A New Formulation of Coupled Propagation Equations in Periodic Nanophotonic Waveguides for the Treatment of Kerr-induced Nonlinearities

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Abstract— Nonlinear phenomena could be used to implement important signal processing functionalities in future nanophotonic integrated optical devices. In this paper, a semi-analytical model incorporating the influence of Kerr-induced non-linearity in the propagation of an optical signal inside a periodic nanophotonic waveguide is derived. The approach consists of a system of nonlinear coupled mode propagation equations and is applicable to both single and multi-mode waveguides. The influence of the mode group velocity on the value of the self phase modulation (SPM) coefficient $\gamma$ is analyzed and the impact of higher order nonlinear terms is also investigated both at the middle and edge of the guided band. The model is also applied to estimate the nonlinear coupling coefficients of a photonic crystal waveguide coupler and provides an efficient method to analyze the influence of nonlinear phenomena in periodic nanophotonic waveguide devices.

Index Terms— Electromagnetic propagation in nonlinear media, Nonlinear optics, Nonlinear wave propagation, Periodic structures.

I. INTRODUCTION

Nanophotonic structures are constantly attracting increased attention for the realization of future optical integrated circuits with increased scale of integration. Particular attention is given to artificial periodic dielectric structures, usually referred to as Photonic Crystals (PC) [1]. PCs can exhibit photonic badgaps, i.e. a range of frequencies where no guided mode exists. By introducing defects in a PC structure, one can realize waveguides and cavities in which light is tightly confined. PC waveguides provide an efficient means of guiding light by allowing the design of sharp optical bends [2]. As in the case of optical fibers, signal processing could be accomplished in the nonlinear regime [3]-[12]. In another context, a large chain of coupled cavities [14] can be thought of as a novel type of waveguide where light propagates through evanescent wave coupling from cavity to cavity. This new type of waveguide is called the Coupled Resonator Optical Waveguide (CROW) [15] and has many interesting properties. By appropriately positioning the resonators, it is possible to construct sharp, lossless and reflection-less bends throughout the entire CROW band. Another important property of the CROW is its ability to drastically slow down the optical wave (the slow light concept) [16],[17] which can find important applications in the realization of compact optical delay lines. The low group velocity and large optical field amplitudes of the localized modes lead to an enhancement of nonlinear effects [18]-[24], which could potentially be useful for all-optical signal processing purposes. Both the CROW and the PC waveguide constitute examples of periodic nanophotonic waveguides and in view of the potential applications, the study of nonlinear phenomena in such structures is beginning to receive increased attention. Finite Difference Time Domain (FDTD) [25] methods can be modified to include nonlinear effects and although in principle might be used to the study the nonlinear propagation phenomena inside a nanophotonic waveguide, they usually require extensive memory resources which renders such simulations
impractical for long devices. Numerical techniques based on nonlinear transfer matrix methods have been also discussed in order to model the propagation inside finite nonlinear periodic media [12],[13].

An alternative method, very similar to the one used in conventional constant cross-section optical waveguides is to expand the optical field in terms of the modes of the structure and derive Schrödinger type evolution equations for the envelope functions of the modes [26]. The propagation equation, describing the z-evolution of the envelope function of the field inside a weakly guiding, single mode optical fiber has been used for many years to model the various nonlinear effects, affecting the signal propagation [27]. In periodic nanophotonic waveguides, the derivation of a similar equation is more complex. In the special case of a CROW, a model describing the time evolution (t-evolution) of the optical field has been derived based on the reciprocity relations assuming nearest neighbor coupling interactions [23]. In [8], a Schrödinger like, t-evolution nonlinear equations have been derived in the case of a general periodic waveguide as well, using a multiple scale analysis.

In this paper, a model based on nonlinear z-evolution coupled mode propagation equations for a general nanophotonic periodic waveguide is derived for the first time, using a straight forward application of reciprocity relations [28],[30] in Maxwell’s equations. From a practical point of view, the advantage of using a z-evolution equation is that eye-diagram evaluations [31] can be more easily accomplished since the entire t dependence of the optical field is calculated at the end of the waveguide, and optical noise can be easily added in the time domain. The equations derived in this paper include both linear and nonlinear mode coupling and are used in order to estimate the Self Phase Modulation (SPM) coefficient γ and determine its relation to the group velocity of the mode. It is also shown that in periodic nanophotonic waveguides, γ is not constant but a periodic function of z. The value of γ is theoretically compared to the value of the SPM coefficient obtained by the CROW discrete equation model derived in [23]. In the case of weak guidance it is also shown that γ reduces to its well known expression [26]. Higher order terms are also included in the model and their influence depending on the pulse duration and launch point inside the guided band is discussed. The model is also applied in the case of a waveguide coupler consisting of two coupled PC waveguides resulting in a system of coupled propagation equations. The nonlinear coupling coefficients are calculated and compared to the SPM terms.

The rest of the paper is structured as follows: In section II, the optical field’s expansion in terms of the periodic waveguide’s Bloch modes is briefly outlined, while in section III, the envelope functions for narrowband signals are introduced. In section IV the nonlinear coupled mode propagation equations are derived using reciprocity relations while in section V, the model is applied to a single mode nanophotonic waveguide in order to obtain the nonlinear SPM coefficient. The nonlinear PC coupler is discussed in section VI while concluding remarks are presented in section VII.

II. MODAL EXPANSION

In this section the preliminary equations regarding the expansion of the optical field inside the nonlinear waveguide in terms of its guided modes are presented. These equations will be used in later sections to derive the system of coupled propagation equations for the envelope functions of the modes.

