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SLOW SCALE MAXWELL-BLOCH EQUATIONS FOR ACTIVE PHOTONIC CRYSTALS

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Abstract—We present a theory to describe the transient and steady state behaviors of the active modes of a photonic crystal with active constituents (active photonic crystal). Using a couple mode model, we showed that the full vectorial Maxwell-Bloch equations describing the physics of light matter interaction in the active photonic crystal can be written as a system of integro-differential equations. Using the method of moments and the mean value theorem, we showed that the system of integro-differential equations can be transformed to a set of differential equations in slow time and slow spatial scales. The slow time (spatial) scale refers to a duration (distance) that is much longer than the optical time period (lattice constant of the photonic crystal). In the steady state, the slow scale equations reduce to a nonlinear matrix eigenvalue problem, from which the nonlinear Bloch modes can be obtained by an iterative method. For cases, where the coupling between the modes are negligible, we describe the transient behavior as an one-dimensional problem in the spatial coordinate, and the steady behaviors are expressed using simple analytical expressions.

1. INTRODUCTION

Photonic crystals (PCs) [1, 2] with active constituents [active PCs] have profound applications such as ultrafast and low threshold lasers, and implementation of nonlinear optical switching effects [3–11]. Active PCs are also used as band edge lasers [12–18]. Band edge lasers provide large area, coherent single mode operations with stable lasing wavelengths. They also provide a mean to tailor the laser beam

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shape [17], and control the polarization mode of the laser [18]. Examples of the active constituents used in PC include quantum dots [8–10, 19–21], Erbium ions [22, 23], organic dyes [24, 25], and active semiconductor materials [12–16].

The physics of semiclassical light-matter interaction in the active PCs can be described using the coupled Maxwell-Bloch equations. The coupled Maxwell-Bloch equations can be solved using a finite difference time domain (FDTD) method by directly discretizing the time and the space [26–28]. However, the direct discretization of the Maxwell-Bloch equation is computationally ineffective, since it will result in very fine spatial and time grids. For an example, the time grid for an optical simulation has to be smaller than the optical time period, which is on the scale of femtoseconds. However, typical electronic transitions occurs on much slower time scale (i.e., on the order picoseconds [29–31]). On the other hand, the spatial grid in the direct discretization has to be smaller than the lattice constant of the PC. However, one is normally interested to know how the light evolves in distances that are much longer than the lattice constant of the PC, so that on can decide on the length of the required PC for lasing etc.. Therefore, the slow scale [time and spatial scales that are much longer than the optical time period and the lattice constant of the PC, respectively] versions of Maxwell-Bloch equations are extremely useful. In addition to the efficient spatial and time discretization, the slow scale formulation is powerful to provide deep analytical insights. An attempt to derive the slow scale Maxwell-Bloch equations was made in Ref. [32], using a multiscale perturbation theory for the E-polarization (electric field is perpendicular to the periodic plane) of a two-dimensional (2D) PC. This multiscale perturbation analysis is a scalar formulation, and valid for near threshold operating condition, where the electric field is small.

In a time independent framework, Maxwell-Bloch equations for the active PC reduce to the time independent Maxwell equation [also called as master equation in PC literatures [2]) with an active dielectric constant. The time independent Maxwell equation with the active dielectric constant has been solved using a couple wave model [33–36], and a couple mode model [37, 38], and the existence of Nonlinear Bloch modes have been shown. In the couple wave model, the electric field, the periodic dielectric constant, and the periodic gain are expanded in term of plane waves, and only plane waves with significant Fourier coefficients are retained, to formulate coupled wave equations for the electric field. The number of coupling waves varies with the problem. In 1D PCs, two coupling waves are normally used [33], and in 2D square lattice PCs at Γ point, eight coupling waves have been used [34–36]. The couple wave model is only valid for active PCs with very weak dielectric modulations and small active perturbations. In the couple mode model, however, the active mode is formulated as a result of a coupling of various modes of a backbone PC, where the backbone PC has a passive and a linear dielectric constant. In Refs. [37, 38], the couple mode model is formulated for scalar version of Maxwell equation [i.e., valid for 1D PC and E-polarization of 2D PC], and it is shown that the couple mode model can be solved as a nonlinear eigenvalue problem. In contrast to the couple wave model, the couple mode model is exact, and thus can handle active PCs of large dielectric modulations and large active dielectric perturbations.

In this paper we give a consistent formulation for both time dependent and time independent problem by extending the couple mode model into the time dependent and a vectorial framework. We show the couple mode model in the time dependent framework give rises to a system of integro-differential equations. Using the method of moments [39–42], and the mean value theorem [43] we transform the system of integro-differential equations to a set of differential equations, in which all the dynamic quantities varies on the slow time, and slow spatial scales. The slow scale equations contain the spatially averaged information on the fast scale which is of relevance to the evolution of the active mode on the slow scale. By invoking a small field approximation, we also show that our slow scale equation recaptures the result of multiscale expansion theory [32], in the vicinity of a near threshold operation.

In the steady state, the slow scale equations reduce to a nonlinear matrix eigenvalue problem. The nonlinear eigenvalue problem can be solved by an iterative procedure to obtain the nonlinear Bloch modes in an infinite active PC, or the lasing modes in a finite sized active PC. Further, we also show that the nonlinear matrix eigenvalue problem reduces to a simple nonlinear integral problem under a single mode assumption. Our formulation also accurately reproduces the time independent results of the couple mode model which is previously proposed for the specialized case of E-polarization in a 2D PC [37, 38].

The presented model can handle active PC with large dielectric modulations and large active perturbation. In contrast to the previous formulations [32, 37, 38], where only scalar version of Maxwell equation is considered, in the present formulation we consider the full vectorial problem with anisotropic dipole moments, and therefore can be used to accurately treat i) H-polarization of 2D PC, ii) 3D PC iii) membrane of PC and PCs with defect: using a supercell, iv) PCs with quantum dots of specific orientation and shapes: this is handled with an anisotropic dipole moment v) finite size PCs: this is handled with a cavity leakage term.

Our paper is organized as follows. In Section 2 we present the general equations describing the physics of light-matter interaction in an active PC. Section 3 outlines the equations for the dynamic quantities: electric field, polarization and population inversion density, in the slow time scale. In Section 4, we formulate the dynamic equations in both slow time and slow spatial scales. Section 5 presents the results of Section 4 in the adiabatic limit. In Section 6 we derive the steady state results, and finally in Section 7, we give summary and conclusion for the paper.

2. GENERAL EQUATIONS

In this section we will outline the general equations that describe the physics of semiclassical light-matter interaction in an active PC.

We model the active constituents as two level dopants. The active dopants are doped in a backbone PC having a linear and frequency independent dielectric constant $\varepsilon(\mathbf{r})$. Maxwell equations for such a system reduce to a nonlinear wave equation of the form

$$\nabla \times \nabla \times \vec{\mathbf{E}}(\mathbf{r}, t) + \frac{\varepsilon(\mathbf{r})}{c^2} \frac{\partial^2 \vec{\mathbf{E}}(\mathbf{r}, t)}{\partial t^2} + \mu_o \left\{ \sigma(\mathbf{r}) \frac{\partial \vec{\mathbf{E}}(\mathbf{r}, t)}{\partial t} + A(\mathbf{r}) \frac{\partial^2 \vec{\mathbf{P}}^{real}(\mathbf{r}, t)}{\partial t^2} \right\} = 0, \tag{1}$$

where the real quantities $\mathbf{r}$, t, $\vec{\mathbf{E}}(\mathbf{r}, t)$, $\vec{\mathbf{P}}^{real}(\mathbf{r}, t)$, $\sigma(\mathbf{r})$, μ_o and c are position vector, time, electric field, polarization, conductivity, vacuum permeability, and the speed of light respectively. The distribution of the active dopants is described by the dimensionless function, $A(\mathbf{r})$. The function $A(\mathbf{r})$ equals to 1 if $\mathbf{r}$ pointing towards the position of the active dopant, and zero otherwise. For an example, in a 2D PC of periodic dielectric cylinders, if the cylinders are actively doped, then $A(\mathbf{r}) = 1$ for $\mathbf{r}$ vectors within the cylinder, and $A(\mathbf{r}) = 0$ for $\mathbf{r}$ vectors outside the cylinder.

