

and the derivative of the transfer matrix with respect to $\gamma$ is

$$
T_n^{\gamma y} = h_n^l
\begin{pmatrix}
-\sin h_n^ldl & -
\cos h_n^ldl \\
\sin h_n^ldl & \cos h_n^ldl
\end{pmatrix} (d(A_n^l - B_n^l)/h_n^l) -h_n^l(d(A_n^l + B_n^l)/h_n^l).
$$

(54)

The results above will be applicable for all layers including grating layers. In a non-grating layer $h_n^{\gamma y} = (\gamma + jnK)/h_n^l$ whereas in a grating layer $h_n^{\gamma y} = n^{(1)}/2h_n^l$.

**G. THE SECULAR EQUATION**

Matching of the proper tangential fields, $E_y$, and $H_z$, at the various layer interfaces will produce the secular equation. Recall that the fields are functions of both $x$ and $z$. At layer boundaries, fields could be point-matched at several $z$ locations. However, it suffices to match only the space harmonics and the field components will be matched for all values of $z$.

Assuming the structure of Fig. 1, matching fields will produce a set of nine equations for each space harmonic

$$
A_n^l = \sum_i V_{Li}(A_i^3 A_i^l + B_i^3 B_i^l),
$$

$$
B_n^l = \sum_i V_{Li}(C_i^3 A_i^l + D_i^3 B_i^l),
$$

$$
\sum_i V_{Li}A_i^3 = A_n^l A_n^l + B_n^l B_n^l,
$$

$$
\sum_i V_{Li}B_i^3 = C_n^l A_n^l + D_n^l B_n^l,
$$

$$
A_n^l = A_n^l A_n^l + B_n^l B_n^l,
$$

$$
B_n^l = C_n^l A_n^l + D_n^l B_n^l,
$$

$$
A_n^l = A_n^l A_n^l + B_n^l B_n^l,
$$

$$
B_n^l = C_n^l A_n^l + D_n^l B_n^l,
$$

$$
A_n^l = A_n^l A_n^l + B_n^l B_n^l,
$$

$$
B_n^l = C_n^l A_n^l + D_n^l B_n^l,
$$

$$
A_n^l = A_n^l A_n^l + B_n^l B_n^l,
$$

$$
B_n^l = C_n^l A_n^l + D_n^l B_n^l,
$$

The first 9 $(2N - 3)$ where $N$ is the number of layers in the structure) equations pertain to $n = L$, the lowest space harmonic and these 9 equations will be reproduced for each $n = L + 1, \ldots, H$. Assuming $N$ layers and $M = H - L + 1$ space harmonics the set of above equations can be represented by a grand matrix $G$ with dimension $M(2N - 3) \times M(2N - 3)$.

The matrix can be written in block form as

$$
G = (B_{\mu \nu}), \quad \text{for } \mu, \nu = L, \ldots, H,
$$

(55)

and the derivative of $G$ with respect to $\gamma$ is

$$
G_{\gamma} = (B_{\mu \nu \gamma}), \quad \text{for } \mu, \nu = L, \ldots, H.
$$

(56)

The diagonal block matrices have band shapes (one lower diagonal, and two upper diagonals) and are identical for each space harmonic. For example, the $B_{nn}$ block for the $n$th space harmonic in (57), as shown at the bottom of the next page.

For sake of clarity, a superscript is placed on the matrix elements of $V$ to denote that the grating is in Layer 3. If Layer 2 was also a grating layer, the matrix elements $V_{2n}^{2n}$ would appear in columns 2 and 3. The block matrix $B_{nn}$ and its derivative are formed from a series of sub-block-matrices: For the $l$th layer (non-grating) and $n$th space harmonic, the modified transfer matrix $T_{nn}^l$ and its derivative $T_{\gamma nn}^l$ are

$$
T_{nn}^l = \begin{pmatrix}
A_n^l & B_n^l \\
C_n^l & D_n^l
\end{pmatrix},
$$

$$
T_{\gamma nn}^l = \begin{pmatrix}
A_n^l & B_n^l \\
C_n^l & D_n^l
\end{pmatrix}.
$$

For the $l$th grating layer and $n$th space harmonic, the modified transfer matrices and their derivatives are

$$
T_{mn}^l = \begin{pmatrix}
V_{mn}^l A_n^l & V_{mn}^l B_n^l \\
V_{mn}^l C_n^l & V_{mn}^l D_n^l
\end{pmatrix},
$$

$$
T_{\gamma mn}^l = \begin{pmatrix}
V_{mn}^l A_n^l & V_{mn}^l B_n^l \\
V_{mn}^l C_n^l & V_{mn}^l D_n^l
\end{pmatrix}.
$$

The off-diagonal block matrices are composed of modified transfer matrices that have six non-zero elements, which is six times the number of grating layers. The off-diagonal blocks, $B_{mn}$, are given by

$$
B_{mn} = \begin{pmatrix}
0 & 0 \\
0 & 0 \\
V_{mn}^3 A_n^3 & V_{mn}^3 B_n^3 \\
V_{mn}^3 C_n^3 & V_{mn}^3 D_n^3
\end{pmatrix}.
$$