The total electromagnetic field (E, H) obeys the usual time dependent Maxwell’s equations:

\[ \nabla \times E = -\mu \frac{\partial H}{\partial t} \quad (1) \]

\[ \nabla \times H = \varepsilon \frac{\partial E}{\partial t} \quad (2) \]
where the dielectric constant $\varepsilon$ corresponds to the actual waveguide structure under consideration and can be decomposed into a linear part $\varepsilon_L$ and a nonlinear part $\varepsilon_{NL}[|E|^2]$ (which is due to the Kerr phenomenon), i.e.

$$
\varepsilon = \varepsilon_L + \varepsilon_{NL}[|E|^2] \quad (3)
$$

The electromagnetic field can be expressed as a linear combination of the guided modes at every frequency $\omega$

$$
E(r,t) = \sum_m d_m(z,\omega)E_m(\omega)e^{j\omega t} \quad (4)
$$

$$
H(r,t) = \sum_m d_m(z,\omega)H_m(\omega)e^{j\omega t} \quad (5)
$$

where $d_m(z,\omega)$, $E_m(\omega)$ and $H_m(\omega)$ are the expansion coefficient, the electric and the magnetic modal fields respectively of $m^{th}$ guided mode at frequency $\omega$. Equations (4) and (5) express the fact that the electromagnetic field can be decomposed as a sum over all waveguide guided modes $m$ at every frequency $\omega$. At each frequency $\omega$, there may also be a continuous mode spectrum corresponding to radiation modes, which will be ignored in this study.

There is some degree of freedom in choosing the guided modal fields in the above expansion depending on the problem at hand. The modal fields can either be the actual modes of the waveguide structure or some other approximate modal fields. For example, in the case of an optical coupler formed by two coupled waveguides, one can either expand the optical field in terms of the actual modes (supermodes) of the coupler, or approximately in terms of the modes of the isolated waveguides [33]. The latter formulation results in significant simplifications and will be adopted in the study of the nonlinear PC coupler in section VI. In any case $E_{m,\omega}$ and $H_{m,\omega}$ obey the following Maxwell equations

$$
\nabla \times H_{m,\omega} = -j\omega \varepsilon_m E_{m,\omega} \quad (6)
$$

$$
\nabla \times E_{m,\omega} = j\omega \mu_m H_{m,\omega} \quad (7)
$$

where $\varepsilon_m$ is the dielectric constant for mode $m$ and $\mu_m$ is the magnetic permeability. If $\varepsilon_m$ is periodic along the $z$-direction, then using Bloch’s theorem [32] one may write the modal fields as:

$$
E_m(\omega) = e_m e^{k_m(\omega)z} \quad (8)
$$

$$
H_m(\omega) = h_m e^{k_m(\omega)z} \quad (9)
$$

where $e_m$ and $h_m$ are periodic vector functions and $k_m(\omega)$ is the propagation constant of the mode. The fields can be normalized such that

$$
N_m = \int_S dS(e_{m,\omega} \times h_{m,\omega}^* + h_{m,\omega} \times e_{m,\omega}^*) \cdot \mathbf{z} = \pm 1 \quad (10)
$$

where $N_m$ is 1 for the forward guided modes and $N_m=-1$ for the backward guided modes. For two different Bloch modes ($m \neq l$) with the same dielectric constant ($\varepsilon_m=\varepsilon_l$) one obtains the orthogonality relation [28]:

$$
\int_S dS(e_{m,\omega} \times h_{l,\omega}^* + h_{m,\omega} \times e_{l,\omega}^*) \cdot \mathbf{z} = 0 \quad (11)
$$

Figure 1(a) illustrates the dispersion relation of the guided mode of a CROW, based on 2D photonic crystal defect cavities (see figure inset). The modes were calculated using the Plane Wave Expansion (PWE) method [32]. In this case the electric field is polarized along the $y$ direction, i.e. $e_{1,\omega} = \mathbf{y} c(x,z)$. The refractive index of the rods was taken $n_g=3.4$ while that of the surrounding medium was taken $n_b=1.0$. The PC lattice constant is taken $a=0.6 \mu m$ while the adjacent cavity spacing $D$ and the rod radius $r_a$ is $D=2a$ and $r_a=0.18a$ respectively. The guided mode band extends from 185.7THz to 204.8THz. The slow down factor $S=c/v_g$, where $c$ is the speed of light in vacuum and $v_g$ is the group velocity of the mode is also shown in the same figure. Near the band edges, $S$ is large, implying larger amplitudes for the modal fields and hence an enhancement of nonlinear effects.
This is illustrated in Figure 1(b) and (c), where the normalized modal fields $e_i(x,z)$ are plotted assuming $k=\frac{\pi}{2}D$ (middle of the band) and $k=0.05\frac{\pi}{D}$ (near the band edge) respectively and it is deduced that the modal amplitude is stronger in the latter case. This enhancement of the modal fields is in agreement with the integral equations relating the field intensity and the group velocity. If $W_m$ and $S_{z,m}$ are defined as

$$S_{z,m} = (e_{m,o_{m}} \times \mathbf{h}_{m,o_{m}}^* + e_{m,o_{m}} \times \mathbf{h}_{m,o_{m}}^*) \cdot \mathbf{z}$$

and

$$W_m = \frac{1}{2} \left( \mu \left| \mathbf{h}_{m,o_{m}} \right|^2 + e_L \left| e_{m,o_{m}} \right|^2 \right)$$

then the group velocity is given by

$$v_{g,m} = \frac{\langle S_{z,m} \rangle}{\langle W_m \rangle} = \frac{D}{\langle W_m \rangle V} = D \left( \int W_m dV \right)^{-1}$$

where $V$ is the volume of the waveguide cell and $<>$ denotes spatial average along the entire waveguide unit cell. According to equation (14), as the group velocity is reduced, the average field intensity increases and hence the modal amplitudes are enhanced. Equation (14) will be used in order to study the influence of $v_{g}$ in the value of the SPM coefficient in section V.

It is interesting to note that, except an amplitude enhancement, the distribution of the modal fields does not vary significantly, especially in the vicinity of the cavity. This is illustrated in Figure 1(d), where both fields are plotted along the $x$-axis, at $z=z_1=-a/2$, with amplitudes normalized to unity. Note that the fields have identical main lobes, while there is some small difference in the sidelobes. Consequently, the shape of $e_{m,o}$ approximately remains the same and near $\omega \approx \omega_0$, one may approximate the mode variation using

$$\left| e_{m,o} \right| \approx N_{e,m}(\omega)$$

where $N_{e,m}(\omega)$ is a function of $\omega$ describing the enhancement of the modal amplitude around $\omega=\omega_0$. The equations of this section will be used in order to derive a set of coupled propagation equations for the modal envelope functions defined in the next section.