The two level dopant is modeled with a resonant frequency ω_0, and with a dopant density of N_T. The population inversion density and the polarization of the two level system can be written in term of density matrix elements, ρ_{11}, ρ_{22}, ρ_{12}, and ρ_{21}. If we define $\vec{\mathbf{P}}(\mathbf{r}, t) = \mathbf{d}_0 N_T \rho_{21}$, where $\mathbf{d}_0$ is the dipole moment of the dopant, then the polarization can be written as $\vec{\mathbf{P}}^{real}(\mathbf{r}, t) = \vec{\mathbf{P}}(\mathbf{r}, t) + \vec{\mathbf{P}}^*(\mathbf{r}, t)$. The dynamics of $\vec{\mathbf{P}}$ can be obtained from the dynamics of ρ_{21} [29], and it is

$$\frac{\partial \vec{\mathbf{P}}(\mathbf{r}, t)}{\partial t} = -i\omega_0 \vec{\mathbf{P}}(\mathbf{r}, t) - \frac{\vec{\mathbf{P}}(\mathbf{r}, t)}{T_2} - \frac{i d_0^2}{\hbar} N(\mathbf{r}, t) \hat{s} \vec{\mathbf{E}}(\mathbf{r}, t), \tag{2}$$

where T_2 is the polarization relaxation time, and $\hat{s}\vec{\mathbf{E}}(\mathbf{r},t) = \mathbf{d}_0[\mathbf{d}_0 \cdot \vec{\mathbf{E}}(\mathbf{r},t)]/d_0^2$ with $\hat{s}$ is a second rank tensor. The matrix $\hat{s}$ accounts for the anisotropic response of the dipole with respect to the electric field. If the dipole aligns parallel to the electric field, then $\hat{s}$ is an unit identity matrix. For the cases of quantum dots and nanocrystals with fixed shapes and orientations [with respect to the underlying PC structure], the dipole moment may not be parallel to the electric field [44], and thus anisotropic form of $\hat{s}$ is necessary. The equation of motion for the population inversion density, $N = N_T(\rho_{22} - \rho_{11})$, is

$$\frac{\partial N(\mathbf{r},t)}{\partial t} = -\frac{N(\mathbf{r},t) - N_0}{T_1} - \frac{2i}{\hbar}\vec{\mathbf{E}}(\mathbf{r},t) \cdot \left[\vec{\mathbf{P}}(\mathbf{r},t) - \vec{\mathbf{P}}(\mathbf{r},t)^*\right], \tag{3}$$

where T_1 is the population decay time, and N_0 is the population inversion density created by the external pumping.

Before proceeding further, let's introduce the slow and the fast scales of time and space, which are relevant to the evolutions of the active modes. The fast time scale refers to a duration on the order of the optical period of the light [i.e., $2\pi/\omega$, where ω is the frequency of the light], and slow time scale refers to a duration that is much longer than $2\pi/\omega$. On the other hand, the fast spatial scale refers to a distance on the order of the PC's lattice constant, and the slow spatial scale refers to a distance that is much longer than the PC's lattice constant.

In Section 3 we will outline the evolution of the dynamic quantities (electric field, polarization and population inversion density) on the slow time scale. In Section 4 the evolution of the dynamic quantities in both slow time and slow spatial scales will be described.

3. EQUATIONS ON THE SLOW TIME SCALE

The population inversion decay time is usually very long compared to the time period of the light [29–31]. This tells us that the population inversion density [i.e., $N(\mathbf{r},\, t)$ in Eq. (3)] does not vary on the fast time scale, and the amplitudes of polarization and electric field will change slowly in time (i.e., on the slow time scale). This section will outline the equations for slowly varying (in time) envelopes of the electric field and the polarization vectors.

Let's assume an harmonic time dependence, and define slowly varying envelopes (i.e., on the slow time scale) $\mathbf{E}(\mathbf{r},\, t)$ and $\mathbf{P}(\mathbf{r},\, t)$ using,

$$\vec{\mathbf{E}}(\mathbf{r},t) = \mathbf{E}(\mathbf{r},t)e^{-i\omega t} + \text{c.c}, \tag{4}$$

and

$$\vec{\mathbf{P}}(\mathbf{r},t) = \mathbf{P}(\mathbf{r},t)e^{-i\omega t}, \tag{5}$$

respectively. With the definitions in Eqs. (4)–(5) and neglecting the second order terms of the time derivative, we can write Eqs. (1)–(3) in the rotating wave approximation as,

$$\nabla\times\nabla\times\mathbf{E}(\mathbf{r},t) - \frac{\omega^2}{c^2}\varepsilon(\mathbf{r})\mathbf{E}(\mathbf{r},t)$$
$$= \left\{\frac{2i\omega}{c^2}\varepsilon(\mathbf{r})\frac{\partial}{\partial t} + i\mu_o\omega\sigma(\mathbf{r})\right\}\mathbf{E}(\mathbf{r},t) + \mu_o A(\mathbf{r})\left\{2i\omega\frac{\partial}{\partial t} + \omega^2\right\}\mathbf{P}(\mathbf{r},t), \tag{6}$$

$$\frac{\partial\mathbf{P}(\mathbf{r},t)}{\partial t} = \frac{(i\Omega-1)\mathbf{P}(\mathbf{r},t)}{T_2} - \frac{id_0^2}{\hbar}\hat{s}N(\mathbf{r},t)\mathbf{E}(\mathbf{r},t), \tag{7}$$

$$\frac{\partial N(\mathbf{r},t)}{\partial t} = -\frac{N(\mathbf{r},t)-N_0}{T_1} - \frac{2i}{\hbar}\left[\mathbf{E}^*\cdot\mathbf{P} - \text{c.c}\right], \tag{8}$$

where $\Omega = (\omega - \omega_0)T_2$. Eqs. (7)–(8) are the Bloch equations for the two level dopants [29–31].

Equations (6)–(8) constitute to dynamic equations for the electric field, polarization and population inversion density in the slow time scale. In the following section, we will develop equations for these dynamic quantities in both slow time and slow spatial scales.

4. EQUATIONS ON THE SLOW TIME AND SPATIAL SCALES

In this section we will derive equations for the electric field, polarization and population inversion density on the slow time and the slow spatial scales. Unless explicitly stated, in the rest of the paper, we will use the term "slow scale" to denote "slow time and slow spatial scales".

Consider the following ansatz for the slowly varying time envelope of the electric field,

$$\mathbf{E}(\mathbf{r},t) = \sum_n \mathcal{E}_n(\mathbf{r},t)\vec{\phi}_n(\mathbf{r}), \tag{9}$$

where we have assumed, the envelope is given by a linear combination of Bloch modes of a backbone PC structure, $\vec{\phi}_n(\mathbf{r})$, with the expansion coefficients, $\mathcal{E}_n(\mathbf{r},t)$. $\mathcal{E}_n(\mathbf{r},t)$ is assumed to vary on the slow scale, and the Bloch mode $\vec{\phi}_n(\mathbf{r})$ varies on the fast spatial scale. The letter in the subscript of $\vec{\phi}_n(\mathbf{r})$ is used as a labeling index of the mode. The mode with the label-n is the solution to the time independent version of Eq. (1) with $A(\mathbf{r}) = \sigma(\mathbf{r}) = 0$,

$$\nabla \times \nabla \times \vec{\phi}_n(\mathbf{r}) - \left[\omega_n^2/c^2\right] \varepsilon(\mathbf{r})\vec{\phi}_n(\mathbf{r}) = 0, \tag{10}$$

where ω_n is the backbone PC's mode frequency. The modes of the backbone PC satisfy the orthogonality condition, $\langle\vec{\phi}_m^*(\mathbf{r}) \cdot \varepsilon(\mathbf{r})\vec{\phi}_n(\mathbf{r})\rangle_{uc} = \delta_{nm}$, where $\langle\ldots\rangle_{uc} = (1/V) \int_{unit\,cell} (\ldots)d^3\mathbf{r}$, and V is the unit cell volume. In PCs each Bloch mode with the label-n is identified with a unique set of symmetry representation and band index. There are two kinds of symmetries in the PC [45–50], namely translational symmetry and point group symmetry. The symmetry representation for the translational symmetry is simply the Bloch wavevector in the first Brillouin zone (BZ), and the symmetry representation for the point group symmetry is usually denoted with the Mulliken's symbols such as A_1, A_2, B_1, B_2 etc. [50, 51]. It is worth to note that only modes with the same symmetry representations couple to each other, and therefore in the summation of Eq. (9), only modes of the backbone PC with the same wavevectors and the same symmetry representations for the point group symmetry need to be kept.

Let's define a slow scale electric field vector as $\boldsymbol{\mathcal{E}} = [\mathcal{E}_1, \mathcal{E}_2, \mathcal{E}_3, \ldots]^T$. This vector contains the expansion coefficients $\mathcal{E}_n$ which vary on the slow scale. Note that $\boldsymbol{\mathcal{E}}$ also can be considered as an array of electric field mode amplitudes, where the modes are referred to those of the backbone PC. Therefore, for a multimode lasing in an active PC, the evolution of various lasing modes can be tracked using the vector $\boldsymbol{\mathcal{E}}$. Consistent with the definition of $\boldsymbol{\mathcal{E}}$, we will define a slow scale polarization vector as $\bar{\boldsymbol{\mathcal{P}}}$, containing the projections of $\mathbf{P}$ onto the subspace spanned by the modes of the backbone PC [a mathematical definition will be given later]. As we will show, the equations connecting $\bar{\boldsymbol{\mathcal{P}}}$ and $\boldsymbol{\mathcal{E}}$ will be in a similar form to the one connecting $\mathbf{P}$ and $\mathbf{E}$ (i.e., Bloch Eqs. (7)–(8)). Consistent with the vectorial definitions for the slow scale electric field and the slow scale polarization vectors, we will encounter matrix representation for the slow scale population inversion density $\hat{\bar{\mathcal{N}}}$, and in the adiabatic limit, we will encounter a matrix representation for the slow scale susceptibility $\hat{\bar{\mathcal{X}}}$. In the adiabatic limit, we will show that,the relationship between the slow scale polarization and the slow scale electric field vectors can be simply written in a familiar form as $\bar{\boldsymbol{\mathcal{P}}} = \varepsilon_0\hat{\bar{\mathcal{X}}}\boldsymbol{\mathcal{E}}$.