The matrix $0_s$ is a $9 \times 3$ block of 0’s while $0_t$ is a $9 \times 4$ block of 0’s. The non-zero elements line up with the $V$ elements of (57). The transfer matrix in $B_{mn}$ is $T_{nn}^l$. If Layer 2 is also a grating layer, then $0_s$ would be replaced with one column of 0’s and two columns of $T_{mn}^2$ placed at row one.
The field coefficients $A_n^l$ and $B_n^l$ can also be partitioned or blocked as follows:

$$
\mathbf{r}_n^T = \begin{pmatrix} A_n^1 & A_n^2 & \cdots & A_n^5 & B_n^5 \end{pmatrix}, \tag{58}
$$

so that all coefficients are contained in the vector $\mathbf{r}$:

$$
\mathbf{r}_n^T = \left( \mathbf{r}_n^T \mathbf{r}_{n-1}^T \cdots \mathbf{r}_0^T \right), \tag{59}
$$

and the complete system of equations is represented by

$$
G(\gamma, k) \mathbf{r} = \mathbf{0}, \tag{60}
$$

where $G$ is a function of the complex propagation constant, $\gamma$, and the free-space wave number, $k$. Eq. (60) is the secular equation for the system and its solution describes a forward-propagating Floquet-Bloch mode. In regard to numerical computations, we are interested only in a single eigenvector whose eigenvalue is zero.

Assuming all layers that form the waveguide have no ohmic losses, then typically, one specifies the free-space wave number and a value of $\gamma$ near a singular condition on $G$, then $\gamma$ is perturbed in such a fashion as to make $G$ more singular. In waveguides near the second Bragg condition, $\gamma$ has real and imaginary parts, but when all space harmonics reside in the slow-wave region, the real part of $\gamma$ is zero. In this latter case, $G$ is a function of two real variables, $\beta$ and $k$. Thus, $\beta$ could be specified, then the problem is to find the proper value of $k$ that makes $G$ singular. However, with proper mathematical methods, $\gamma$ could be specified and then the problem at hand would be to find the free-space wave number that makes the determinant of $G$ as close to zero as possible.

The grand matrix $G$ is typically very large and sparse. It has a dimension of $M(2N - 3)$ where $M$ is the number of space harmonics and $N$ is the number of layers. For example, using 17 space harmonics and six layers, $G$ has a dimension of 153 and has 23,409 elements. Assuming one grating layer, the number of non-zero elements of $G$ is $M(6N - 10) + 6M(M - 1) = 2074$. To find $\gamma$ to make $G$ singular requires the solution of the matrix $X$ for the linear system of equations $G_0X = G_\gamma$ (See (A.4)) using a sparse matrix solver [40].

### H. NODES AND LAYER INTERFACE LOCATIONS

A node is defined as a transverse position $x$, where the field is calculated from the solution of (60). In the derivation of (60), the nodes are specified as points that lie at the interface of two distinct layers, including the different layers of the grating region. In general, nodes may be placed at any point in the transverse direction $x$.

Fig. 10 (a) shows five node positions where the nodes are placed at layer interfaces so that the node position is $\xi_i = x_i$. However, Fig. 10 (b) has eight nodes with the addition of four new nodes, while two nodes are moved from that shown in (a). The two end nodes are anchor nodes and cannot be deleted but they can be moved to cladding regions one and six. For the node positions shown in Fig. 7 (b), the field quantities $A$ and $B$ would be computed at all eight node positions for each space harmonic. When a node does not lie on an interface the transfer matrix will be computed as a product of two single layer transfer matrices. For example, when the material between $x_5$ and $x_6$ is different from the material between $x_4$ and $x_3$ the transfer matrix from $\xi_7$ to $\xi_6$ would be the product of two simple transfer matrices.

### I. SOLUTION OF THE SECULAR EQUATION

The number and location of nodes affect the accuracy of the calculation of the eigenvalue $\gamma$ and the corresponding eigenvector (58). The characteristics of the simple dielectric structure [3], [31] with an etched grating will be derived. The dielectric structure described by Table 2 is a basic four–layer waveguide where the superstrate, Layer 1, is air. (This particular structure has been extensively investigated by many different techniques.) A grating with a 50 percent duty cycle is formed in Layer 2 where the dielectric constant, varying between 3.0 and 1.0 along the propagation direction, produces an average value of 2.0.

$$
B_{nn} = \begin{pmatrix}
-1 & A_n^2 & B_n^2 & 0 & 0 \\
0 & A_n^3 & V_n^3 & m_n^3 & 0 \\
0 & 0 & A_n^4 & V_n^4 & m_n^4 \\
-1 & V_n^3 & 0 & A_n^5 & B_n^5 \\
0 & 0 & 0 & 0 & 1
\end{pmatrix} \tag{57}
$$
The angles for the leaky waves for the structure listed in Table 2 are computed for \( \lambda = 1 \) and \( \Lambda = 1/2 \), which is less than \( \Lambda_B \). For Mode I, as illustrated in Fig. 5 (a), \( \alpha > 0 \) because of power loss via radiation. The propagation constant \( \gamma \) has \( \alpha \lambda = 0.018713 \) and the mode’s effective index of refraction is \( n_e = \beta/k = 1.58075 \). Mode II has \( \alpha \lambda = -0.018713 \) and an identical effective index of refraction, as that of Mode I. Modes III and IV have \( \alpha \lambda = \pm 0.016894 \) (positive sign for Mode III and negative sign for Mode IV) and \( n_e = 1.56840 \). Modes I and II have an outgoing and incoming angle in the superstrate of \( \sim 114.8^\circ \) relative to the \( z \) axis and an outgoing and incoming angle in the substrate of \( \sim -106.0^\circ \) relative to the \( z \) axis. The outgoing and incoming angles for Modes III and IV are \( \sim 115.6^\circ \) and \( \sim -106.5^\circ \) for the superstrate and substrate respectively. For the particular structure analyzed, the radiation angles for Modes I and II are almost indistinguishable from the radiation angles of Modes III and IV.

