

MODELING TRANSMISSION OF PHOTONIC CRYSTAL WAVEGUIDE MODES ENHANCED BY KERR NONLINEARITY

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Nonlinear modes of electromagnetic fields propagating in photonic crystal systems have been studied by implementing various computer simulation techniques using electromagnetic theory. The fundamentals of simulation of photonic crystals are analyzed using general purpose methodologies such as the FDTD or PWE methods. Information derived from the underlying physical insights into the systems could be utilized to describe the control mechanisms over the propagation of the modes around impurities in the photonic crystal lattice. The impurities trap the resonantly localized electromagnetic modes having a frequency in a stop band of the photonic crystal, suggesting novel optical controls in the photonic crystal systems. Our focus is on deepening understanding of the nonlinear modes existing within photonic crystal waveguides which interact with the Kerr nonlinearity of the controlling medium; this enables us to reveal specific mechanisms of the nonlinear systems and their potential nonlinear functions and applications. To gain full generality of the nonlinear modes of increasing complexity, we propose a novel theoretical approach, the difference equation waveguide, using Green's function theory of the non-homogeneous system. The recursive difference equations for the photonic crystal waveguides are solved for the guided modes interacting with multiple bound modes localized on the impurity features. The interest is on the transmissivity of resonant scattering of the nonlinear

modes arising from in- or off-channel features formed in Kerr dielectrics in a 2D photonic crystal. Here, the modes display the wide and interesting varieties of behavior present in the system including optical bistability and induced transparency. More interestingly, the transmissions are fully treated for the case in which the field dependence of Kerr dielectric properties, with enhancing nonlinear effects, allows two different frequency waveguide modes to interact with one another by a modulation of the Kerr properties. In this regard, we show the observation of one mode used to model numerically the transmission characteristics of the other, e.g., the propagation of one frequency mode can turn on and off the resonant transmission of the other along the waveguide channel.

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by

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*To the memory of my parents. Bhadra and Muga, who gave birth to me
To my very special, Lurette, for making me complete
And,
To my son, Abuditi, for the joy you bring us*

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CHAPTER I

Introduction and Motivation

During my Ph.D. years, I have worked on several different projects related to computational/theoretical electromagnetics using concepts of condensed matter physics. As it seems to me, I am supposed to put all of them under the roof of one theme in an introduction to the dissertation. It is hard to integrate things that are different, though. Meaning, the introduction of my dissertation should be rather general as shown in the following paragraphs.

1.1 A General Overview

One of the novel class of optical materials of interest to us is a photonic crystal, a periodic dielectric structure with lattice parameters on the order of the wavelength of the electromagnetic wave. Such a photonic structure supports only a limited number of electromagnetic fields to propagate through it. These are called its modes. In this dissertation, the propagation properties of the electromagnetic modes in photonic crystals will be investigated by using various numerical simulation techniques for deriving information about the underlying physical insights into the light modes of photonic crystals. Typical for a photonic crystal is that its structure, if designed correctly, affects the properties of light flowing through it and allows us to achieve a complete control (moulding, manipulating, and guiding) over the propagation of light energy. This gives an opportunity for a number of applications based on the implementation of this control [1–3]. Essentially, the impurity structures embedded into the photonic crystal determine the control mechanisms over the light modes. Recently, these endeavors were the focus of a number of

theoretical and experimental efforts on the systems of linear dielectric media [4–6], yet we know little about the specific mechanisms of the systems formed of nonlinear optical media and the potential for nonlinear functions that might be revealed with further study. In this dissertation research, we are focussing on better understanding nonlinear modes existing within photonic crystal waveguides. In order to explore these possibilities for applications, a theoretical study of the fundamental characteristics of periodic dielectric structures is necessary.