We can derive the equation of motion for $\boldsymbol{\mathcal{E}}$ by substituting Eq. (9) into Eq. (6), and neglecting the second order terms. The equation of motion for $\boldsymbol{\mathcal{E}}$ is (see Appendix A for the details of the mathematical derivation).

$$\left(\hat{\bar{D}} + \hat{I}_u \frac{\partial}{\partial t}\right) \boldsymbol{\mathcal{E}} + \frac{\omega}{2}\left\{\hat{\bar{\gamma}} + i\hat{\Delta}\right\} \boldsymbol{\mathcal{E}} = -\frac{1}{\varepsilon_0}\left(\frac{\partial}{\partial t} - i\frac{\omega}{2}\right) \hat{I}_u \bar{\boldsymbol{\mathcal{P}}}, \qquad (11a)$$

where $\hat{I}_u$ is a unit identity matrix. The above equation contain quantities (identified with a bar "$-$" on top) that represent the averaged information on the fast spatial scale which is of relevance to the evolution of the active modes on the slow scale. The definition for the quantities $\bar{\boldsymbol{\mathcal{P}}}$, $\hat{\bar{D}}$, $\hat{\bar{\gamma}}$ and $\hat{\Delta}$ are as follows.

The quantity $\bar{\boldsymbol{\mathcal{P}}} = [\bar{\mathcal{P}}_1, \bar{\mathcal{P}}_2, \bar{\mathcal{P}}_3, \ldots]^T$ in Eq. (11a) is defined as a slow scale polarization vector. The definition for the vector element $\bar{\mathcal{P}}_m$ is

$$\bar{\mathcal{P}}_m = \left\langle A(\mathbf{r})\vec{\phi}^*_m(\mathbf{r}) \cdot \mathbf{P} = \right\rangle_{uc}, \qquad (11b)$$

The matrix element of the operator $\hat{\bar{D}}$ is $\bar{\mathbf{v}}_{mn} \cdot \nabla$. The j-th Cartesian component of $\bar{\mathbf{v}}_{mn}$ [see Eq. (A2)] is

$$\bar{v}^j_{mn} = i\frac{c^2}{2\omega}\left\langle \phi^{*j}_m \left(\partial^l \phi^l_n\right) + \left(\phi^{*l}_m \partial^l\right)\phi^j_n - 2\phi^{*l}_m \partial^j \phi^l_n \right\rangle_{uc}, \qquad (11c)$$

where we assumed a summation over the repeated indices. The expression for the diagonal element $\bar{\mathbf{v}}_{mm}$ represents the actual group velocity of the m-th mode. This group velocity expression, which is in general applicable for any 3D inhomogeneous dielectric structure, has been verified with respect to the one obtained using $\mathbf{k} \cdot \mathbf{p}$ perturbation theory [see Appendix B for details]. In Eq. (11a), the matrix elements of $\hat{\Delta}$ and $\hat{\bar{\gamma}}$ have the following definitions:

$$\Delta_{mn} = \left[\left(\omega^2_m/\omega^2\right) - 1\right]\delta_{mn}, \qquad (11d)$$

$$\bar{\gamma}_{mn} = \frac{1}{\varepsilon_0 \omega}\left\langle \vec{\phi}^*_m(\mathbf{r}) \cdot \sigma'(\mathbf{r})\vec{\phi}_n(\mathbf{r})\right\rangle_{uc}. \qquad (11e)$$

In Eq. (11e), $\sigma'(\mathbf{r}) = \sigma(\mathbf{r}) + \kappa_m \delta_{mn}$, where additional losses [apart from the material loss, $\sigma(\mathbf{r})$] such as scattering and output losses associated with the mode-m is phenomenologically included via the cavity leakage parameter κ_m. An estimation of κ_m for a finite sized PC with a length L along the direction $\hat{\mathbf{q}}$ is [32, 50],

$$\kappa_m = \frac{2}{cL}\left|\hat{\mathbf{q}}.\bar{\mathbf{v}}_{mm}\right|^2. \qquad (11f)$$

A single mode assumption can be applied if the gain lineshape function of the active dopant is very narrow compared to the frequency distribution of the backbone PC's modes. In this assumption, we neglect the couplings between neighboring modes, and hence Eq. (9)

can be written in only one mode. In the single mode assumption, Eq. (11a) can be reduced to a scalar equation as

$$\left(\bar{\mathbf{v}}\cdot\nabla+\frac{\partial}{\partial t}\right)\mathcal{E}+\frac{\omega}{2}\left\{\bar{\gamma}+i\Delta\right\}\mathcal{E}=-\frac{1}{\varepsilon_0}\left(\frac{\partial}{\partial t}-i\frac{\omega}{2}\right)\bar{\mathcal{P}} \tag{11g}$$

where $\bar{\mathbf{v}}=\bar{\mathbf{v}}_{mm}$, $\mathcal{E}=\mathcal{E}_m$, $\bar{\gamma}=\bar{\gamma}_{mm}$, $\Delta=\Delta_{mm}$, and $\bar{\mathcal{P}}=\bar{\mathcal{P}}_m$. Note that spatial variation of $\mathcal{E}$ in Eq. (11g) only occurs on the direction of the group velocity. By a coordinate transformation we can show that the directional derivative $\bar{\mathbf{v}}\cdot\nabla$ in Eq. (11g), can be written as $\partial/\partial Z$, where the Z-axis is parallel to the direction of the group velocity. Therefore, Eq. (11g) constitute to an one dimensional problem in the spatial direction of the group velocity.

Equations (7), (8) and (11a) form a system coupled differential equations of mixed spatial scales. The bridge between the fast spatial scale [Eqs. (7)–(8)] and the slow spatial scale [Eq. (11a)] differential equations are provided by the integral definition of the slow scale polarization vector [$\bar{\boldsymbol{\mathcal{P}}}$] in Eq. (11b). In order to have a complete set of equations in which all the dynamic quantities vary on the slow scale, we have to formulate Eqs. (7) and (8) in term of $\bar{\boldsymbol{\mathcal{P}}}$ and the slow scale version of the population inversion density. One easy way to accomplish this task is by spatially integrating Eqs. (7)–(8) over an unit cell of the PC, and we will show that, this procedure will not completely remove the dependence on the fast spatial scale.

Firstly, let's dot product $A(\mathbf{r})\vec{\phi}^*_m(\mathbf{r})$ to Eq. (7). The result can be casted in a vector form as

$$\frac{\partial\boldsymbol{\mathcal{P}}}{\partial t}=\frac{(i\Omega-1)\boldsymbol{\mathcal{P}}}{T_2}-\frac{id_0^2}{\hbar}A\hat{S}N\boldsymbol{\mathcal{E}}, \tag{12}$$

where the vector element of $\boldsymbol{\mathcal{P}}$ is $\mathcal{P}_m=A(\mathbf{r})\vec{\phi}^*_m(\mathbf{r})\cdot\mathbf{P}$ and the matrix element of $\hat{S}$ is $S_{mn}(\mathbf{r})=\vec{\phi}^*_m(\mathbf{r})\cdot\hat{s}\vec{\phi}_n(\mathbf{r})$. Integrating Eq. (12) over the unit cell of the PC, we obtain the equation of motion for the slow scale polarization vector $\bar{\boldsymbol{\mathcal{P}}}$ as

$$\frac{\partial\bar{\boldsymbol{\mathcal{P}}}}{\partial t}=\frac{(i\Omega-1)\bar{\boldsymbol{\mathcal{P}}}}{T_2}-\frac{id_0^2}{\hbar}\hat{\bar{\mathcal{N}}}\boldsymbol{\mathcal{E}}, \tag{13}$$

where now we have a matrix representation for the slow scale population inversion density, $\hat{\bar{\mathcal{N}}}=\langle A\hat{S}N\rangle_{uc}$. Note the striking similarity between Eqs. (7) and (13). One can simply arrive at Eq. (13) by simply replacing the fast scale dynamic quantities $\mathbf{E}$, $\mathbf{P}$ and $\hat{s}N$ with the slow scale version of the quantities $\boldsymbol{\mathcal{E}}$, $\bar{\boldsymbol{\mathcal{P}}}$, and $\hat{\bar{\mathcal{N}}}$.