### III. Narrow Band Signals

In this section the envelope function of the modes will be introduced. Assuming narrowband real signals of bandwidth $\delta \omega$ around a central frequency $\omega_0$ (Figure 2), the electric field in (4) can be expressed in terms of two complex electric fields $E_P$ and $E_N$ with spectra lying inside $P=[\omega_0-\frac{1}{2}\delta \omega, \omega_0+\frac{1}{2}\delta \omega]$ and $N=[-\omega_0-\frac{1}{2}\delta \omega, -\omega_0+\frac{1}{2}\delta \omega]$ respectively,

$$E(r,t) = E_p(r,t) + E_N(r,t) = E_p(r,t) + c.c.$$

where c.c. stands for complex conjugate and

$$E_p(r,t) = \sum_m \int_P d\omega a_m(z,\omega) E_{m,o} e^{j\omega t}$$

$$E_N(r,t) = \sum_m \int_N d\omega a_m(z,\omega) E_{m,o} e^{j\omega t}$$

The complex conjugation in (16) originates from the fact that $E(r,t)$ is a real quantity and hence the portion of the spectrum located in $N$ (around $-\omega_0$) is the complex conjugate of the spectrum located inside $P$ (around $+\omega_0$), i.e. $E_N=E_P^*$. The envelope functions $A_m(z,t)$ of the modes can be defined as

$$A_m(z,t) = \int_P d\omega a_m(z,\omega) e^{j\Delta k z - j\Delta \omega t}$$

where $\Delta \omega=\omega-\omega_0$ and $\Delta k=k(\omega)-k(\omega_0)$. Taking the time derivative in (19)
The envelope functions can be used to provide an alternative representation of the electromagnetic field. First, the electric Bloch function and the propagation constant are expanded around the central frequency $\omega_0$ as

$$ e_{l,n}(\omega) = \sum_{n=0}^{\infty} \frac{\partial^n}{\partial \omega^n} e_{l,n} \Delta \omega^n $$

$$ k_j(\omega) = \sum_{n=0}^{\infty} k_{ln} \frac{\Delta \omega^n}{n!} $$

with $k_{ln} = \frac{\partial^n}{\partial \omega^n} (\omega_0)$. Substituting (22), (21), (20) into (17), one obtains:

$$ E(r,t) = \sum_{n} \frac{\partial^n}{\partial t^n} A_m(z,t) \frac{j^n}{n!} e^{i\Delta(k_o-z-\Delta \omega t)} + c.c. \approx \sum_{n} A_n(z,t) e_{m,n} e^{i\Delta(k_o-z-\Delta \omega t)} + c.c. $$

where $k_{m0} = k_{m}(\omega_0)$ and the second approximate equality is obtained by keeping only the zero order terms. Equation (23) reveals the importance of the envelope functions in the representation of a narrow band optical signal: The electric field can be approximated by an expansion over the Bloch modes at $\omega = \omega_0$ oscillating as $\exp(-j \omega_0 t)$, modulated by the slowly varying envelope functions $A_m(z,t)$. The complex conjugate ensures that the field is real in the time domain.

To derive the coupled propagation equations for the envelope functions, (19) is differentiated with respect to $z$

$$ \frac{\partial A(z,t)}{\partial z} = \int d\omega \left[ \frac{\partial a_m}{\partial z} + j \Delta k_m \right] e^{i\Delta(k_o-z-\Delta \omega t)} $$

The second part of the integral in the Right Hand Side (RHS) of (24) can be simplified in terms of the time derivatives of $A(z,t)$ by expanding $\Delta k_j$ in terms of $\Delta \omega$ and using (22) along with (20), which yields

$$ \int d\omega \Delta k_m a_m e^{i\Delta(k_o-z-\Delta \omega t)} = \sum_{n=1}^{\infty} \frac{j^{n+1} k_{ln}}{n!} \frac{\partial^n}{\partial t^n} A_j $$

The above integral depends only on the dispersion properties of the modes, i.e. the variation of their propagation constants $k_m$ with respect to $\omega$. In the next section, the first part of the integral of (24) will be shown to originate from the linear and nonlinear coupling of the modes and will also be expressed in terms of the envelope functions. Defining the vector $A = (A_m(z,t))^T$, $b = (b_m)^T$, where

$$ b_m = \frac{\partial a_m}{\partial z} e^{i\Delta k_m z} $$

and the diagonal matrices $K_n = [k_{pq}^{(n)}]$ with $k_{pq}^{(n)} = k_{pq} \delta_{pq}$, equation (24) can be written in vector form

$$ \frac{\partial A(z,t)}{\partial z} = \int d\omega b(\omega) e^{-\Delta \omega t} + \sum_{n=1}^{\infty} \frac{j^{n+1}}{n!} K_n \frac{\partial^n}{\partial t^n} A(z,t) $$

The field intensity needed in the calculation of the nonlinear part of the dielectric constant $\varepsilon_{NL}|E|^2$ in (3) can be expressed solely in terms of the spectrum in $P$ using the fact that

$$ |E|^2 = E \cdot E = E_p^2 + E_N^2 + 2E_p \cdot E_N $$

In (28), the term $E_p^2$ is oscillating around $2\omega_0$ and the field $E_N^2$ is oscillating around $-2\omega_0$ and if included in (3) will account for third harmonic generation. Ignoring this effect and using (17), one may approximate the electric field intensity as:

$$ |E(r,t)|^2 \approx 2|E_p|^2 = 2 \sum_{pq} e^{i(k_p-k_q)z} \int d\omega_1 a_p(z,\omega_1) \int d\omega_2 a_q^*(z,\omega_2) e^{i\Delta k_o-z-\Delta \omega_1 t-\Delta \omega_2 t} e_{p,\omega_1} \cdot e_{q,\omega_2} $$

(29)
IV. DERIVATION OF THE NON-LINEAR PROPAGATION EQUATIONS

In this section, the reciprocity relations are applied in order to obtain a relation between \( \partial a_l / \partial z \) in (24) and the linear and nonlinear coupling of the modes. These expressions can provide a system of coupled \( z \)-evolution propagation equations for the envelope functions \( A_l \).