Photonic crystals have been a subject of great interest in the last few decades, particularly due to the wide range of their applications in photonic device components such as waveguides, resonators, filters, multiplexers, switches, and new optical fibers [7–17]. The guided modes in such structures and other promising designs [18–22] of photonic crystals allow control of light within the structures at the wavelength scale. Photonic crystals are artificially formed optical media with periodic modulation of dielectric constant ε_r (or equivalently the refractive index). This modulation occurs in 1D, 2D, or 3D, respectively, as a layering of dielectric slabs, a two-dimensional array of dielectric rods, or a three-dimensional array of dielectric cubes (Figure 1.1). The optical properties of

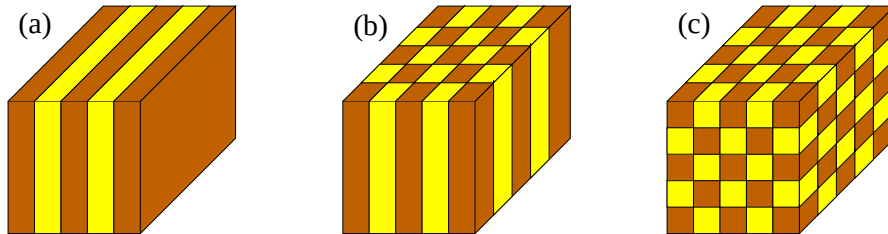


Figure 1.1: Schematic views of periodic dielectric (a) slabs, (b) rods, and (c) cubes representing 1D, 2D, and 3D periodic dielectric structures (photonic crystals). The two colors represent the two types of materials composing the period.

such structures depend on the dielectric constant of the materials composing the crystal as well as the period of the crystal.

The photons (or electromagnetic waves) traveling through a photonic crystal experience a periodic variation of the dielectric constant similar to the periodic potential of an electron in an atomic lattice of solid state physics. Due to this analogy, the periodic dielectric constant for photon motion in a photonic crystal leads to the division of the photonic modes into pass and stop band frequency states. The modes at pass band frequencies can propagate through the photonic crystal, while modes at stop band frequencies do not propagate through the photonic crystal. Here, the stop band, more popularly known as a photonic band gap, is the most important property that determines the practical significance of the photonic crystal as it allows us to block and confine certain stop band frequency modes.

As there is a similarity between solid state physics and photonic crystals, the concepts of solid state crystals, viz., reciprocal space, Brillouin zones, dispersion relations, Bloch wave functions, etc., can also be applied to photonic crystals [23]. That is why it is logical to call the periodic dielectric structures photonic crystals, and this subject has received an increasing interest since the authors [24,25] in 1987 demonstrated theoretically the potential use for the structures in the control of light. In general, however, the periodicity of photonic crystals is in the operating wavelength scale (micrometers) and that of the electronic crystals is in the atomic scale (nanometers). Consequently, the Brillouin zone for photonic crystals is about 1000 times smaller (and the reciprocal lattice translation vector for them is much larger) than that for the electronic crystals.

Unlike naturally periodic solid state crystals, photonic crystals have a universe of possible geometries, which provide possibilities of creating many different novel photonic devices. The stop band property of a pure photonic crystal can be directly implemented for device applications like frequency filters of light or dielectric mirrors, because when light with frequency inside the stop band is incident on the structure, it appears to be completely reflected or scattered. But incident light with pass band frequencies appears to be completely transmitted through the structure. Such a property can be implemented to use photonic crystals as optical filters.

However, intentionally introduced site defects (single impurities) in the photonic crystal lattice can lead to localized electromagnetic modes or, in cases of multiple defects, to localized propagating modes. The localized states are formed in the stop band, since these states cannot propagate through the surrounding photonic crystal materials. Many useful devices can be designed using impurities in the photonic crystals. Examples are microcavities (single impurities) and linear waveguides (lines of multiple impurities). The localized and propagating modes on such designs will be a primary interest later in this dissertation. The impurity media are generally formed of linear or nonlinear dielectric materials depending on the types of impurity light modes to be treated in the problem, and they actually enable us to localize the light modes about a particular region in the lattice of the crystal.

Impurities destroy the perfect translational symmetry in the photonic crystals. This can be achieved in a periodic dielectric by a number of different methods. For example, such methods include: adding impurity dielectric materials to a unit cell (a period) or removing dielectric materials from a unit cell or by changing the dielectric

constant of materials in a cell or by changing the size/geometry of materials in a cell in the lattice. The total effect will be a localized change of the average dielectric constant of the medium. As a general rule, if the impurity causes the average dielectric constant to increase, the eigen frequency at the frequency will drop and one or more bands from the upper pass band edge may drop into the stop band, creating so called ‘donor’ impurity bands; if the impurity causes the average constant to decrease, the eigen frequency will shift upwards, and one or more bands from the lower pass band edge may emerge into the stop band, creating the so called ‘acceptor’ impurity bands. The concepts of ‘donor’ and ‘acceptor’ are from solid state crystals [26–31], and we will discuss them in greater detail in Chapter III. It is important to note that single impurities and linear arrays of impurities are the two fundamental forms of impurity structures in the photonic crystal lattice.