We can try to get an equation for the slow scale population inversion density matrix [$\hat{\bar{\mathcal{N}}}$] by performing the operation, $\langle A\hat{S}(\ldots)\rangle_{uc}$

to Eq. (8), and using the ansatz in Eq. (9). The resulting equation will be,

$$\frac{\partial \hat{\bar{\mathcal{N}}}}{\partial t} = -\frac{\hat{\bar{\mathcal{N}}} - \left\langle A\hat{S}\right\rangle_{uc} N_0}{T_1} - \frac{2i}{\hbar}\left[\sum_m \mathcal{E}_m^* \left\langle \mathcal{P}_m \hat{S}\right\rangle_{uc} - \text{c.c}\right] \tag{14}$$

However, as we can see from Eq. (14), this procedure introduces a new dynamic variable $\langle \bar{\mathcal{P}}_m \hat{S}\rangle_{uc}$. In order to evaluate this variable in which $\mathcal{P}_m = A(\mathbf{r})\vec{\phi}_m^*(\mathbf{r}) \cdot \mathbf{P}$, one still required to use the dynamic equation for $\mathbf{P}$ [Eq. (7)], which is on the fast spatial scale. In the following we will illustrate three methods to overcome this, and generate complete system of equations in the slow scale. These methods are the method of mean field approximation, the method of moments, and the method of small field approximation.

4.1. Mean Field Approximation

Applying the mean value theorem [43] to the integral $\langle \mathcal{P}_m \hat{S}\rangle_{uc}$ in Eq. (14), yields $\langle \mathcal{P}_m \hat{S}\rangle_{uc} = \hat{\zeta}\langle \mathcal{P}_m\rangle_{uc} = \hat{\zeta}\bar{\mathcal{P}}_m$, where $\hat{\zeta}$ is the mean value of the matrix $\hat{S}$. With the mean value theorem, Eq. (14) can be rewritten as,

$$\frac{\partial \hat{\bar{\mathcal{N}}}}{\partial t} = -\frac{\hat{\bar{\mathcal{N}}} - \left\langle A\hat{S}\right\rangle_{uc} N_0}{T_1} - \frac{2i}{\hbar}\hat{\zeta}\left[\boldsymbol{\mathcal{E}}^* \cdot \bar{\boldsymbol{\mathcal{P}}} - \text{c.c}\right]. \tag{15}$$

With the above equation and Eqs. (11a) and (13), we have a complete system of self-consistent equations in the slow quantities, $\boldsymbol{\mathcal{E}}$, $\bar{\boldsymbol{\mathcal{P}}}$, and $\hat{\bar{\mathcal{N}}}$. For numerical evaluations, one has to approximate $\hat{\zeta}$. Although, this could be done in various ways, a simplest approximation would be $\hat{\zeta} \approx \langle \hat{S}\rangle_{uc}$.

4.2. The Method of Moments

Another method to transform a system of integro-differential equations such as a system of Eqs. (7)–(8), and (11a) to a set of differential equations is the method of moments [39–42]. Here, we will use this method to generate a set of differential equations in which all the dynamic quantities vary on the slow scale. For a simplicity of mathematics,we will illustrate the method of moments under a single mode assumption.

The single mode dynamic equation for the slow scale electric field is given by Eq. (11g). To derive dynamic equations for the slow scale polarization and the slow scale population inversion density, let's start with the unaveraged equations, Eqs. (12) and (8). These equation for a single mode become

$$\frac{\partial \mathcal{P}}{\partial t} = \frac{(i\Omega-1)\mathcal{P}}{T_2} - \frac{id_0^2}{\hbar} ASN\mathcal{E}$$
$$\frac{\partial N}{\partial t} = -\frac{N-N_0}{T_1} - \frac{2i}{\hbar}\left[\mathcal{E}^*\vec{\phi}^*\cdot\mathbf{P} - \text{c.c}\right]$$

where $\vec{\phi}=\vec{\phi}_m$ and $S=S_{mm}$. Define the k-th moment of $\mathcal{P}$ and N as $\bar{\mathcal{P}}^{(k)}=\langle S^k\mathcal{P}\rangle_{uc}$ and $\bar{\mathcal{N}}^{(k)}=\langle AS^{k+1}N\rangle_{uc}$, where k is a positive integer. We can obtain the equations of motions for these moments by performing the operations $\langle S^k[\ldots]\rangle_{uc}$ and $\langle AS^{k+1}[\ldots]\rangle_{uc}$ to the above equations. The resulting equations of motions are

$$\frac{\partial \bar{\mathcal{P}}^{(k)}}{\partial t} = \frac{(i\Omega-1)\bar{\mathcal{P}}^{(k)}}{T_2} - \frac{id_0^2}{\hbar}\bar{\mathcal{N}}^{(k)}\mathcal{E}, \tag{16}$$
$$\frac{\partial \bar{\mathcal{N}}^{(k)}}{\partial t} = -\frac{\bar{\mathcal{N}}^{(k)} - \left\langle AS^{k+1}\right\rangle N_0}{T_1} - \frac{2i}{\hbar}\left[\mathcal{E}^*\cdot\bar{\mathcal{P}}^{(k+1)} - \text{c.c}\right]. \tag{17}$$

Equations (16)–(17) constitute to a system of infinite hierarchy of equations in the slow scale quantities $\bar{\mathcal{P}}^{(k)}$ and $\bar{\mathcal{N}}^{(k)}$. Using the moment definitions, we can see that the slow scale polarization $\bar{\mathcal{P}}$ is simply the zeroth moment of $\mathcal{P}$ (i.e., $\bar{\mathcal{P}}=\bar{\mathcal{P}}^{(0)}$), and it is coupled to the higher order moments of $\mathcal{P}$ and N for all values of $k>0$ [i.e., $\bar{\mathcal{P}}=\bar{\mathcal{P}}^{(0)}$ is coupled with $\bar{\mathcal{N}}^{(0)}$, $\bar{\mathcal{N}}^{(0)}$ is coupled with $\bar{\mathcal{P}}^{(1)}$, $\bar{\mathcal{P}}^{(1)}$ is coupled with $\bar{\mathcal{N}}^{(1)}$, $\bar{\mathcal{N}}^{(1)}$ is coupled with $\bar{\mathcal{P}}^{(2)}$, and so on].

One can always truncate the infinite hierarchy of equations in (16)–(17) to a finite number of equations by noticing that S^k is small for a large value of k. This can be easily noticed for isotropic dipole moments [i.e., $\hat{s}$ is a unit matrix], where we have $S^k=\phi_m^{2k}$. Using the normalization condition $\langle\varepsilon\phi_m^2\rangle_{uc}=1$ with ε being a positive function, we have $\phi_m^2<1$, and thence $S^k\to 0$ for $k\to\infty$. As we will show in Section 6, in the steady state, the hierarchy of moment equations [Eqs. (16)–(17)] will simply reduce to a Binomial series in S^k.

Equations (11g), (16) and (17) form a self-consistent formulation of differential equations in the slow scale quantities $\mathcal{E}$, $\bar{\mathcal{P}}^{(k)}$ and $\bar{\mathcal{N}}^{(k)}$. Note that the formulation based on the method of moments is exact if one takes the limit $k\to\infty$, under the single mode assumption.

4.3. Small Field Approximation

Here, we will assume a near threshold operation, where the electric field is small and $N\approx N_0$. We will show that under the single mode assumption, this approximation yields the same results with the one obtained using the multiscale perturbation theory [32],

With $N = N_0$, the single mode version of Eq. (12) becomes

$$\frac{\partial \mathcal{P}}{\partial t} = \frac{(i\Omega - 1)\mathcal{P}}{T_2} - \frac{id_0^2}{\hbar} N_0 A S \mathcal{E}$$

Let's postulate an ansatz $\mathcal{P} = ASp$, where p is a quantity that depends on both time and space. If we substitute this ansatz into the above equation, we will arrive at $\partial p/\partial t = (i\Omega - 1)p/T_2 - (id_0^2/\hbar)N_0\boldsymbol{\mathcal{E}}$, for which the right hand side, has no dependence on the fast spatial scale, and thus shows that p varies only on the slow scale. Therefore, for operations near the threshold condition, we can write approximately write $\mathcal{P} = ASp$. Thus, by averaging $\mathcal{P}$, we have $\bar{\mathcal{P}} = \langle AS \rangle_{uc} p$. With this factorization of $\bar{\mathcal{P}}$, we can write Eqs. (13)–(14) for a single mode as

$$\frac{\partial p}{\partial t} = \frac{(i\Omega - 1)p}{T_2} - \frac{id_0^2}{\hbar} \bar{n} \mathcal{E} \tag{18}$$

$$\frac{\partial \bar{n}}{\partial t} = -\frac{\bar{n} - N_0}{T_1} - \frac{2i}{\hbar} \beta [\mathcal{E}^* p - \text{c.c}], \tag{19}$$

where $\bar{n} = \bar{\mathcal{N}}/\langle AS \rangle_{uc}$ and $\beta = \langle AS^2 \rangle_{uc}/\langle AS \rangle_{uc}$. These equations are in exact agreement with the results of the multiscale perturbation theory for the E-polarization of the 2D PC doped with the dopants of isotropic dipole moments [32]. Note that for the isotropic dipole moments, $\beta = \langle A\phi_m^4 \rangle_{uc}/\langle A\phi_m^2 \rangle_{uc}$.