A. Application of the Reciprocity Relations

Using the time domain reciprocity relation (A3) and the electromagnetic field expansion in (4),(5) one easily obtains

\[
\sum_m \int d\omega a_m R_{lm} e^{-j\omega t} = j \sum_m \int d\omega a_m M_{lm} e^{-j\omega t}
\]

where

\[
R_{lm} = \int dS \left( E_{m,\omega} \times H_{l,\omega}^* + E_{l,\omega}^* \times H_{m,\omega} \right) z
\]

\[
M_{lm} = \int dS \left\{ \mu \Delta \omega H_{m,\omega} H_{l,\omega}^* + (\epsilon \Delta \omega - \epsilon_0 \epsilon_f) E_{m,\omega} E_{l,\omega}^* \right\}
\]

Using the frequency domain reciprocity relations (A1) yields an expression for the derivative of \( R_{lm} \)

\[
\frac{\partial R_{lm}}{\partial z} = j \int dS \left\{ \mu \Delta \omega H_{m,\omega} \cdot H_{l,\omega}^* + (\epsilon \Delta \omega - \epsilon_0 \epsilon_f) E_{m,\omega} \cdot E_{l,\omega}^* \right\}
\]

Substituting (33) in (30) and using (32), the following equation is derived:

\[
\sum_m \int d\omega \frac{\partial a_m}{\partial z} e^{j\Delta \omega z} u_{lm} e^{-j\omega t} = Q_l(t) + G_l(t)
\]

with

\[
u_{lm} = \int dS \left( e_{m,\omega} \times h_{l,\omega}^* + e_{l,\omega}^* \times h_{m,\omega} \right) z
\]

\[
Q_l(t) = j \sum_m \int d\omega a_m(z, \omega) \omega e^{-j\omega t} \int dS \left( \epsilon_{m,\omega} - \epsilon_f \right) e_{m,\omega} \cdot e_{l,\omega}^*
\]

\[
G_l(t) = j \sum_m \int d\omega a_m(z, \omega) \omega e^{-j\omega t} \int dS \epsilon_{NL} |E|^2 e_{m,\omega} \cdot e_{l,\omega}^*
\]

Equations (34)-(36) relate the derivatives \( \partial a_m / \partial z \) to the linear and nonlinear perturbations corresponding to the functions \( Q_l(t) \) and \( G_l(t) \) respectively. Defining the matrix \( U=[u_{lm}] \) and the vectors \( G=[G_l]^T \), \( Q=[Q_l]^T \), equation (34) can be written in vector form as follows:

\[
\sum_m \int d\omega U(\omega) b(\omega) e^{-j\omega t} = Q + G
\]

Inverting the Fourier transforms in (38) and Fourier transforming inside \( P \), the following equation is derived:

\[
\int_P b(\omega) e^{-j\omega t} = \int_P U^{-1}(\omega) \left( \tilde{G}(\omega) + \tilde{Q}(\omega) \right) e^{-j\omega t}
\]

where \( \tilde{G}(\omega) \) and \( \tilde{Q}(\omega) \) are the Fourier transforms of \( G \) and \( Q \) respectively. Expanding the matrix \( U^{-1}(\omega) \) around \( \omega=\omega_0 \), i.e.

\[
U^{-1}(\omega) = \sum_{n=0}^\infty U \frac{(\Delta \omega)^n}{n!}
\]

and using (27), one obtains
where the elements of the vectors $G_P$ and $Q_P$ are given by

$$Q_{P,j}(t) = j \sum_p \int d\omega \omega e^{i\Delta \omega} \int dS (\epsilon_p - \epsilon_m) e_{m,\omega} \cdot \epsilon^*_{j,\omega}$$

$$G_{P,j}(t) = j \sum_p \int d\omega \omega e^{i\Delta \omega} \int dS e_{NL} |E| e_{m,\omega} \cdot \epsilon^*_{j,\omega}$$

In the next subsections, the vectors $Q_P$ and $G_P$ will be expressed in terms of the envelope functions in order to complete the derivations of the coupled mode non-linear propagation equations.

### B. Linear Coupling

The vector function $Q_P$, given by (42) and corresponding to the linear coupling perturbation, can be expressed in terms of the envelope functions by defining a coupling matrix $C=[c_{lm}]$, whose elements are

$$c_{lm} = \omega e^{i\Delta \omega} \int dS (\epsilon_p - \epsilon_m) e_{m,\omega} \cdot \epsilon^*_{j,\omega}$$

and $\Delta k_{ml} = k_m(\omega) - k_l(\omega)$. Using this matrix, (42) is written as

$$Q_P = j \int d\omega e^{-i\Delta \omega} C(\omega) \bar{A}(\omega)$$

where the elements of $\bar{A}(\omega) = (\bar{A}_m)^T$ are the spectra of the envelope functions,

$$\bar{A}_m = a_m(z,\omega) e^{i\Delta \omega}$$

Expanding $C$ around $\omega = \omega_0$,

$$C(\omega) = \sum_n C_n (\Delta \omega)^n$$

and using (45) the vectors $Q_P$ are written as:

$$Q_P = \sum_n \frac{j^{n+1}}{n!} C_n \frac{\partial^n A}{\partial \epsilon^n}$$

Equation (48) expresses the linear perturbation in terms of the envelope functions.

### C. Nonlinear Coupling

A similar procedure can be used in order to express the vector $G_P$ in terms of the envelope functions. To facilitate the derivations, the tensor $T=[T_{pml}]$ is defined, where

$$T_{pml} = 2 \omega e^{i\Delta \omega} \int dS e_{NL} (e_{p,\omega} \cdot \epsilon^*_{j,\omega}) (e_{m,\omega} \cdot \epsilon^*_{l,\omega})$$

with $\Delta k_{pml} = k_p(\omega_0) - k_m(\omega_0) - k_l(\omega_0)$. As in the case of the linear coupling matrix, the tensor $T$ is expanded in Taylor series around $\omega_1 = \omega_2 = \omega = \omega_0$,

$$T = \sum_{\mu\nu\kappa} T^{\mu\nu\kappa} \frac{(\Delta \omega)^\mu (\Delta \omega_1)^\nu (\Delta \omega_2)^\kappa}{\mu!\nu!\kappa!}$$

and using (29) and (50) in (43), the vector $G_P$ may be written as:

$$G_P = j \sum_{\mu\nu\kappa} \frac{j^{\mu+\nu+\kappa}}{\mu!\nu!\kappa!} T^{\mu\nu\kappa} \frac{\partial^\mu A}{\partial \epsilon^\mu} \frac{\partial^\nu A}{\partial \epsilon^\nu} \frac{\partial^\kappa A}{\partial \epsilon^\kappa}$$
Equation (51) expresses the nonlinear perturbation in terms of the envelope functions.