As the grating period approaches the second Bragg condition the electric field, \( \mathbf{R}(x, z) \) in (6) starts to rapidly change along the propagation direction. Fig. 6 shows the field distribution for the four different modes when the grating period is \( \Lambda = 0.61 \lambda \). Modes I and II have attenuation coefficients \( \alpha = \pm 0.0157744/\lambda \), whereas Modes III and IV have attenuation coefficients \( \alpha = \pm 0.0202065/\lambda \).

To address the accuracy of the computational method two different node sets are discussed below. A profile of the structure given in Table 2 is illustrated in Fig. 11. The dielectric profiles across the tooth and fill regions are also illustrated. When the number of nodes (properly chosen) increase in number, the calculation time increases as \( \mathcal{O}(N^2) \) where \( N \) is the number of nodes. However, the overall accuracy is better, particularly with increasing number of space harmonics. In fact, the node spacing must be decreased as the number of space harmonics increases. For a non-trivial solution of (60), the grand matrix \( G \) must be singular, or equivalently, its determinant must be zero. Newton’s method [37], [38] can be used to find the propagation constant that makes the matrix \( G(\gamma, k) \) singular. Assuming the free-space wave number is fixed, \( G \) is expanded about \( \gamma = \gamma_0 \) as

\[
G(\gamma, k) = G_0(\gamma_0, k) + G_\gamma(\gamma_0, k)(\gamma - \gamma_0)
\]

where \( \gamma_0 \) is the initial guess value of the propagation constant, and the matrix \( G_\gamma \) is the derivative of the \( G \) matrix elements with respect to \( \gamma \) at \( \gamma = \gamma_0 \). The next iteration point is

\[
\gamma_1 = \gamma_0 - 1/\chi,
\]

where \( \chi \) is the maximum eigenvalue of \( G_0^{-1} \). However, as the number of space harmonics increases, for a given node distribution, the matrix \( G_0 \) becomes ill conditioned because of the large imaginary parts of \( h_v \) in (34) and of \( h_v^\prime \) in (45). When \( h_v^\prime d_i \) in the latter equation has a large imaginary part, the cosine and sine expressions are identical, for a given precision, and the transfer matrix is singular and the grand matrix (55) becomes ill-conditioned for \( \gamma \) values in regions near the root.

The condition number of a matrix can be used as a gauge to determine if it is singular [34], [41], [42], [43]. When the condition number is approximately zero, the matrix is well conditioned or non singular, whereas if the condition number is large, the matrix is singular and its determinant is approximately zero. Contemporary linear algebra software is used here to estimate the reciprocal condition number, \( R_c \), of \( G \). In particular, the reciprocal condition number of \( G \) will be driven from a value close to unity, for the initial guess of \( \gamma_0 \), to a value close to zero, at the desired complex root.

For the structure in Fig. 11 and a grating period \( \Lambda = 0.62 \lambda \) which is below the second Bragg condition, the initial value \( \gamma_0/k = 0.0004 + j 1.57 \) yields a root \( \gamma/k = 0.0023668 + j 1.5812627 \) for Mode I. The roots for the other modes are \( -0.0023668 + j 1.5812627 \) for Mode II and \( -0.00276343 + j 1.57210132 \) for Modes III and IV. Thus, the initial guess for \( \gamma_0 \) should produce a large value of \( R_c \) for the grand matrix compared to the machine precision. Starting with a small number of space harmonics, the reciprocal condition number for the initial guess is illustrated in Fig. 12.

The first iteration of the Newton search involves the calculation of \( R_c \) for the initial value \( \gamma_0 \). For the uniform node spacing of \( 0.2 \lambda \), and three space harmonics, the initial \( R_c \) is about \( 10^{-3} \). Using Newton iterations (3-4), \( R_c \rightarrow 10^{-20} \) and the Newton step (for \( \gamma \)) is less than \( 10^{-12} \) which is close to machine precision. On the other hand, as the number of space harmonics is increased above \( 10 \) the initial computed value of \( R_c \) drops below \( 10^{-15} \), and consecutive iterations are unsuccessful in reducing \( R_c \). Indeed, for the number of space harmonics above about 27, \( R_c \) fluctuates and step sizes approach zero.

When the node separation is \( 0.1 \lambda \), initial values of \( R_c \) are higher for identical numbers of space harmonics. Indeed, the lower node spacing produces stable results for a number of space harmonics exceeding 45. The cost for the additional accuracy is computation cycles.