Throughout this paper, we assume a constant value for the population inversion created by the pumping, N_0. (i.e., a continuous wave pumping). It is straightforward to generalize N_0 to $N_0(t)$ to include the time dependence, and thus allow modeling of step and pulsed pumping conditions. In the slow scale formalism, when a pulsed pumping condition is used, $N_0(t)$ must be replaced with the averaged version, $(1/T) \int_t^{t+T} N_0(t')dt'$, with $T = 2\pi/\omega$ is the optical time period.

5. SLOW SCALE EQUATIONS IN ADIABATIC LIMIT

Assuming the polarization relaxation time is very fast compared to the population decay time [i.e., adiabatic approximation [29–31]), we can neglect the slow variation of the polarization amplitude [i.e., $\partial \mathbf{P}/\partial t \approx 0$], and re-write Eq. (7) as

$$\mathbf{P}(\mathbf{r}, t) = \varepsilon_0 \chi(\mathbf{r}, t) \hat{s} \mathbf{E}(\mathbf{r}, t), \tag{20}$$

where the dynamic susceptibility is defined as $\chi(\mathbf{r}, t) = g \frac{\Omega - i}{1 + \Omega^2} N(\mathbf{r}, t)$ with the constant $g = d_0^2 T_2/\varepsilon_0 \hbar$ representing the maximum of the imaginary part of the susceptibility (and thus the maximum gain) per unit dopant density. Using Eqs. (9) and (20), we can show that in the adiabatic limit, the equation for the population inversion density [Eq. (8)] becomes,

$$\frac{\partial N(\mathbf{r},t)}{\partial t}=-\frac{N(\mathbf{r},t)-N_0}{T_1}-\frac{\boldsymbol{\mathcal{E}}\cdot\hat{S}\boldsymbol{\mathcal{E}}^*}{T_1 I_s\left(1+\Omega^2\right)}N(\mathbf{r},t), \tag{21}$$

where the constant $I_s = \hbar^2/(4d_0^2 T_1 T_2)$ represents the saturation intensity [29–31]. Since χ is directly proportional to N, the dynamic equation for χ can be obtained from Eq. (21) by multiplying with $g\frac{\Omega-i}{1+\Omega^2}$. The resulting equation is

$$\frac{\partial \chi(\mathbf{r},t)}{\partial t}=-\frac{\chi(\mathbf{r},t)-\chi_0}{T_1}-\frac{\boldsymbol{\mathcal{E}}\cdot\hat{S}\boldsymbol{\mathcal{E}}^*}{T_1 I_s(1+\Omega^2)}\chi(\mathbf{r},t), \tag{22}$$

where $\chi_0 = gN_0\ [\Omega-i]/(1+\Omega^2)$.

One can see that in adiabatic limit, the dynamic equations only involves two dynamic quantities, electric field and population inversion density. Instead of the population inversion density, one can also use the susceptibility to formulate the dynamics of the system. In the following we will derive dynamic equations for the electric field and susceptibility in the slow scale.

If we dot product $A(\mathbf{r})\vec{\phi}_m^*(\mathbf{r})$ to Eq. (20), perform averaging over an unit cell of the PC, and then write the results in a vector form, we can show that the slow scale electric field and polarization vectors are related through

$$\bar{\boldsymbol{\mathcal{P}}}=\varepsilon_0\hat{\bar{\mathcal{X}}}\boldsymbol{\mathcal{E}} \tag{23}$$

where $\hat{\bar{\mathcal{X}}}=\langle A\hat{S}\chi\rangle_{uc}$ is defined as the slow scale susceptibility matrix. For the single mode assumption, Eq. (23) reduces to a scalar equation $\bar{\mathcal{P}}=\varepsilon_0\bar{\mathcal{X}}\mathcal{E}$ with $\bar{\mathcal{X}}=\langle AS\chi\rangle_{uc}$. We also can show this result by letting Eq. (16) for $k=0$, to zero, and noticing that $\bar{\mathcal{P}}=\bar{\mathcal{P}}^{(0)}$ and $\bar{\mathcal{N}}=\bar{\mathcal{N}}^{(0)}$. With the result in Eq. (23), the equation of motion for the slow scale electric field vector [Eq. (11a)] becomes,

$$\left(\hat{D}+\hat{I}_u\frac{\partial}{\partial t}\right)\boldsymbol{\mathcal{E}}=\frac{\omega}{2}\left\{i\hat{\bar{\mathcal{X}}}-\hat{\bar{\gamma}}-i\hat{\Delta}\right\}\boldsymbol{\mathcal{E}}. \tag{24a}$$

Equation (24a) is a continuity equation describing the slow evolution of the electric field in the time and space, with the presence of loss and gain. Note that the real and imaginary parts of $\hat{\bar{\mathcal{X}}}$ in Eq. (24a), are responsible for the frequency and gain of the laser oscillation, respectively. The single mode version of Eq. (24a) is

$$\left(\bar{\mathbf{v}}\cdot\nabla+\frac{\partial}{\partial t}\right)\mathcal{E}=\frac{\omega}{2}\left\{i\bar{\mathcal{X}}-\bar{\gamma}-i\Delta\right\}\mathcal{E}, \tag{24b}$$

which is an one dimensional problem in the spatial direction of the group velocity [see Eq. (11g)].

Equations (22) and (24a), and the integral definition of $\hat{\bar{\mathcal{X}}} = \langle A\hat{S}\chi\rangle_{uc}$ forms a system of integro-differential equations with mixed spatial scales in the adiabatic limit. Note that χ in Eq. (22) varies on the fast spatial scale and $\boldsymbol{\mathcal{E}}$ in Eq. (24a) varies on the slow spatial scale. The bridge between the two equations is provided by the integral definition of $\hat{\bar{\mathcal{X}}}$, which washes away the fast spatial variation from χ.

In the following we will use the method of mean field approximation, and the method of moments to obtain self-consistent formulations of the dynamic equations in the slow scale for the adiabatic limit.

5.1. Mean Field Approximation

In order to describe $\hat{\bar{\mathcal{X}}} = \langle A\hat{S}\chi\rangle_{uc}$, let's perform the operation $\langle A\hat{S}[\ldots]\rangle_{uc}$ to Eq. (22) to obtain

$$\frac{\partial\hat{\bar{\mathcal{X}}}}{\partial t} = -\frac{\hat{\bar{\mathcal{X}}} - \chi_0\left\langle A\hat{S}\right\rangle_{uc}}{T_1} - \frac{\left\langle A\hat{S}\boldsymbol{\mathcal{E}}\cdot\hat{S}\boldsymbol{\mathcal{E}}^*\chi\right\rangle_{uc}}{T_1 I_s(1+\Omega^2)}$$

Applying the mean value theorem to the integral $\langle A\hat{S}\boldsymbol{\mathcal{E}}\cdot\hat{S}\boldsymbol{\mathcal{E}}^*\chi\rangle_{uc}$ in the above equation, we have $\langle A\hat{S}\boldsymbol{\mathcal{E}}\cdot\hat{S}\boldsymbol{\mathcal{E}}^*\chi\rangle_{uc} = \boldsymbol{\mathcal{E}}\cdot\hat{\zeta}\boldsymbol{\mathcal{E}}^*\langle A\hat{S}\chi\rangle_{uc} = (\boldsymbol{\mathcal{E}}\cdot\hat{\zeta}\boldsymbol{\mathcal{E}}^*)\hat{\bar{\mathcal{X}}}$. Consequently, we obtain the equation of motion for the slow scale susceptibility matrix from the above equation as

$$\frac{\partial\hat{\bar{\mathcal{X}}}}{\partial t} = -\frac{\hat{\bar{\mathcal{X}}} - \chi_0\left\langle A\hat{S}\right\rangle_{uc}}{T_1} - \frac{\boldsymbol{\mathcal{E}}\cdot\hat{\zeta}\boldsymbol{\mathcal{E}}^*}{T_1 I_s\,(1+\Omega^2)}\hat{\bar{\mathcal{X}}}. \tag{25}$$

With Eqs. (24a) and (25) we have a self-consistent formulation of the dynamic equations in the slow scale for the adiabatic limit, under the mean field approximation.