D. Coupled Mode Propagation Equations

Having expressed the linear and nonlinear coupling perturbations in terms of the envelope functions, one may proceed to derive the coupled mode propagation equations. Substituting (51) and (48) in (41), the following equations are obtained:

\[
\frac{\partial \mathbf{A}(z,t)}{\partial z} = \sum_{\nu} \frac{j^{\nu+1}}{n!} \mathbf{K}_{\nu} \frac{\partial^n \mathbf{A}(z,t)}{\partial t^n} + \sum_{\mu} j^{\mu+1} \mathbf{U}_{\mu} \frac{\partial^{\mu+1} \mathbf{A}}{\partial t^{\mu+1}} + \sum_{\kappa} j^{\kappa+1} \mu! \nu! \mathbf{K}_{\kappa} \frac{\partial^\kappa}{\partial t^\kappa} \mathbf{T}^{\mu\nu\kappa} \left[ \frac{\partial^n \mathbf{A}}{\partial t^n} \frac{\partial^{\mu} \mathbf{A}^*}{\partial t^{\mu}} \frac{\partial^\kappa \mathbf{A}}{\partial t^\kappa} \right]
\]

(52)

The first sum in the right hand side of (52) accounts for the linear dispersion effects of each mode, while the second sum accounts for the linear coupling of the modes. The Kerr-induced nonlinear coupling is accounted for in the third sum where the higher order nonlinear coupling contributions are also included. In section V, equation (52) will be used to derive the nonlinear propagation equation in the case of single mode periodic waveguides, while in section VI, a system of equations describing the pulse evolution inside a photonic two mode coupler will also be derived.

V. SINGLE MODE CASE

In this section, the propagation equation for a single mode periodic waveguide will be derived and the properties of the SPM coefficient \( \gamma \) and higher order nonlinear terms will be discussed.

A. Propagation Equation and Influence of \( v_g \)

In the case of a single mode periodic nonlinear waveguide, there is no linear coupling and neglecting higher order nonlinear terms, equation (52) is reduced

\[
\frac{\partial A}{\partial z} = \sum_{\nu} \frac{j^{\nu+1} k_{\nu}}{n!} \frac{\partial^n A}{\partial t^n} + j \gamma |A|^2 A
\]

(53)

where \( A \) is the envelope function of the mode and the subscript \( l = 1 \) is dropped for convenience. Note that in the single mode case \( U \) is a scalar and the coefficients \( U_u \) of the expansion of its inverse \( U^{-1} \) are obtained from the Taylor expansion coefficients of \( 1/u = 1/u_{11} \), where \( u_{11} \) is given by (35). Using the fact that \( u(\omega_0) = u_{11}(\omega_0) = 1 \), one easily deduces that \( U_u = 1/u(\omega_0) = 1 \) and the SPM coefficient is given by

\[
\gamma(\omega_0) = U_u T^{\text{mono}} = 2 \epsilon_0 \int_S |e_{\omega_0}^l|^4
\]

(54)

Figure 3 illustrates the value of \( \gamma \) across the unit cell of the CROW considered in Figure 1, in the case where \( k = \sqrt{2} \pi / D \) (middle of the band) and \( k = 0.05 \pi / D \) (near the band edge). The nonlinear refractive index of the rods was taken \( n_2 = 1.5 \times 10^{-17} \text{m}^2/\text{W} \). Note that unlike conventional waveguides, the SPM coefficient is periodic and varies along the propagation direction. Also, as explained in section II, near the band edge, the modal fields \( e_{\omega_0} \) are enhanced and hence the value of \( \gamma \) increases accordingly.

Equation (54) can be used to estimate the nonlinear phase shift in a photonic crystal waveguide and compare the results of the present model with that of the 2D finite element mode solver for nonlinear periodic waveguides [29]. Despite the fact that in contrast to the model of the present paper, the FEM method computes the nonlinear modes \( (e, h) \) of the structure assuming complex continuous wave (CW) fields oscillating as \( \exp(j \omega_0 t) \). Besides a change in the propagation constant one can roughly expect that the nonlinear modes will be approximately proportional to the linear Bloch modes, i.e.

\[
e = B e_{\omega_0} e^{j (\beta z + j \delta_{\omega_0} z) - j \omega_0 t}
\]

(55)

\[
h = B h_{\omega_0} e^{j (\beta z + j \delta_{\omega_0} z) - j \omega_0 t}
\]

(56)
The constant $B$ can be considered as the envelope function of the mode. In [29], $\varepsilon_{NL}\|e\|^2$ is written as $\varepsilon_{NL}\|e\|^2$ and the power is measured as

$$P_0 = \frac{1}{4} \int (e \times h^* + e^* \times h)z dx = \frac{1}{4} \int (e_{v_0} \times h_{v_0} + e_{v_0}^* \times h_{v_0}^*)z dx$$

which is the power carried by the CW wave. In our case and assuming that $A(z,t)=A_0$ is constant with respect to $t$, the optical power is measured as

$$P = \int (E \times H) \cdot zdz = |A|^2 \int (e_{v_0} \times h_{v_0} + e_{v_0}^* \times h_{v_0})zdz$$

(57)

Notice that the $1/4$ factor is not present in (58) since the fields are in the time domain and the $\exp(-j\omega_0 t)$ must be accounted for. In addition, in our case the field intensity in the FEM model is $|e|^2 = |B|^2 |e_{v_0}|^2$ while $|E|^2 = 2|A|^2 |e_{v_0}|^2$. Therefore in order to have the same electric field intensity in both model and hence the same change in both models one must choose $2|A|^2 = |B|^2$ which using (57) and (58), implies that in order to have the same field intensity one must choose $P=2P_0$. Figure 4, depicts the rate of the nonlinear phase shift $\delta\phi_{NL}$ calculated using

$$\delta\phi_{NL} = \frac{\gamma P_0}{a}$$

(59)

assuming “Type I” PC waveguides as in [25] and that $a=0.4 \mu m$, $r_a=0.18a$, $\varepsilon_a=3.5^2$, $\varepsilon_b=1.5^2$, $a/\lambda=0.263$. These results are very close to the results obtained by the FEM mode solver (see figure 7(a) of [29]).