The process of adding space harmonics to obtain a Cauchy-type convergence for \( \gamma \) is addressed below. The circle
markers in Fig. 13 were obtained with the large inter node spacing while the square markers pertain to the small inter node spacing. When the number of space harmonics is greater than $\sim 20$, the solutions for $\gamma$ obtained for the 0.2 $\lambda$ inter node spacing become unstable as the grand matrix becomes ill conditioned at initial root guesses. The square markers result from the calculations with 0.1 $\lambda$ inter node spacing.

Convergence of $\gamma_n$ will be assumed if for two different roots obtained with increasing $n$ and $m$ space harmonics, $|\gamma_n - \gamma_m| \rightarrow \varepsilon$, where $\varepsilon$ represents machine precision. There are two sets of points illustrated and the lower set represents $|\gamma_n - \gamma_{n-6}|$, whereas the upper set represents $|\gamma_n - \gamma_{n-4}|$. The number of space harmonics are $n = 9, 13, 17, \ldots$. The first point in the lower set is $|\gamma_7 - \gamma_7|$ while the last point in the set is $|\gamma_9 - \gamma_5|$. These numbers were used because of the formation of the Toeplitz matrix $K$. When three space harmonics are used to form $K$, the matrix has a diagonal and the first upper and lower diagonal elements; for five space harmonics, there are two upper and lower diagonal entries. However, for the 50 percent duty cycle, $\kappa_2 = \kappa_{-2} = 0.0$, as illustrated in Table 1. Thus, to get proper root differences, two different cases were computed: (1) when the maximum space harmonic produces a zero value on the diagonal and (2) when the maximum space harmonic produces a non-zero value on the diagonal. Thus, the difference $|\gamma_7 - \gamma_5|$ is more meaningful than say $|\gamma_7 - \gamma_5|$ for the 50 percent duty cycle.

**IV. FLOQUET-BLOCH SOLUTIONS**

This section will be concerned with properties of the waveguide mode and its various space harmonics in the grating layer for the structure given in Table 2 and illustrated in Fig. 11. The free-space wavelength of all computations use a real fixed wavelength, $\lambda = 1.0 \mu m$. Variations of the grating tooth duty cycle are shown to greatly influence the propagation properties.

In general there are three parameters that characterize each layer: the real and imaginary parts of the complex dielectric constant and the layer thickness. However, additional parameters such as the grating duty cycle affect the mode characteristics. The material in the grating regions, specified in Table 2 represent the material that forms the tooth regions. The material of the fill regions is air.

Calculations for Mode I are made for the structure given in Fig. 11 with seven nodes and a node spacing of 0.1 $\mu m$. The number of space harmonics are indicated in the various figures. Calculations for various modal characteristics are plotted in Figs. 14–17 as a function of $(\beta - K)/K$ where the grating period $K$ will be varied and the complex propagation constant $\gamma = \alpha + j\beta$.

**A. GRATINGS-LAYER EIGENVALUES**

The calculations for the wave eigenvalues illustrated in Figs. 12–16 assume the tooth duty cycle of 50 percent. The 17 space harmonics included in the calculation shown in Fig. 14 are $n = -9, \ldots, 7$. Near the second Bragg condition, space harmonics come in pairs centered about $n = -1$, such as space harmonics $n = -2$ and $n = 0$. Fig. 14 illustrates the
$\sigma_{-1}$ eigenvalue. Note that $|\sigma_{-1}'| \gg |\sigma_{-1}''|$ and that $\sigma_{-1}'' \to 0$ at the second Bragg condition. Fig. 15 shows the $m = -2$ and $m = 0$ grating eigenvalues. Fig. 16 illustrates the grating eigenvalues for all high-order space harmonics. The imaginary part of $\sigma_m$ has the property that $\Im(\sigma_m) \geq 0$ for all positive space harmonics while $\Im(\sigma_m) \leq 0$ for all negative space harmonics. The two high-order space harmonics $m = -9$ and $m = 7$ have $\Im(\sigma_m) \approx -6000$ ($\mu$m)$^{-2}$ and the corresponding wavenumbers $h_m \approx j75$ ($\mu$m)$^{-1}$. Indeed, in the grating region, near the second Bragg condition, all space harmonics, save $m = -1$, are evanescent.

We show that the modes may have both positive and negative values of $\alpha$ as shown corresponding to (6) and (18). Fig. 17 plots the attenuation constants for the various Floquet-Bloch modes. In Fig. 17(a), the solid curve shows that $\alpha$ is positive before the second Bragg (outward leaking) whereas $\alpha$ is negative after (inward leaking). The dashed curve represents the other mode. Without sources at $x = \pm \infty$, modes leak outward so that a wavelength scan across the second Bragg condition will cause the operating mode to switch from Mode I to Mode II or vice versa.