Single site impurities serve as high Q microcavities. Such structures bind or trap resonantly localized light modes (cavity modes) about themselves having a frequency in a stop band of the photonic crystal. Since no light in the stop band can pass through the surrounding bulk materials, the impurity mode will be evanescent in the bulk material. Thus a resonance occurs in a very narrow frequency range inside the stop band. The structure is then called a resonant microcavity, and the confined resonant mode about the structure is called the resonant excitation. The efficiency of the resonant cavity is characterized by a quality factor or Q value, a measure of the number of oscillations of light in the cavity before damping eventually causes the original excitation to decay away. The resonant excitations in such cavities are the basis of laser systems, Fabry-Perot oscillators, and photonic microcavities.

Linear arrays of impurities can be achieved in a similar manner, for instance, by removal (addition, replacement, etc.) of a row/column of unit cells from the photonic crystal lattice. They cause light localization about the line of defects, resulting in highly efficient waveguides known as photonic crystal waveguides. The mechanism of localization around these structures is described by stop band effects in a manner similar to those in the case of microcavities. Such waveguides can have unusual properties, e.g., guiding of light without radiation loss or with only minimal loss of radiation energy through a very sharp bend. This is not possible to achieve in conventional waveguides based on total internal reflection. For example, fiber optics can transport only a portion of the incident light around a waveguide (fiber) bend, and the remaining portion escapes out as loss. This is due to the angular constraint for total internal reflection in the curved waveguide system. But the photonic crystal waveguides (or photonic crystal fiber optics) can transport incident light in arbitrarily tight bends [17, 32, 33].

More interestingly, photonic crystal waveguides have received a lot of attention because of their possible use as components in optical integrated circuits that would be analogous to electronic integrated circuits but that would operate entirely with light. The optical circuits not only transmit light signals optically but they also may perform switching, routing, and other device functions more efficiently. Additionally, the exponential growth of information data processing at present in the world (optical networks) demands faster speeds and larger bandwidths than electronic circuits can provide (switching speeds ≈ 50 GB per second). Many researchers have been engaged in recent years in adjusting such operational abilities to optimize the size and performance of the photonic crystal integrated circuit components [10, 13–16, 32, 34–39]. One focus of particular

recent interest has been on the modeling of waveguide modes arising in photonic crystals containing nonlinear optical modes [11, 16, 40–43]. These types of systems have potential applications in switching and optical transistors which require the interaction of light with itself or other optical beams. Another focus has been on multiplexing designs which may be of importance in routing and uploading and downloading information carried in optical networks. This important function can be accomplished in systems composed solely of linear optical media.

Of particular interest is the Kerr nonlinear effect and its nature in photonic crystal waveguide systems as well as photonic crystal impurities in the hope that these systems can be used for all-optical switching purposes. Kerr nonlinearity is a third-order nonlinearity [44–49] in the electric field which arises in some dielectric materials and which is introduced into photonic crystal lattices in the form of a nonlinear dielectric impurity. The nonlinearity of the Kerr medium allows light to interact with itself and other optical beams while maintaining the frequency of the original beam of light. Based on this idea, this dissertation attempts to investigate the waveguide modes interacting with various in- and off-channel sites Kerr impurities and the modes associated with Kerr impurities isolated in a photonic crystal lattice. Theoretical modeling studies on such systems of interest will be conducted by using the methods of the classical electrodynamics and numerical simulation techniques.

Photonic crystals are complex scattering problems [50], which make wave propagation in photonic crystals difficult to analyze. Therefore, numerical simulations are crucial for most theoretical analyses. In this regard, a wide range of simulation techniques [33] have been developed and utilized for investigating the scattering and guidance

properties of electromagnetic modes in complex photonic crystal structures. Typically, they fall into three categories: (1) time-domain simulations, such as the finite-difference time-domain method (FDTD) [51, 52], which can simulate the electromagnetic fields propagating in time, (2) frequency-domain eigenproblems, primarily, the plane wave expansion method (PWE) [34, 53–55], which has proved very successful in computing band structure in different geometries, and (3) transfer matrix [56], scattering matrix, difference equation [10, 57, 58], and beam propagation methods. The difference equation method, which is classified as one of the methods in (3), will be implemented in Kerr nonlinear problems in this dissertation.