Equation (54) can be also used to study the dependence of the SPM coefficient with respect to the group velocity. Applying the 3D divergence theorem [30] on the vector function $F = E_{v_0} \times H_{v_0}^*$, one obtains

$$\int \int \mu |h_{v_0}|^2 dV = \int \int e_{v_0} |e_{v_0}|^2 dV$$

(60)

Using (15) and (60), the SPM coefficient is approximately written as:

$$\gamma(\omega) \equiv \left[N(\omega)\right]^{\dagger} \gamma(\omega_0)$$

(61)

and hence the group velocity $v_g$ given by (14), can be expressed in terms of the electric field alone to yield,

$$v_g^{-1}(\omega) \equiv (N_\epsilon(\omega))^2 \frac{1}{D} \frac{1}{\int W(\omega_0) dV} = (N_\epsilon(\omega))^2 v_g^{-1}(\omega_0)$$

(62)

Using (61), (62) and (54) the SPM coefficient is written as

$$\gamma(\omega) \equiv \frac{2\omega_b v_g^2(\omega_0) \int dS e_{NL} |e_{v_0}|^4}{v_g^2(\omega)}$$

(63)

Equation (63) shows that near $\omega=\omega_b$, the SPM coefficient is inversely proportional to the square of $v_g$, implying that the reduction of the group velocity enhances the nonlinear effects [3]. Equation (63) expresses the fact that, as light is slowed down, it has more time to sample the nonlinear perturbation and this leads to an enhancement of the nonlinear effects. The frequency dependence of the SPM coefficient is depicted in Figure 5, where the normalized inverse of the effective SPM coefficient $\gamma_{eff}$ is plotted and

$$\gamma_{eff} = \frac{1}{D} \int_{D/2}^{D/2} \gamma(z)dz = \frac{2\omega_b}{D} \int_{D/2}^{D/2} dV e_{NL} |e_{v_0}|^4$$

(64)
Also plotted in the figure is the normalized $v_g^2$. Comparing the two curves it is deduced that the SPM coefficient roughly exhibits a $1/v_g^2$ behavior. The difference in the two curves is due to the fact that although (15) is valid inside the defect cavity (as shown in Figure 1(a)), it is not a very accurate on the dielectric rods. Consequently (61) is only a rough approximation in this case.

**B. Higher Order Nonlinear Terms**

Equation (52) can be used to derive the higher order nonlinear contributions. Keeping the nonlinear terms up to first order, one obtains:

$$\frac{\partial A}{\partial z} = \sum_{n} \frac{j^{n+1} k_n}{n!} \frac{\partial^n A}{\partial t^n} + j \gamma |A|^2 A + \delta_1 \frac{\partial}{\partial t} \left( |A|^2 A \right) - \left( \delta_2 + \delta_3 \right) \frac{\partial A}{\partial t} + \delta_4 A^* \frac{\partial A^*}{\partial t}$$  \hspace{1cm} (65)

The nonlinear term with coefficient $\delta_1$ corresponds to $r=1$ and $\mu=\nu=k=0$ in (52) and is given by

$$\delta_1 = -U_1 T^{000} = u_1 \gamma$$  \hspace{1cm} (66)

where $U_1=\partial(u^{-1})/\partial \omega = -u_1/u_0^2 = -u_1$ and

$$u_1 = \int dS \left( \frac{\partial e_{n_0}}{\partial \omega} \times h_{n_0} + e_{n_0}^* \times \frac{\partial h_{n_0}}{\partial \omega} \right) z$$  \hspace{1cm} (67)

The term $\delta_3$ is obtained for $\nu=1$ and $r=\nu=k=0$ in which case,

$$\delta_3 = 2 \omega_b \int dS \delta_{NL} \left| e_{n_0} \right|^2 \left( \frac{\partial e_{n_0}}{\partial \omega} \cdot e_{n_0}^* \right)$$  \hspace{1cm} (68)

The term $\delta_2$ corresponds to $\mu=1$ and $r=\nu=k=0$ and is given by

$$\delta_2 = 2 \omega_b \int dS \delta_{NL} \left| e_{n_0} \right|^2 \left( \frac{\partial e_{n_0}}{\partial \omega} \cdot e_{n_0}^* \right) = \gamma + \delta_3$$  \hspace{1cm} (69)

The last nonlinear term is obtained for $k=1$ and $r=\nu=\mu=0$ and is written as

$$\delta_4 = 2 \omega_b \int dS \delta_{NL} \left| e_{n_0} \right|^2 \left( \frac{\partial e_{n_0}}{\partial \omega} \cdot e_{n_0}^* \right) = \delta_4^*$$  \hspace{1cm} (70)

Inspecting equations (66)-(70), one deduces that, as expected the higher order nonlinear contributions arise from the frequency dependence of the Bloch function $e_{n_0}$ (Figure 1). In Figure 6, the value of the higher order nonlinear coefficients at the middle of the CROW band ($k=\pi/2D$) are plotted. The influence of the terms also depends on the magnitude of the derivatives of the envelope functions. Assuming Gaussian incident pulses $A(0,t)=A_0 \exp(-t^2/2T_0^2)$, these derivatives are proportional to $A_0/T_0$ and hence the magnitude of the higher order terms is roughly $\delta_4 A_0/T_0$ while the magnitude of the SPM terms is $\gamma A_0$. For 10ps pulses, $T_0=10^{-11}$s and hence the maximum of $\delta_4/T_0$ will be of the order of $5 \times 10^4$ W^{-1}m^{-2} which is about three orders of magnitude less than the maximum of the SPM coefficient which is $\gamma_{max}=6 \times 10^3$ W^{-1}m^{-2} for $k=\pi/2D$. It is therefore reasonable to deduce that the higher order nonlinear terms will not significantly affect the pulse propagation. The value of the higher order nonlinear coefficients near the band edge ($k=0.05\pi/D$) are plotted in Figure 7. For $T_0=10^{-11}$s, the maximum of $\delta_2/T_0$ becomes $1.4 \times 10^3$ W^{-1}m^{-2}, which is now 2 order of magnitude less than $\gamma_{max}=1.3 \times 10^4$ W^{-1}m^{-2}. This means that the higher order terms have a more pronounced influence near the band edges and for pulse durations less than 10ps, they have to be included in the analysis.
C. Weak Guidance