5.2. The Method of Moments

Let's extend the results of the method of moments presented in Section 4.2, to the adiabatic limit. The adiabatic condition $\partial\mathbf{P}/\partial t = 0$, implies $\partial\bar{\mathcal{P}}^{(k)}/\partial t = 0$ for all values of k in Eq. (16) [recall that $\bar{\mathcal{P}}^{(k)} = \langle S^k(A\vec{\phi}^*\cdot\mathbf{P})\rangle_{uc}$]. Thus in the adiabatic limit, we have

$$\bar{\mathcal{P}}^{(k)} = \varepsilon_0\bar{\mathcal{X}}^{(k)}\mathcal{E}, \tag{26}$$

where $\bar{\mathcal{X}}^{(k)} = g\frac{\Omega-i}{1+\Omega^2}\bar{\mathcal{N}}^{(k)} = g\frac{\Omega-i}{1+\Omega^2}\langle AS^{k+1}N\rangle_{uc} = \langle AS^{k+1}\chi\rangle_{uc}$. By substituting Eq. (26) [for $k+1$] into Eq. (17), and multiplying the resulting equation with $g\frac{\Omega-i}{1+\Omega^2}$, we can show that,

$$\frac{\partial\bar{\mathcal{X}}^{(k)}}{\partial t} = -\frac{\bar{\mathcal{X}}^{(k)} - \chi_0\left\langle AS^{k+1}\right\rangle_{uc}}{T_1} - \frac{\mathcal{E}^2}{T_1 I_s\left(1+\Omega^2\right)}\bar{\mathcal{X}}^{(k+1)}. \tag{27}$$

Equation (27) represents a system of infinite hierarchy of coupled moment equations, and together with Eq. (24b) form a self-consistent formulation of the dynamic equations in the slow scale, under the single mode assumption. The slow scale susceptibility can be obtained as the first moment of χ [i.e., $\bar{\mathcal{X}} = \bar{\mathcal{X}}^{(0)} = \langle AS\chi\rangle_{uc}$].

Note that, as in Section 4.2, the infinite hierarchy of equations defined in (27), can be terminated to obtain finite number of equations by noticing that the higher order moments of χ should be small.

6. STEADY STATE EQUATIONS

For a non-growing and a non-decaying mode amplitude in both time and space [i.e., $\boldsymbol{\mathcal{E}}$ is independent of $\mathbf{r}$ and t], we require the right hand side of Eq. (24a) to be zero. This results in

$$\left\{i\hat{\bar{\mathcal{X}}}^{ss} - \hat{\bar{\gamma}} - i\hat{\Delta}\right\}\boldsymbol{\mathcal{E}} = 0. \tag{28}$$

Here, we have written the steady state $\hat{\bar{\mathcal{X}}}$ as $\hat{\bar{\mathcal{X}}}^{ss}$. The steady state mode amplitudes are therefore, can be found from the null space of the matrix $i\hat{\bar{\mathcal{X}}}^{ss} - \hat{\bar{\gamma}} - i\hat{\Delta}$. Using the matrix elements, Eq. (28) can be written in a symmetrized form as (after some rearrangement),

$$\sum_n \frac{\delta_{mn} + \bar{\mathcal{X}}^{ss}_{mn} + i\bar{\gamma}_{mn}}{\omega_m\omega_n}\left(\omega_n\mathcal{E}_n\right) = \frac{1}{\omega^2}\left(\omega_m\mathcal{E}_m\right). \tag{29}$$

In writing the above equation we used $\Delta_{mn} = [(\omega_m^2/\omega^2) - 1]\delta_{mn}$ [Eq. (11d)]. Recall the definition of $\hat{\bar{\mathcal{X}}}^{ss} = \langle A\hat{S}\chi^{ss}\rangle_{uc}$ in Eqs. (28)–(29). The exact steady state value of χ can be found from Eq. (22) as,

$$\chi^{ss} = gN_0\frac{\Omega - i}{1+\Omega^2+\boldsymbol{\mathcal{E}}\cdot\hat{S}\boldsymbol{\mathcal{E}}^*/I_s}$$

This leads to

$$\hat{\bar{\mathcal{X}}}^{ss} = gN_0\left\langle A\hat{S}\frac{\Omega - i}{1+\Omega^2+\boldsymbol{\mathcal{E}}\cdot\hat{S}\boldsymbol{\mathcal{E}}^*/I_s}\right\rangle_{uc}. \tag{30a}$$

Now let's compare Eq. (30a) with the results of the mean field approximation, and the method of moments. By letting Eq. (25) to zero, we can show that mean field approximation yields

$$\hat{\bar{\mathcal{X}}}^{ss}_{MF} = gN_0 \left\langle A\hat{S} \right\rangle_{uc} \frac{\Omega - i}{1 + \Omega^2 + \boldsymbol{\mathcal{E}} \cdot \hat{\zeta}\boldsymbol{\mathcal{E}}^*/I_s}. \tag{30b}$$

The mean field approximation simply replaces $A\hat{S}$ (in the numerator of Eq. (30a)) and $\hat{S}$ (in the denominator of Eq. (30a)) with the averaged versions $\langle A\hat{S}\rangle_{uc}$ and $\hat{\zeta}$. To compare the method of moment, which is derived under the single mode assumption, let's first write Eq. (30a) for a single mode. The single mode version of Eq. (30a) is

$$\bar{\mathcal{X}}^{ss} = gN_0 \left\langle AS \frac{\Omega - i}{1 + \Omega^2 + \mathcal{E}^2 S/I_s} \right\rangle_{uc}. \tag{30c}$$

To get a steady state description from the method of moments, let's equate Eq. (27) to zero. This yields a recursive equation,

$$\bar{\mathcal{X}}^{(k)} = \chi_0 \left\langle AS^{k+1} \right\rangle_{uc} - \frac{\mathcal{E}^2}{I_s(1 + \Omega^2)} \bar{\mathcal{X}}^{(k+1)}.$$

Starting from $k = 0$, and recursively using the above equation for higher values of k, we can show that the steady state susceptibility from the method of moments $\bar{\mathcal{X}}^{ss}_{mm}$ can be written as,

$$\bar{\mathcal{X}}^{ss}_{mm} = \bar{\mathcal{X}}^{(0)} = \sum_k \left\langle AS\chi_0 \left[-\frac{\mathcal{E}^2 S}{I_s(1 + \Omega^2)} \right]^k \right\rangle_{uc}. \tag{30d}$$

The right hand side of Eq. (30d) is a Binomial series in the powers of the electric field, and will converge for $|\mathcal{E}^2 S/I_s| < 1$. If we assume $k \to \infty$, use the definition $\chi_0 = gN_0[\Omega - i]/(1 + \Omega^2)$, and move the average out of the summation in Eq. (30d), we can readily verify that the method of moment reproduces the exact result in Eq. (30a).

Equation (29) is a nonlinear eigenvalue problem, with eigenvalues, $1/\omega^2$, and eigenvectors, $[\omega_1\mathcal{E}_1, \omega_2\mathcal{E}_2, \omega_3\mathcal{E}_3, \ldots]^T$. The nonlinearity comes from the fact, $\bar{\mathcal{X}}^{ss}_{mn}$ [Eq. (30a)] depends on the eigenvalue and the eigenvectors in Eq. (29). The nonlinear eigenvalue problem [Eq. (29)] can be numerically solved using a self-consistent iterative procedure [52], to obtain the nonlinear Bloch modes (i.e., the steady state modes of the active PC [37]). One also can use Eq. (29) to evaluate the lasing characteristic [i.e., frequency, threshold, and the intensity] of a finite sized PC. The lasing mode in a finite sized PC is usually the Nonlinear Bloch modes at the photonic band edge [12–18]. This is because, the loss term in Eqs. (28)–(29) depends on the cavity leakage rate [see Eqs. (11e) and (11f)], and therefore depends on the group velocity. Modes at the photonic band edges will have small group velocity. Small group velocity will yield small cavity leakage rate [Eq. (11f)] and thus, we can expect the corresponding threshold for the modes close to the photonic band edge should be smaller, than those of the modes far from the photonic band edge.

The result for the steady state obtained in this section, generalizes and simplifies the resultin Refs. [37, 38], which is obtained using the scalar formulation for the specific case of E-polarization in a 2D PC. The vectorial nature of the current formulation allows one to consider time independent analysis of variety of new cases that cannot be modeled using the scalar formulation such as

i) H-polarization of 2D PC,
ii) 3D PC,
iii) membrane of PC and PCs with defect: In this case, the unit cell is actually a supercell,
iv) PCs with quantum dots of specific orientation and shapes: this can be handled with the matrix $\tilde{s}$,
v) finite size PCs: this is handled with the cavity leakage term κ_m.

Previous formulation does not take advantage over the symmetry of the bands for the given wavevector in the formulation. In the previous formulation, the summation in Eq. (29) includes Bloch modes of all bands for a given wavevector. However, as we have mentioned in Section 4, the coupling of modes of the same wavevector but with different symmetry representations for the point group symmetry are zero. Therefore, the summation in Eq. (37) only should include Bloch modes of the same wavevector and the same symmetry representations for the point group symmetry. This will result in much smaller matrices to solve. Furthermore, the numerical solution to Eq. (29) with the exact version of $\bar{\mathcal{X}}^{ss}_{mn}$ [i.e., Eq. (30a) and also in Refs. [37, 38] requires integration at each iteration step, since the unknown quantity $\boldsymbol{\mathcal{E}}$ is inside the integral [see Eq. (30a)]. Performing integration at each iterative step is computationally time demanding. One can use the approximate version [i.e., Eq. (30b)] in which $\boldsymbol{\mathcal{E}}$ is separated from the integration, and this is numerically much effective to handle.

6.1. Steady State Results under a Single Mode Assumption

In this section we present the results of the steady state under the single mode assumption. The results in this section serve as an approximation for the nonlinear matrix eigenvalue problem [Eqs. (28)–(29)].