The FDTD technique may be the most generally used method. It is based on the numerical time-integration of Maxwell’s curl equations. In this technique, the computational space is replaced by a discrete set of nodes where finite differences to the spatial and temporal derivatives of the electromagnetic fields are used as approximations. The numerical approximations lead to a system of algebraic equations which are solved sequentially starting from initial and boundary conditions.

The particular interest in FDTD methods derives from recent research in photonic crystal device modeling, particularly for computing the field distribution inside the photonic crystal structures with non-uniform dielectric distribution, including various material properties of interest. Since this method can treat almost any type of structure, it has been extensively used for predicting behavior of electromagnetic wave scattering and radiation for a variety of practical problems. Some of these works have been initiated by John D. Joannopoulos, J.B. Pendry, Y. Kivshar and others [13, 35, 52, 59–61]. In this

dissertation, we will deal with similar work on modeling of waveguides and cavities used as components of photonic crystal designs for prospective applications.

The PWE method is a popular modeling tool applied to photonic crystal devices. In this method, the plane wave incident on an infinite periodic structure is modulated by a Fourier series expansion of Bloch functions describing the crystal structure. The result is an infinite matrix eigenvalue problem, which can be truncated to a fixed number of terms and the resulting finite matrix can be solved numerically for the photonic band spectrum and eigenmodes.

The difference equation method is a new analytical approach that consists in describing the electric field of the guided modes at stop band frequencies into the waveguide channel sites or localized modes onto Kerr nonlinear sites. This method offers a quick investigation of the general types of the modal behaviors to be expected in the system. The field solutions of the modes are taken in the form of planewaves with fixed incident wave vectors. The solutions, in general, result in a system of linear and nonlinear simultaneous equations which are used to numerically investigate the transmission characteristics of the modes in the system. For numerical treatment of the nonlinear modes in this dissertation, the focus is directed towards difference equation approach, as this method is convenient to formulate in- or off-channel features of photonic crystal waveguides and to adapt in computer simulation models without complex mathematics. In addition, the method in my dissertation provides more physical insights into the characteristics of the problem.

The in- or off-channel impurity features formed in photonic crystal waveguides are constantly demanded in optical applications because of their characteristics to support the resonantly localized states of the light modes. But, such modal characteristics for

applications are not easily tunable in the linear media photonic crystals. If the intensity dependence, known as the Kerr effect, of the Kerr-type dielectric constant is significant in the impurity features of the nonlinear photonic crystal waveguides, then the system may allow us to manipulate the light modes and to design the photonic crystals for applications that may rely on the powerful principle of the optical bistability [62–65]. The dissertation will attempt to exploit this principle in order to achieve the switching action in a model of photonic crystal. Other useful applications (optical tricks) for the Kerr effect include the frequency conversion or frequency generation, solitons, logic gates, and memory, among others [66–68]. However, the theory or analytical solution for Kerr-type nonlinearity in photonic crystals is not well understood yet, and, hence, we will thoroughly study this subject in the dissertation. By using an appropriate computer technique, it is also possible to link the numerical results of a Kerr model to the theory and the experiment for the nonlinear photonic crystals. The dissertation work mainly focuses on how to model and simulate the modes in the 2D photonic crystal waveguides. The objective is to develop theoretical analysis and numerical tools to design photonic crystal waveguides mediated by the Kerr dielectrics in the in- or off-channel sites.

The systems of in- and/or off-channel resonant scattering of guided modes in photonic crystal waveguides have been studied by many other researchers in the past few years. These studies have mainly focused on systems composed of linear dielectric media [5, 11, 14, 16, 20–22, 42, 69–74]. Noda and co-workers initiated the off-channel work, conducting experimental and numerical (computer simulation) investigations on 2D photonic crystal slabs. In their work, the resonant interaction of guided modes with modes localized on single off-channel sites were treated [5, 20–22, 72, 73]. The system was origi-

nally proposed as a multiplexer for downloading signals of various frequencies transported by a photonic crystal waveguide. For these applications, the ability to design a system with high selectivity in the download of a large number of modes is important. This requires a high Q resonant interaction of the guided modes with those on the off-channel sites. The transmission and confinement properties of the modes in the photonic crystal square lattice with nonlinear impurities at various lattice sites were investigated by Mingaleev *et al.* [14, 16, 37, 69, 75]. They observed bistability phenomenon and indicated possible applications in photonic integrated circuits. In this regard, in Reference [13, 76], Soljacic *et al.* showed the possibility of using optical bistability for telecommunications. Besides these studies, a significant number of simulation (and to our knowledge few experimental) studies on the similar types of the systems were made [77–79].