**B. GRATING-LAYER DUTY CYCLES**

The characteristics of the various modes are strongly influenced by the value of the duty cycle of the tooth in the grating layer. To illustrate the effect of the tooth duty cycle on the fields, the eigenvalues for the four modes are computed for three duty cycles, 25, 50 and 75 percent. Figs. 7 and 9 illustrate the complex propagation constant for the 50 percent duty cycle, producing a Bragg condition occurring at $\lambda_B \equiv \lambda_{S0} \approx 0.631072 \lambda$. For the 25 percent duty cycle, the second Bragg condition occurs at $\lambda_{25} \approx 0.638383 \lambda$. For the 75 percent duty cycle, the second Bragg condition occurs at $\lambda_{75} \approx 0.618379 \lambda$.

Fig. 18 shows the normalized components of the complex propagation constant $\alpha/k$ and $\beta/k$ for Modes I and III. Figs. 18 (a) and (b) pertain to Mode I while Figs. 18 (c) and (d) pertain to Mode III. (The propagation constant $\beta$ for Mode II is identical to that of Mode I, i.e., $\beta_{II} = \beta_{I}$, however, $\alpha_{II} = -\alpha_{I}$. Similarly, $\beta_{IV} = \beta_{III}$ and $\alpha_{IV} = -\alpha_{III}$.)

Computations for the three duty cycles show that Mode I, Fig. 18 (a), has a positive attenuation coefficient before the second Bragg condition but it changes sign after the second Bragg condition when $\Lambda > \Lambda_B$. Mode III shows similar behavior for the 50 and 75% duty cycles but the 25% duty cycle case has $\alpha_{III} < 0$ for $\Lambda < \Lambda_B$ and $\alpha_{III} > 0$ for $\Lambda > \Lambda_B$. In particular, when $d_c \approx 0.3 \Lambda$, $\alpha_{III} > 0$ but $\alpha_{III} \approx 0$ for $\Lambda < \Lambda_B$. Fig. 19 shows Mode III attenuation for the duty cycles 25,
FIGURE 18. Characteristics of Modes I and III for duty cycles of 25, 50 and 75% as a function of the grating period relative to the second Bragg condition: (a) and (b) pertain to Mode I with the real (a) and imaginary (b) parts of the propagation constant. Mode III characteristics for $\alpha/k$ and $\beta/k$ are shown in (c) and (d) respectively. Characteristics of Modes II and IV are similar except for the sign change of $\alpha$.

FIGURE 19. Mode III relative attenuation near the second Bragg condition for 25, 30 and 35% duty cycles. The 30 percent duty cycle has $\alpha_{\text{III}} \approx 0$ before the second Bragg condition, but it rises rapidly for $\lambda > \Lambda_B$. The 30 and 35 percent. Because $\alpha_{\text{III}} \approx 0$ below the second Bragg condition the amount of power entering the 30% duty cycle waveguide mode from the substrate and the power radiated from the mode are similar. Nevertheless, at $\Lambda = \Lambda_B$, there is no radiation to or from the waveguide mode. Fig. 19 shows abrupt changes in the value of $d\alpha/d\Lambda$ at the second Bragg condition. However, Fig 20, using a different scale below and above the second Bragg condition, indicates $d\alpha/d\Lambda \rightarrow -\infty$ as $\Lambda \rightarrow \Lambda_B$. Fig. 21 also indicates $d\alpha/d\Lambda \rightarrow -\infty$ as $\Lambda \rightarrow \Lambda_B$.

FIGURE 20. Mode III relative attenuation near the second Bragg condition for the 30% duty cycle with different scales before and after the second Bragg condition. The top curve starts at $\Lambda = 0.631\lambda$ and progresses toward the second Bragg condition, whereas, the bottom curve starts at $\Lambda = 0.645\lambda$ and ends near the second Bragg condition.

FIGURE 21. Mode III relative attenuation near the second Bragg condition for three duty cycles near the 30% duty cycle. The 29.8% duty cycle has the relative attenuation changing from a negative value to a positive value.

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30, and 35 percent. Because $\alpha_{\text{III}} \approx 0$ below the second Bragg condition the amount of power entering the 30% duty cycle waveguide mode from the substrate and the power radiated from the mode are similar. Nevertheless, at $\Lambda = \Lambda_B$, there is no radiation to or from the waveguide mode. Fig. 19 shows abrupt changes in the value of $d\alpha/d\Lambda$ at the second Bragg condition. However, Fig 20, using a different scale below and above the second Bragg condition, indicates $d\alpha/d\Lambda \rightarrow -\infty$ as $\Lambda \rightarrow \Lambda_B$. Fig. 21 also indicates $d\alpha/d\Lambda \rightarrow -\infty$ as $\Lambda \rightarrow \Lambda_B$.

Fig. 21 further illustrates the sensitivity of the mode attenuation as a function of the tooth duty cycle. The curve illustrating the attenuation coefficient of the 29.8 percent tooth duty cycle indicates $\alpha_{\text{III}} = 0$ not only at $\Lambda = \Lambda_B$, but also near $\Lambda = 0.6335\lambda$, which implies equal amounts of power leak into the mode from the substrate and leak out of the mode into the superstrate. If the output power from the superstrate can be directed into the substrate, the mode will lossless. If the waveguide has a finite-depth substrate, then two waveguides could coupled by way of leaky mode radiation.