The single mode version of Eq. (28) is $i\bar{\mathcal{X}}^{ss} - \bar{\gamma} - i\Delta = 0$. With $\bar{\gamma}$ and Δ being real quantities, this equation splits into two equations,

$\mathrm{Re}(\bar{\mathcal{X}}^{ss}) = \Delta$ and $\mathrm{Im}(\bar{\mathcal{X}}^{ss}) + \bar{\gamma} = 0$ which can be written as,

$$\frac{\omega_m^2}{\omega^2} = 1 + gN_0\Omega \left\langle \frac{AS}{1+\Omega^2+\mathcal{E}^2 S/I_s} \right\rangle_{uc}, \tag{31}$$

$$\bar{\gamma} = gN_0 \left\langle \frac{AS}{1+\Omega^2+\mathcal{E}^2 S/I_s} \right\rangle_{uc}, \tag{32}$$

where the frequency of the backbone PC's mode is ω_m, and the frequency of the Nonlinear Bloch mode is ω. In Eqs. (31)–(32), the quantity N_0 depends on the external pumping value. We can cancel the term $\langle \ldots \rangle_{uc}$ in the Eqs. (31)–(32) to show a cubic equation for ω,

$$(\bar{\gamma}T_2)\,\omega^3 + [1 - (\bar{\gamma}T_2)\,\omega_0]\,\omega^2 - \omega_m^2 = 0. \tag{33}$$

If we simply replace the effective loss (i.e., the average loss) parameter in the above equation with a bulk loss, then the resulting equation for ω is in perfect agreement with the results of the first order semiclassical theory for a spatially homogeneous active media [53].

Once ω is solved from Eq. (33), the rest of the unknowns can be solved. For a threshold calculation we have $\mathcal{E} = 0$, and the unknown is $N_0 = N_{th}$. For pumping level greater than the threshold level (i.e., $N_0 > N_{th,m}$), the unknown is $\mathcal{E}$.

The threshold population inversion density $[N_{th}]$ can be found from Eq. (32) by setting $\mathcal{E} = 0$, as

$$N_{th} = \frac{\bar{\gamma}}{g\langle AS\rangle_{uc}}\left(1+\Omega^2\right). \tag{34a}$$

If we define a dimensionless quantity $g_0 = gN_T$ that characterize the maximum gain [recall that N_T is the total density of the active dopants, and $g = d_0^2 T_2/\varepsilon_0\hbar$ is the maximum of the imaginary part of the susceptibility (and thus the maximum gain) per unit dopant density], we can write Eq. (34) in an intuitive form as

$$\frac{N_{th}}{N_T} = \frac{\bar{\gamma}}{\bar{g}}. \tag{34b}$$

In Eq. (34b), we have casted the ratio of the threshold population inversion density to the total population density as the ratio between the effective loss $[\bar{\gamma}]$ to an effective gain, $\bar{g} = \frac{g_0\langle AS\rangle_{uc}}{1+\Omega^2}$. As we can see from the expression for the effective gain, the effective gain depends on g_0 (which is a material property), the confinement of the backbone PC's mode in the active region of the unit cell (which is quantified through $\langle AS\rangle_{uc}$), and the deviation of the atomic resonant frequency from the frequency of backbone PC's mode [which is quantified through $\Omega = (\omega - \omega_0)T_2$].

For a finite sized PC, the cavity leakage rate must be included in the effective loss parameter. Using the estimation of the cavity leakage rate in Eq. (11f), we can write the threshold population inversion density for a finite sized PC as

$$N_{th} = \frac{1+\Omega^2}{2cgL\langle AS\rangle_{uc}} \left|\hat{\mathbf{q}}\cdot\bar{\mathbf{v}}\right|^2, \tag{34c}$$

In writing Eq. (34c), we have neglected the material loss. Eq. (34c) shows that, the threshold population inversion density is small for a small group velocity. Therefore, the photonic band edge modes (which possesses smaller group velocities) will have smaller threshold population inversion densities, and thus emerge as lasing modes.

From Eq. (33), we can see that the steady state mode frequency does not depend on the pumping level, but it depends on $\bar{\gamma}$, ω_0, ω_m and T_2 [i.e., parameters that control N_{th}]. One can expect increasing the pumping, will increase the real part of the susceptibility, and therefore the frequency of the active mode should change as a function of pumping. The real part of the susceptibility depends on the steady state population inversion density. In steady state, for pumping level beyond the threshold value, increasing the pumping value will not change the population inversion density significantly, however the energy from the pumping will be used to generate more light (i.e., to increase the steady state intensity) [29–31]. Therefore for in steady state, the population inversion density is approximately equal to the threshold population inversion density N_{th}, and therefore the steady state frequency will depend on the parameters that control N_{th} [see Eq. (34)].

The amplitude of the Nonlinear Bloch mode $\mathcal{E}$, has to be solved numerically from the nonlinear integral equation, Eq. (32). Defining an intensity ratio as $\mathcal{I} = \mathcal{E}^2/I_s$, we can get an approximate value of $\mathcal{I}$, using the mean field approximation [Eq. (30b)] for the single mode gain. Using $\mathrm{Im}(\bar{\mathcal{X}}^{ss}_{MF}) + \bar{\gamma} = 0$ we can show that

$$\mathcal{I} = g\frac{\langle A\hat{S}\rangle_{uc}}{\bar{\gamma}\zeta}\left(N_0 - N_{th}\right). \tag{35}$$

6.2. Threshold Pumping and Steady State Intensity in Three Level System

Population inversion cannot be created in a purely two level system. Additional energy levels apart from the two radiating energy levels are needed to create the realistic pumping mechanism. For this purpose, two widely studied energy level configurations are three and four level systems [29–31].

For a discussion of a realistic pumping mechanism and the corresponding threshold pumping, let's consider PC structures with active dopants of three energy levels [37]. The analysis can be easily extended for active dopants with four levels. In a three level system, the pumping will excite the dopants from level 1 to level 3. We assume the excited dopant will decay very fast to level 2 (almost instantaneously). As before, levels 2 and 1 remain as radiating energy levels. In this system, N_0, population inversion decay time, and saturation intensity can be written as $N_0 = N_T(\rho - 1)/(\rho + 1)$, $T_1/(\rho + 1)$, and $I_s(\rho + 1)$, respectively [30, 31]. In these expressions, ρ stands for the ratio of the pumping rate from level 1 to level 3, to the population decay rate from level 2 to level 1. With this notations for the three level dopants, the threshold pumping, ρ_{th}, with the help of Eq. (34b) can be shown to be,

$$\rho_{th} = \frac{\bar{g} + \bar{\gamma}}{\bar{g} - \bar{\gamma}} = 1 + 2\sum_{l\geq 1}\left(\frac{\bar{\gamma}}{\bar{g}}\right)^{l}, \tag{36}$$

For a finite ρ_{th}, Eq. (36) requires $\bar{g} > \bar{\gamma}$ [i.e., the effective mode gain must be larger than the effective mode loss]. Recall that $\bar{g}$ and $\bar{\gamma}$ depend on the parameters of the backbone PC (such as radius and dielectric constant of rods). Therefore, the inequality $\bar{g} > \bar{\gamma}$, will set limits on the parameters of the backbone PC.

For an exact calculation of the steady state intensity ratio ($\mathcal{I}$) as a function of ρ, one has to numerically evaluate Eq. (32) with $N_0 = N_T(\rho - 1)/(\rho + 1)$. Approximate version of $\mathcal{I}$ can be obtained from Eq. (35) as $\mathcal{I} = \frac{\bar{g}-\bar{\gamma}}{\bar{\gamma}\zeta}[1 + \Omega^2](\rho - \rho_{th})$.

7. CONCLUSION

In conclusion we have presented a theory to describe the transient and steady state behaviors of the modes in an active PC. We model the active constituents as two level atoms, and assumed the electric field in the active PC can be expanded in term of modes of a backbone PC [i.e., a couple mode model], with the expansion coefficient varying slowly in the time and spatial scales. We defined a slow scale electric field vector [i.e., $\boldsymbol{\mathcal{E}}$] as an array of the expansion coefficients. The equation of motion for $\boldsymbol{\mathcal{E}}$ together with the Bloch equations forms a system of integro-differential equations. Using the method of moments and the mean value theorem, we showed the system of integro-differential equations can be transformed to a set of differential equations in slow time and slow spatial scales. In the adiabatic limit, the couple mode model results in a familiar relationship $\bar{\boldsymbol{\mathcal{P}}} = \varepsilon_0 \hat{\hat{\mathcal{X}}} \boldsymbol{\mathcal{E}}$, where $\bar{\boldsymbol{\mathcal{P}}}$ is the slow scale polarization vector and $\hat{\hat{\mathcal{X}}}$ the slow scale susceptibility matrix. In steady state, the entire formalism reduces to a nonlinear matrix eigenvalue problem. The nonlinear matrix eigenvalue problem can be solved to obtain the Nonlinear Bloch modes in an infinite PC, or lasing modes in a finite sized PC.