In the special case of weak guidance, one may use the above equation to obtain the well known expression for the SPM coefficient derived in [26] using perturbation theory. Assuming a constant cross-section waveguide, with small variations in the refractive index (weak guidance case) one can approximate the guided mode as

\[ \mathbf{e}_{n_0} = \phi(x,y) \mathbf{x} \]  

(71)

\[ \mathbf{h}_{n_0} \equiv \left( \epsilon_L / \mu \right)^{1/2} \phi(x,y) \mathbf{y} \]  

(72)

In this case, the normalization condition (10) is written as

\[ N_i \equiv 2 \left( \epsilon_L / \mu \right)^{1/2} \int_S |\phi|^2 dS = 1 \]  

(73)

while the SPM coefficient becomes

\[ \gamma = \frac{\omega_0 \epsilon_{NL} \mu}{2 \epsilon_L A_{eff}} \]  

(74)

where \( A_{eff} \) is given by

\[ A_{eff} = \left( \int_S |\phi|^2 dS \right)^{1/2} \int_S |\phi|^4 dS \]  

(75)

The average power density carried by the electromagnetic wave is

\[ P_z = (\mathbf{E} \times \mathbf{H}) z dS \equiv 2 |A|^{2} \sqrt{\frac{\epsilon_L}{\mu}} |\phi|^2 \]  

(76)

Assuming that both \( \epsilon_L \) and \( \epsilon_{NL} \) do not vary significantly over the waveguide section (weak guidance approximation), the nonlinear properties of the medium can be described in terms of the nonlinear refractive index coefficient \( n_2 \) measured in m^2/W^2 and for which

\[ \epsilon_{NL} |\mathbf{E}|^2 = 2 \epsilon_{NL} |A|^2 |\phi|^2 \equiv 2 \epsilon_0 n_2 P_z \]  

(77)

where \( n=(\epsilon_L/\epsilon_0)^{1/2} \) is the refractive index of the medium approximately equal to the effective refractive index of the mode. Using (77) and (76), one obtains:

\[ \epsilon_{NL} \equiv 2 \epsilon_0 n_2 \left( \epsilon_L / \mu \right)^{1/2} \]  

(78)

Substituting (78) into (74) and using the fact that \( n=(\epsilon_L/\epsilon_0)^{1/2} \), the following expression is obtained:

\[ \gamma \equiv \frac{\omega_0 \epsilon_0 n_2}{c A_{eff}} \]  

(79)

which is derived in [26] using perturbation theory in the case of weakly guiding, constant cross-section waveguides.

D. Comparison to the Discrete Equation Model

Before turning our attention to multimode waveguides, it is useful to compare the results of our derivations to the Discrete Equation Model (DEM) developed for CROWs in [23] using the tight-binding approximation, according to which the shift in phase in a small time interval \( \Delta t \), due to SPM is

\[ \Delta \phi_{nl} = \gamma_z |A|^2 \Delta t \]  

(80)

where
and $\mathbf{e}$, $\mathbf{h}$, are the electric and magnetic field modes of the isolated cavities of the CROW and $V_2$ is the entire space. The cavity fields decay exponentially outside the cavities and hence one may replace $V_2$ with the volume of the unit cell $V$. In addition, inside the cavities, the intensities $|\mathbf{e}|^2$ and $|\mathbf{h}|^2$ of the modes of the isolated cavities closely resemble the intensities of the fields of the guided mode of the CROW and $|\mathbf{e}_0|^2 \equiv |\mathbf{e}|^2$ and $|\mathbf{h}_0|^2 \equiv |\mathbf{h}|^2$. Hence, using (13), (14) and (64), equation (81) is written as

$$\gamma_z \approx \frac{\gamma_{eff} D}{(V)} = \gamma_{eff} v_g$$

(82)

In addition, the propagation length $\Delta z$ corresponding to the time interval $\Delta t$ is $\Delta z = v_g \Delta t$, where $v_g$ is given by (14). Using (80) and (82), one obtains

$$\frac{\Delta \phi_{eff}}{\Delta z} = \frac{\gamma_z}{v_g} \approx \gamma_{eff}$$

(83)

Equation (83) dictates that the SPM coefficient obtained by the model in [23] is the same as the average SPM coefficient $\gamma_{eff}$ obtained by (64), and this is another indication of the validity of the present model.

VI. PHOTONIC CRYSTAL COUPLER

In this section, the model is applied to another example structure, this time having multiple modes. The structure in question is a photonic crystal coupler such as the one illustrated in Figure 8 formed by two coupled single mode waveguides. Considerable simplification is gained if the field is expanded in terms of the isolated guided modes of the two waveguides which obey Maxwell’s equations (6)-(7) for $\varepsilon_m=\varepsilon_1$ and $\varepsilon_m=\varepsilon_2$. The dielectric distributions $\varepsilon_1$ and $\varepsilon_2$ are illustrated in Figure 8. Due to the symmetry of the structure, the linear coupling matrix up to zero order is

$$C_0 = \begin{bmatrix} c_s & c_s \\ c_s & c_s \end{bmatrix}$$

(84)

where

$$c_s = \omega_0 \int_S dS (\varepsilon_L - \varepsilon_1) |\mathbf{e}_{0s}|^2$$

(85)

$$c_s = \omega_0 \int_S dS (\varepsilon_L - \varepsilon_2) |\mathbf{e}_{0s}|^2$$

(86)