The previously mentioned research used mainly the linear impurity media or nonlinear media with simple modes. This dissertation demonstrates our interest and research in the difference equation waveguide modes that resonantly scatter with the modes of the in- and/or off-channel Kerr nonlinear impurity features. This will be done by expanding studies recently made by McGurn [11, 42, 70, 71] in the context of a simple mode in photonic crystal waveguides. We elaborate in our work for new systems containing two different frequency guided modes with the following motivation: In the present work both guided modes will be taken to affect each other’s dielectric properties through the Kerr media. In the earlier treatment by McGurn, the Kerr parameter at the frequency of one of the frequency modes was taken to be zero. This meant that while the dielectric properties of the system as seen by one of the modes depended on the field intensity of both modes,

the other mode saw only a linear dielectric effect. This simplified the solution and the focus of the present work will be to treat the full generality of the nonlinear system.

By implementing difference equation formalism for two frequencies of the present problem, we study both the linear and nonlinear transmissions of the waveguide modes. Particularly, we analyze the effect of the Kerr nonlinearity in the resonant scattering of the waveguide modes. We first review specific cases of the two modes, ω_1 and ω_2 , introduced in this dissertation. This not only simplifies the problem, but also allows us to consider the ω_1 mode as the primary interest for the numerical analysis without the loss of its qualitative nature of transmission, or reflection coefficient, or its interaction with the ω_2 mode through off-channel nonlinearity. Both ω_1 and ω_2 modes fall within the same stop band of the photonic crystal. Indeed, the presence of the ω_2 mode in the problem gives rise to unusual features in the transmission of the ω_1 mode, which will be examined later in a case study of the ω_1 mode. The ω_2 mode induces the localized field of the Kerr defect, hence, causing the modulation in the dielectric or optical properties of the off-channel site; this, in turn, affects the ω_1 mode transmission of interaction. The strength of the nonlinear effect in modulating dielectric constant may become much larger at a resonance of the ω_2 mode in the vicinity of the off-channel Kerr site, which will be discussed later in the numerical results.

1.2 Outline of the Dissertation

The dissertation is organized as follows: This chapter is an introduction of the dissertation and explains the motivation of the work. Chapter II explains the mathematical background of the problems investigated in this dissertation, and also discusses briefly the numerical algorithms implemented for the simulation in the computer experiment. Chap-

ter [III](#) discusses the fundamentals of the computation of photonic crystal characteristics using the FDTD method and also validates the results of the simulation using the PWE method when possible. Chapters [IV](#) and [V](#) explain difference equation approaches to modeling of the guided modes into photonic crystal waveguide channel with the embedded Kerr nonlinearity. Chapter [VI](#) presents the self-interaction theory for the off-channel problem using the two different frequency guided modes. Chapter [VII](#) is a summary and conclusion of the dissertation work.

CHAPTER II

Electromagnetic Approach for Photonic Crystals

In this chapter, the general methods of electromagnetism used for investigating the photonic crystal in the dissertation are reviewed. The main focus is on introducing the various mathematical techniques for the numerical solutions of Maxwell's equations in 1D and 2D photonic crystals described by a dielectric constant function $\varepsilon(\mathbf{r})$. We assume that light propagates in photonic crystals but that there are no external charges and currents, since photonic crystals are dielectric systems.