For cases, where the coupling between the modes are negligible [i.e., a single mode assumption], the transient equations can be casted as an one dimensional problem in the spatial coordinate. Further, in the steady state, we showed that the moment equations describing the transient behavior reduce to a Binomial series in the powers of the electric field. The threshold population inversion density under a single mode assumption is given by a formula which can be calculated using the unit cell averaged parameters, and the steady state mode amplitude is described by a simple nonlinear integral equation. A partial numerical illustration for the steady state results based on the single mode assumption is given in Ref. [55].

This work provides a foundation for the transient and steady state analysis of lasers and nonlinear Bloch modes in PC structures of all dimensions. The presented theory can be easily extended for any active and nonlinear perturbation with more than two levels, and can be used in various investigations of nonlinear phenomena in PCs.

APPENDIX A.

To derive Eq. (11a), we start with Eq. (6). Using Eqs. (9)–(10), and neglecting second order terms [31, 53], we can write Eq. (6) as

$$\frac{1}{c^2}\sum_n \left\{(\omega_n^2-\omega^2)\varepsilon(\mathbf{r}) - i\frac{\omega}{\varepsilon_0}\sigma(\mathbf{r}) - 2i\omega\varepsilon(\mathbf{r})\frac{\partial}{\partial t}\right\}\mathcal{E}_n(\mathbf{r},t)\vec{\phi}_n(\mathbf{r}) + \sum_n \mathcal{V}_n(\vec{\phi}_n,\mathcal{E}_n) = \mu_0 A(\mathbf{r})\left(2i\omega\frac{\partial}{\partial t}+\omega^2\right)\mathbf{P}, \tag{A1}$$

where $\mathcal{V}_n = \nabla\mathcal{E}_n \times \nabla \times \vec{\phi}_n + (\nabla\mathcal{E}_n)\nabla\cdot\vec{\phi}_n - (\nabla\mathcal{E}_n\cdot\nabla)\vec{\phi}_n$. If we dot product Eq. (A1) with $\vec{\phi}_m^*$, and then perform spatial averaging over an unit cell of the PC, we will arrive at Eq. (11a). In writing Eq. (A1), we used the orthogonality relationship $\langle\vec{\phi}_m^*(\mathbf{r})\cdot\varepsilon(\mathbf{r})\vec{\phi}_n(\mathbf{r})\rangle_{uc} = \delta_{nm}$, and the result $\langle\vec{\phi}_m^*(\mathbf{r})\cdot\mathcal{V}_n(\vec{\phi}_n,\mathcal{E}_n)\rangle_{uc} = -i\frac{2\omega}{c^2}\bar{\mathbf{v}}_{mn}\cdot\nabla\mathcal{E}_n(\mathbf{r},t)$, where $\bar{\mathbf{v}}_{mn}$ is defined in Eq. (11c). To prove this result, firstly note that the dot product $\vec{\phi}_m^*(\mathbf{r})\cdot\mathcal{V}_n$ can be written as $(\nabla\mathcal{E}_n)\cdot\mathcal{T}_{mn}$ using the identities of vector calculus. Here the l-th Cartesian component of the vector $\mathcal{T}_{mn}$ is

$$\mathcal{T}^l_{mn} = \phi_m^{*l}\left(\partial^k\phi_n^k\right) + \left(\phi_m^{*k}\partial^k\right)\phi_n^l - 2\phi_m^{*k}\partial^l\phi_n^k \tag{A2}$$

[written in the summation of repeated index convention], where the superscript denotes the Cartesian component of the vector, and $\partial^k(\partial^l)$ represents the partial derivative with respect to k (l)-th Cartesian component. Finally by defining, $\bar{\mathbf{v}}_{mn} = i\frac{c^2}{2\omega}\langle\mathcal{T}_{mn}\rangle_{uc}$, we arrive at $\langle\vec{\phi}^*_m(\mathbf{r})\cdot\mathcal{V}(\vec{\phi}_n,\mathcal{E}_n)\rangle_{uc} = -\frac{2i\omega}{c^2}\bar{\mathbf{v}}_{mn}\cdot\nabla\mathcal{E}_n(\mathbf{r},t)$.

APPENDIX B.

In this appendix, we will show that the group velocity for the m-th mode of the backbone PC can be written as $\bar{\mathbf{v}}_{mm}$ [see Eq. (11c) and Appendix A]. In order to do this we will use $\mathbf{k}\cdot\mathbf{p}$ perturbation theory which is in earlier has been used to derive group velocity expression for 1D Bragg stacks [54].

Let start with Eq. (10), by identifying the mode of backbone PC with a pair of indices to denote the Bloch wavevector, $\mathbf{k}$, and band index, n. If we write $\vec{\phi}_{\mathbf{k},n}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{u}_{\mathbf{k},n}(\mathbf{r})$, then Eq. (10) can be written in an operator form as

$$\mathrm{H}_{\mathbf{k}}\mathbf{u}_{\mathbf{k},n}(\mathbf{r}) = \boldsymbol{\varepsilon}(\mathbf{r})\boldsymbol{\omega}^2_{\mathbf{k},n}\mathbf{u}_{\mathbf{k},n}(\mathbf{r}), \tag{B1}$$

where $\mathrm{H}_{\mathbf{k}}\mathbf{u}_{\mathbf{k},n}(\mathbf{r}) = c^2(\nabla + i\mathbf{k}) \times (\nabla + i\mathbf{k}) \times \mathbf{u}_{\mathbf{k},n}(\mathbf{r})$. For a small increment of $\mathbf{q}$, in $\mathbf{k}$, Eq. (B1) becomes $\mathrm{H}_{\mathbf{k+q}}\mathbf{u}_{\mathbf{k+q},n}(\mathbf{r}) = \boldsymbol{\varepsilon}(\mathbf{r})\boldsymbol{\omega}^2_{\mathbf{k+q},n}\mathbf{u}_{\mathbf{k+q},n}(\mathbf{r})$. $\mathrm{H}_{\mathbf{k+q}}$ can be decoupled as $\mathrm{H}_{\mathbf{k}} + \mathbf{V}_{\mathbf{k},\mathbf{q}}$ where

$$\mathbf{V}_{\mathbf{k},\mathbf{q}}\mathbf{u}_{\mathbf{k+q},n} = c^2\left\{i\mathbf{q}\times(\nabla+i\mathbf{k})+(\nabla+i\mathbf{k})\times i\mathbf{q}-\mathbf{q}\times\mathbf{q}\right\}\times\mathbf{u}_{\mathbf{k+q},n}, \tag{B2}$$

and $\mathbf{V}_{\mathbf{k},\mathbf{q}}$ can be considered as a perturbing operator. Using the first order time independent perturbation theory, we obtain,

$$\boldsymbol{\omega}^2_{\mathbf{k+q},n} = \boldsymbol{\omega}^2_{\mathbf{k},n} + \langle\mathbf{u}_{\mathbf{k},n}\cdot\mathbf{V}_{\mathbf{k},\mathbf{q}}\mathbf{u}_{\mathbf{k},n}\rangle_{uc} \tag{B3}$$

We can expand the frequency in Taylor expansion as $\boldsymbol{\omega}_{\mathbf{k+q},n} = \boldsymbol{\omega}_{\mathbf{k},n} + \mathbf{q}\cdot\mathbf{v}_{\mathbf{k},n} + O(q^2)$, where $\mathbf{v}_{\mathbf{k},n}$ is the group velocity which can be found using Eq. (B3) as,

$$\bar{\mathbf{v}}_{\mathbf{k},n} = \frac{1}{2\omega_{\mathbf{k+q},n}}\nabla_{\mathbf{q}}\langle\mathbf{u}_{\mathbf{k},n}\cdot\mathbf{V}_{\mathbf{k},\mathbf{q}}\mathbf{u}_{\mathbf{k},n}\rangle_{uc}\Big|_{q=0} \tag{B4}$$

where the operator $\nabla_{\mathbf{q}} = \hat{\mathbf{q}}_x(\partial/\partial q_x) + \hat{\mathbf{q}}_y(\partial/\partial q_y) + \hat{\mathbf{q}}_z(\partial/\partial q_z)$. Neglecting the second order terms of $\mathbf{q}$, we can evaluate $\mathbf{u}_{\mathbf{k},n}\cdot\mathbf{V}_{\mathbf{k},\mathbf{q}}\mathbf{u}_{\mathbf{k},n}$ as a function, $\vec{\phi}_{\mathbf{k},n}(\mathbf{r})$. The resulting expression in a single index notation [i.e., $(k,n)\equiv n$], is $\mathbf{u}_n\cdot\mathbf{V}_{\mathbf{k},\mathbf{q}}\mathbf{u}_n = ic^2\mathbf{q}\cdot\mathcal{T}_{nn}$ where $\mathcal{T}_{nn}$ is defined in Eq. (A2). Using this result and the definition of group velocity in Eq. (B4), it is straightforward to show $\bar{\mathbf{v}}_{nn} = i\frac{c^2}{2\boldsymbol{\omega}}\langle\mathcal{T}_{nn}\rangle_{uc}$.

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