The elements of the tensor $T$ in (49) are given by

$$T^{100}_{111} = T^{000}_{222} = \gamma$$

(87)

$$T^{000}_{112} = T^{000}_{212} = T^{000}_{221} = \Gamma_1$$

(88)

$$T^{000}_{121} = T^{000}_{122} = T^{000}_{211} = T^{000}_{212} = \Gamma_1$$

(89)

$$T^{000}_{112} = T^{000}_{212} = T^{000}_{221} = \Gamma_2$$

(90)

$$T^{000}_{121} = T^{000}_{211} = \Gamma_3$$

(91)

where
The coupled mode propagation equations yield to zero order

\[
\Gamma_1 = 2\omega_0 \int_{S_{\text{NL}}} |e_{1,\omega_0}|^2 e_{1,\omega_0}^* \cdot e_{2,\omega_0}^* \quad (92)
\]

\[
\Gamma_2 = 2\omega_0 \int_{S_{\text{NL}}} |e_{1,\omega_0}|
\]

\[
\Gamma_3 = 2\omega_0 \int_{S_{\text{NL}}} (e_{1,\omega_0}^* \cdot e_{2,\omega_0})^2 \quad (94)
\]

The above system of coupled nonlinear equations describes the pulse propagation in the two waveguide arms of the coupler. The first sum in the right hand side of (95) and (96) accounts for the linear dispersion effects of the Bloch mode, while the next two linear terms correspond to the linear mode coupling of each waveguide mode to the core of its adjacent waveguide. The first nonlinear term corresponds to SPM, while the rest of the terms arise from the nonlinear coupling between the waveguide modes. Figure 9 illustrates the value of the linear coupling coefficients \(c_s\) and \(c_x\) in the case of the PC coupler of Figure 8. It is deduced that the self-coupling coefficient \(c_s\) is much smaller than the cross-coupling coefficient \(c_x\), since the modes rapidly decays outside the waveguide core. The nonlinear coupling coefficients are plotted in Figure 10. For this structure \(\Gamma_2 \approx \Gamma_3\) and the nonlinear cross-coupling coefficients \(\Gamma_1, \Gamma_2, \Gamma_3\) are about one order of magnitude smaller than the self-phase coefficient \(\gamma\) and should therefore be included in the analysis.

**VII. CONCLUSIONS**

In this paper, a system of nonlinear coupled z-evolution equations for the amplitudes of the guided modes of periodic nanophotonic waveguides were derived. In the single mode case, the model has been used to estimate the SPM coefficient \(\gamma\) of the waveguide which has been shown to be a periodic function along the propagation direction. The model was applied to verify the \(1/v_g^2\) dependence of \(\gamma\) and estimate the influence of the higher order nonlinear term contributions in the middle and edge of the guided mode band. The model was also applied in the case of a PC waveguide coupler. This model can be used to provide a physical understanding and estimation of the influence of modal dispersion, linear and nonlinear coupling effects in the propagation of an optical signal inside a nonlinear nanophotonic single or multimode waveguide without excessive computational effort.

**VIII. APPENDIX A: RECIPROCITY RELATIONS**

Given two mediums with dielectric constants \(\varepsilon_1\) and \(\varepsilon_2\) the electromagnetic fields \((E_1, H_1)\) and \((E_2, H_2)\) at frequencies \(\omega=\omega_1\) and \(\omega=\omega_2\), one obtains

\[
\frac{\partial}{\partial z} \int_{S} \mathbf{F}_{12} \cdot z dS = \oint \mathbf{F}_{12} \cdot d\mathbf{l} + j \mu \left(\omega_1 - \omega_2\right) \int_{S} \mathbf{H}_1 \cdot \mathbf{H}_2 dV + j \int_{S} \left(\varepsilon_1 \omega_1 - \varepsilon_2 \omega_2\right) \mathbf{E}_2^* \cdot \mathbf{E}_1 dV \quad (A1)
\]

where

\[
\mathbf{F}_{12} = \mathbf{E}_1 \times \mathbf{H}_2^* + \mathbf{E}_2^* \times \mathbf{E}_1 \quad (A2)
\]
and $S$ is a surface enclosed by the closed contour $\partial S$ and $d\mathbf{l}$ is tangential to $\partial S$. Assuming an electromagnetic field $(\mathbf{E}, \mathbf{H})$ obeying Maxwell’s equations (1), (2) the following expression is obtained:

$$\frac{\partial}{\partial z} \int_S \mathbf{F} \cdot d\mathbf{S} = -\int_S \left( \mu \mathbf{H}^\prime \cdot \frac{\partial \mathbf{H}}{\partial t} + \varepsilon \mathbf{E}^\prime \cdot \frac{\partial \mathbf{E}}{\partial t} \right) dS - j\omega \int_S \left( \varepsilon \mathbf{E} \cdot \mathbf{E}^\prime + \mu \mathbf{H} \cdot \mathbf{H}^\prime \right) dS$$  \hspace{1cm} (A3)

with

$$\mathbf{F} = \mathbf{E} \times \mathbf{H}^\prime + \mathbf{E}^\prime \times \mathbf{H}$$  \hspace{1cm} (A4)
Figure 1: a) the dispersion relation and slow down factor $S$ of the guided mode of a coupled resonator optical waveguide (CROW) formed out of 2D photonic crystal defect cavities spaced $D=2a$ apart, b) and c) the modal field distribution of the electric field $e_y$ of the modes inside the waveguide cell at $k=\pi/D/2$ and $k=0.05\pi/D$, d) the waveguide field pattern at $z=z_1=-a/2$. 

$$S = c/v_g$$

$$f(k) = \omega(k)/(2\pi)$$
Figure 2: The spectrum of a narrowband real electric field: The spectrum around $+\omega_0$ corresponds to the signal $E_s(r,t)$ and the part around $-\omega_0$ corresponds to $E_N(r,t)$. 
Figure 3: The SPM coefficient for the CROW of Figure 1 at the middle and the edge of the guided band.
Figure 4: Nonlinear phase shift obtained for a “Type I” PC waveguide of [29].
Figure 5: Frequency dependence of $\frac{1}{\gamma_{\text{eff}}}$ and $v_g^2$
Figure 6: Higher order nonlinear term coefficients for the CROW of Figure 1 at $k=\pi/D/2$
Figure 7: Higher order nonlinear term coefficients for the CROW of Figure 1 at $k=0.05\pi/D$
Figure 8: A photonic crystal coupler
Figure 9: Linear coupling coefficients of the PC coupler of Figure 8
Figure 10: The SPM coefficient and the nonlinear cross coupling coefficients for the PC coupler of Figure 8
REFERENCES