The 30 and 29.9 percent duty cycle curves for Mode III of Fig. 21 also have attenuation coefficients that are zero at different grating periods $\Lambda < \Lambda_B$. On the other hand, Mode I has $\alpha > 0$ while Mode II has $\alpha < 0$ at all values of $\Lambda < \Lambda_B$ provided $\beta_{-1}$ lies in the fast-wave region.

The sharp changes in $\alpha$ around the second Bragg condition ($d\alpha/d\Lambda \rightarrow \pm\infty$) implies a very narrow bandwidth for either no radiation from the waveguide mode or for coupling power into the waveguide mode.
The waveguide structure illustrated in Fig. 1 may be viewed as a collection of waveguides placed back-to-back. If materials in the tooth and fill regions along with all the other layers are lossless, then the modes in each of those regions consist of a set of discrete-spectra modes whose fields tend to zero as $x \to \pm \infty$, resulting in a set of continuous-spectra modes (radiation modes) whose fields remain finite at all positions in the superstrate and substrate regions, along with a set of continuous-spectra evanescent modes confined to the vicinity of the discontinuity. These three sets of modes form a complete orthogonal set. Continuous-spectra modes are induced at the tooth and fill boundaries and thus scatter power into or out of the central waveguide region. The process of matching fields with discrete and continuous spectra, in the tooth region to the those in the fill region produces the fields in the periodic waveguide.

Floquet theory, in essence, condenses the mode sets to one mode whose field has a periodicity and a propagation constant as given in (6). At grating periods near the second Bragg condition, there is a single space harmonic, $n = -1$, that has exponential growth in the claddings with propagation either in or out of the cladding regions. At points $x_1$ and $x_5$ in Layers 1 and 6 of Fig. 1, the Poynting vector indicates the direction of power flow due to the $-1$ space harmonic. Power computed from the Poynting vectors correlates with the power loss or gain of the computed value of $\alpha$.

In a typical application, a periodic waveguide is located longitudinally between waveguides without gratings. The fields of the input waveguide are characterized by incident...
and reflected fields while fields of the output waveguide are characterized only by transmitted fields. The fields in the periodic waveguide will have forward and backward Floquet-Bloch modes given by

\[ \Psi_g(x, z) = a R(x, z)e^{-\gamma z} + b S(x, z)e^{\gamma z}, \]

where \( a \) and \( b \) are constants and the forward mode, \( R(x, z) \), satisfies (17). For symmetric unit cells, the backward mode, \( S(x, z) \), satisfies

\[ \frac{\partial S(x, z)}{\partial z} = -\frac{\partial R(x, z)}{\partial z}. \]

When the input and output waveguide fields approximate the fields in the periodic waveguide, and when radiation modes induced at the interfaces between the input and periodic waveguide and the periodic waveguide and the output waveguide can be ignored, one can obtain accurate results for the coefficients \( a \) and \( b \) in (63) using the overlap integrals of the input and output waveguide fields with the field of the periodic structure. Assuming \( 2N_g \) grating periods are etched into a dielectric waveguide, then the periodic waveguide has a length of \( L_g = 2N_g \lambda \). Because \( R(x, z) \) and \( S(x, z) \) are periodic, with respect to \( z \), input to the periodic waveguide, centered about \( z = 0 \), occurs at \( z = -N_g \lambda \) and the field in the grating region is

\[ \Psi_g(x, -N_g \lambda) = a R(x, 0)e^{N_g \gamma \lambda} + b S(x, 0)e^{-N_g \gamma \lambda}. \]

Similarly, the output field of the periodic waveguide at \( z = N_g \lambda \) is

\[ \Psi_g(x, N_g \lambda) = a R(x, 0)e^{-N_g \gamma \lambda} + b S(x, 0)e^{N_g \gamma \lambda}. \]

With proper analysis, one obtains a system of equations with six unknowns, \( a, b \), and the percentages of reflected and transmitted power along with percentages of power radiated toward the superstrate and substrate resulting from the section of the periodic waveguide can be determined.

**V. CONCLUSION**

A new mathematical approach to calculating the waveguide characteristics near the second Bragg condition is presented. The method relies on the expansion of the fields in terms of the eigenvectors of the matrix, determined from the Fourier expansion of the periodic dielectric constant. The dimension of the vector space is equal to the number of space harmonics used in the expansion of the dielectric constant. For the best numerical accuracy of the field calculations at the second Bragg condition, pairs of space harmonics are chosen above and below the \( m = -1 \) space harmonic, i.e., \((-2, 0), (-3, 1), \) etc. As the number of space harmonics increases, the numerical accuracy increases and then can decrease. The decrease in accuracy with increasing number of space harmonics can be overcome by splitting up large layers into smaller layers with the same material properties, thereby increasing the number of nodes. In particular, when using 17 space harmonics the calculation of \( \gamma \) for the structure in Fig. 11 starts to degrade when the tooth height is greater that 0.6 \( \lambda \) and when the nodes are placed at layer boundaries [3]. However the addition of nodes within a layer allows the number of space harmonics to be increased while providing increased accuracy.

Since the root search for the propagation constant is developed using Newton’s method, one needs the derivative of the eigenvalues and eigenvectors with respect to \( \gamma \), obtained from (29) and by the vector expansion given by (30). Furthermore, Appendix B describes a method of calculating the group velocity of the modes which involves the calculation of the derivative of the grand matrix with respect to \( \gamma \) and the derivative with respect to the free-space wavenumber \( k \). An iteration scheme such as one that varies the grating period \( \Lambda \), after a root is determined, allows a new root at the iteration point to be approximated from the derivative \( d\gamma/d\Lambda \), obtained by differentiation of the grand matrix, (55), with respect to \( \gamma \) and \( \Lambda \). Note that there is a fourth-order zero at the second Bragg condition, so that the Newton root search has trouble. However, Figs. 9 and 17 illustrate sufficient accuracy in the neighborhood of the second Bragg condition. The explanation of why second-order gratings are successfully used as reflectors and outcouplers in optical waveguide devices is explained physically based on the mathematical analysis developed in this paper.

In addition to showing mathematically that there is no mode attenuation at the exact second Bragg condition, we show that some modes with leaky waves coming into the substrate and leaky waves going out of the superstrate have a second zero in the attenuation coefficient at grating periods near the second Bragg condition.

There are two sources of dispersion in dielectric waveguides: (1) material and (2) waveguide geometry. In most waveguide geometries the material dispersion plays a minor role if the operating wavelength is significantly different from the material’s bandgap wavelength. Hence, the source of the derivative of the grand matrix, \( G_\gamma \) in Appendix III-B is due to the parameter \( k \).

**APPENDIX A NEWTON’S METHOD**

An iterative method is used for driving the eigenvalue \( \nu(\gamma, k) \) of the equation

\[ G(\gamma, k) r(\gamma, k) = \nu(\gamma, k) r(\gamma, k), \]

(A.1)

to zero, where the complex variables \( \gamma \) and \( k \) are the propagation constant and free-space wavenumber, respectively. For a given wavelength the matrix \( G \) and its associated eigenvector \( r \) are functions of \( \gamma \). Similarly, for a given propagation constant, \( G \) and its eigenvector are functions of \( k \).

The object here is to determine the value of \( \gamma \) for a specific value of \( k = k_d \) that renders \( G \) as singular and thus maps the non-trivial eigenvector \( r \) to \( 0 \). If \( \gamma = \gamma_d \) makes \( G \) singular, then \( r(\gamma_d) \) is the non-trivial solution vector, or eigenvector whose eigenvalue is 0. (There may be more than one solution.) If for an arbitrary value of \( \gamma \), \( G \) is non-singular, \( G \) cannot map \( r \), whose norm is unity, to \( 0 \), but it can, for example, map the eigenvector associated with its
smallest eigenvalue to the product of the eigenvalue and its eigenvector, so one possibility is to make the vector \( \mathbf{r} \) the vector of the smallest eigenvalue of \( G \). The problem of using a Newton method to drive the smallest eigenvalue of the matrix \( G \) to zero is that the order of the eigenvalues tends to change during the iteration process. The method here tracks the condition number of \( G \). When an arbitrary value of \( \gamma \), say \( \gamma_0 \), is chosen near the point \( \gamma_0 \), then this Newton method converges rapidly as outlined in the following algorithm.

Assume, for a given \( \gamma = \gamma_0 \), \( G \) is non singular, i.e., \( \gamma_0 \neq \gamma_a \). Expanding (A.1) about \( \gamma_0 \) produces, to first order,

\[
G(\gamma) \mathbf{r}(\gamma) = G_0 \mathbf{r}_0 + (G_\gamma \mathbf{r}_0 + G_0 \mathbf{r}_\gamma) \delta \gamma, \tag{A.2}
\]

where \( \delta \gamma = \gamma - \gamma_0 \) is the step toward the singularity, and

\[
G_0 = G(\gamma_0), \quad G_\gamma = \left( \frac{\partial G}{\partial \gamma} \right)_{\gamma=\gamma_0}, \quad \mathbf{r}_0 = \mathbf{r}(\gamma_0), \quad \mathbf{r}_\gamma = \left( \frac{\partial \mathbf{r}}{\partial \gamma} \right)_{\gamma=\gamma_0}.
\]

When \( G_0 \) is singular, \( \delta \gamma = 0 \), but, if \( G_0 \) is non singular, it has an inverse and the right-hand-side of (A.2) can be written as

\[
\mathbf{r}_0 + G_0^{-1} G_\gamma \mathbf{r}_0 \delta \gamma + \mathbf{r}_\gamma \delta \gamma. \tag{A.3}
\]

The object now is to find the value of the step, \( \delta \gamma \), that makes the norm of (A.3) as small as possible. Consider the eigenvalue problem

\[
G_0^{-1} G_\gamma \mathbf{r} = \chi \mathbf{r}. \tag{A.4}
\]

If \( G_0^{-1} G_\gamma \) has a rank of \( N \), then there are \( N \) eigenvalues, \( \chi_n \), and their corresponding eigenvectors, \( \mathbf{r}_n \), \( n = 1, 2, \ldots, N \). The vector \( \mathbf{r}_0 \) will be selected as the eigenvector associated with the largest eigenvalue, \( |\chi_{\text{max}}| = \max(|\chi_1|, |\chi_2|, \ldots, |\chi_N|) \), so that the above expansion becomes

\[
\mathbf{r}_{\text{max}} + \chi_{\text{max}} \mathbf{r}_{\text{max}} \delta \gamma + \mathbf{r}_\gamma \delta \gamma = -\mathbf{r}_\gamma/\chi_{\text{max}}, \tag{A.5}
\]

when the step \( \delta \gamma \) is equal to \(-1/\chi_{\text{max}}\). Thus, when \( \mathbf{r}_0 = \mathbf{r}_{\text{max}} \) the norm of right-hand-side of the above equation, \( \|\mathbf{r}_\gamma/\chi_{\text{max}}\| = 1/\|\chi_{\text{max}}\| \), is minimized. Choosing an eigenvector other than that associated with \( \chi_{\text{max}} \), would slow convergence.

**APPENDIX B GROUP VELOCITY**

The group velocity can be calculated from the matrix \( G(\gamma, k) \) when it is singular. We outline the formulation below.

At the singular point the eigenvalue \( \nu(\gamma_a, k_a) = 0 \) so that \( G(\gamma_a, k_a) \) maps the non-trivial vector \( \mathbf{r}_a \) to \( \mathbf{0} \). In addition to the right-hand eigenvector \( \mathbf{r}_a \) the left-hand eigenvector \( \mathbf{s}_a \) that has the same eigenvalue, \( \nu = 0 \), and satisfies

\[
\mathbf{s}_a^H(\gamma_a, k_a) G(\gamma_a, k_a) = \nu(\gamma_a, k_a) \mathbf{s}_a^H(\gamma_a, k_a) = \mathbf{0}. \tag{B.1}
\]

That is, \( G^H(\gamma_a, k_a) \) maps the vector \( \mathbf{s}_a \) (\( \| \mathbf{s}_a \| \neq 0 \)) to \( \mathbf{0} \).

In this paper there are two types of eigen expansions: a) expansion for Newton’s method for root searching, and b) expansion about singular points for evaluating wave properties by way of eigenvectors. For a) the expansion (A.2) is about the point \( \gamma = \gamma_0 \) and a fixed value of \( k \), where \( G \) is non singular. For b) it is assumed that both \( k \) and \( \gamma \) are independent variables, and (A.1) will be expanded about \( k = k_a \) and \( \gamma = \gamma_a \). When \( G, \nu \) and \( \mathbf{r} \) are expanded about the singularity, (A.1) becomes, keeping first two terms,

\[
\mathbf{r}_a = \mathbf{s}_a \left( \nu(\gamma_a, k_a) \mathbf{r}_a + \delta \gamma \right). \tag{B.2}
\]

where \( \nu(\gamma_a, k_a) = 0 \). The terms with subscripts of \( k \) and \( \gamma \) represent partial derivatives with respect to the variables evaluated at \( k = k_a \), and \( \gamma = \gamma_a \). The first-order terms in (B.2) become

\[
G_a \mathbf{r}_a \delta \gamma + G_a \mathbf{r}_\gamma \delta \gamma + (G_a \mathbf{r}_a \delta \gamma + G_a \mathbf{r}_\gamma \delta \gamma) \mathbf{r}_a = \nu(\gamma_a, k_a) \mathbf{r}_a. \tag{B.3}
\]

Upon taking the product of the transpose conjugate of left-hand eigenvector \( \mathbf{s}_a \), the first two terms of the left-hand side of (B.3) vanish. Assuming the inner product of the two vectors \( \mathbf{s}_a^H \mathbf{r}_a = 1 \), the derivative of the eigenvalue \( \nu \) with respect to \( \gamma \) at the singular point becomes

\[
\nu(\gamma_a, k_a) = \mathbf{s}_a^H \mathbf{G}_k \mathbf{r}_a = \langle \mathbf{s}_a | \mathbf{G}_k | \mathbf{r}_a \rangle. \tag{B.4}
\]

Similarly, the derivative of \( \nu \) with respect to \( k \) at the singular point becomes

\[
u_k(\gamma_a, k_a) = \mathbf{s}_a^H \mathbf{G}_k \mathbf{r}_a = \langle \mathbf{s}_a | \mathbf{G}_k | \mathbf{r}_a \rangle. \tag{B.5}
\]

The ratio of the derivatives is

\[
\frac{dk}{d\gamma} = \left| \frac{\mathbf{s}_a G_k | \mathbf{r}_a}{\mathbf{s}_a G_k | \mathbf{r}_a} \right|. \tag{B.6}
\]

The complex group velocity for a real frequency \( \omega \) and a complex propagation constant \( \beta \) is defined as

\[
\frac{d\omega}{d\beta} = c \frac{dk}{d\gamma} = \frac{dk}{d\gamma}. \tag{B.7}
\]

where \( c \) is the velocity of light in vacuum. We defined mode propagation along the \( z \) direction as \( \exp(j\omega t - \gamma z) \) where \( \gamma \) is complex. However, group velocity which specifies the velocity of a wave packet is usually defined as the real quantity \( 1/(d\beta/d\omega) \). (In (B.7) we use the transformation \( \gamma = j\beta \) so that \( \beta \) is complex.

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