2.1 Formulation of Equations

Nearly one and a half centuries ago [80], James Clerk Maxwell formulated Maxwell's partial differential equations that form the foundation of modern electromagnetism including electrical and optical network technologies. Here, we write Maxwell's equations in a useful form based on electric and magnetic fields in photonic crystals. The Maxwell's equations that govern propagation of light, the electric and magnetic fields, through the photonic crystal under our assumption take the following differential forms [81–83],

$$\nabla \times \mathbf{H} = \partial_t \mathbf{D}, \quad (\text{Ampere's law}), \quad (2.1a)$$

$$\nabla \times \mathbf{E} = -\partial_t \mathbf{B}, \quad (\text{Faraday's law}), \quad (2.1b)$$

$$\nabla \cdot \mathbf{B} = 0, \quad (2.1c)$$

$$\nabla \cdot \mathbf{D} = 0, \quad (2.1d)$$

where the field vectors, $\mathbf{E}$, $\mathbf{D}$, $\mathbf{H}$, and $\mathbf{B}$ are functions of both location and time, and they are related to each other via the material equations $\mathbf{D} = \varepsilon \mathbf{E}$ and $\mathbf{B} = \mu \mathbf{H}$. Any electromagnetic field must satisfy these equations.

The ε and μ , permittivity (dielectric constant) and permeability, are functions of location only, and they are described as $\varepsilon = \varepsilon_0 \varepsilon_r$ and $\mu = \mu_0 \mu_r$, where ε_r and μ_r , respectively, are called the relative permittivity and relative permeability of the crystal. For most dielectric materials of interest used in photonic crystals, the relative permeability is very close to unity and we set $\mu_r = 1$ in this dissertation for simplicity unless stated as a different value. In that case, it is more convenient and more physical to define the relative permittivity as the square of the refractive index n , i.e., $\varepsilon_r \approx n^2$ so that $n = \sqrt{\varepsilon_r}$, but, in general, $n = \sqrt{\varepsilon_r \mu_r}$. The $\varepsilon_0 \approx 8.854 \times 10^{-12}$ Farad/m and $\mu_0 = 4\pi \times 10^{-7}$ Henry/m, respectively, are permittivity and permeability of free space, which are used to describe the velocity of light in a vacuum, $c = 1/\sqrt{\mu_0 \varepsilon_0}$, and the free space impedance, $\eta_0 = \sqrt{\mu_0/\varepsilon_0}$, in the computation.

The $\mathbf{E}$ and $\mathbf{H}$ field solutions are complicated functions of time and space and they are interdependent through Maxwell's equations. However, since the structure of the set of Eqs. (2.1a)-(2.1d) are linear, and assuming the field solutions are time harmonic, we can separate out the time dependence of the solutions by expanding the fields as $\vec{\phi}(\mathbf{r}, t) = \vec{\phi}(\mathbf{r})e^{-i\omega t}$, where $\vec{\phi}$ represents either the $\mathbf{E}$ or $\mathbf{H}$ field at a fixed frequency ω . In the field equation, $\vec{\phi}(\mathbf{r})$ is a periodic function, the so called Bloch function, with periodicity of the photonic crystal lattice that will be explained in Section 2.2.

Depending on the treatment of the problems, for instance, the mathematical techniques, the material property of interest, etc., Eqs. (2.1a)-(2.1d) can be reduced to various convenient forms suitable for numerical computations. The general structures of some of them, particularly the forms of Helmholtz equations used in this dissertation, are briefly reviewed in the following sections/subsections. To that, a detailed survey of a form of

non-homogeneous Helmholtz equation will be given in developing the difference equation theory for 2D photonic crystals in Chapter IV. It is important to note here that solutions to the Helmholtz equations will describe how electric and magnetic fields propagate through a medium.

2.1.1 The Helmholtz Curl Equations

The curl operations reduce Maxwell's equations to equations involving only one type of field. For example, taking the curl of both sides of Eq. (2.1a) and substituting Eq. (2.1b) results in a wave equation for the electric field, and equivalently, carrying out the process in the opposite order results in a wave equation for the magnetic field:

$$\nabla \times \nabla \times \vec{\phi} = \varepsilon \mu \partial_t^2 \vec{\phi} \quad (2.2)$$

where $\vec{\phi}$ represents either the $\mathbf{E}$ or $\mathbf{H}$ field. Since we assume the fields are time-harmonic the operator ∂_t^2 yields $-\omega^2$. The resulting curl-curl equations, known as Helmholtz equations, in only the $\mathbf{E}$ -field or $\mathbf{H}$ -field then can be written as

$$\nabla \times \nabla \times \mathbf{E} = \frac{\omega^2}{c^2} \varepsilon_r \mathbf{E}, \quad (2.3a)$$

$$\nabla \times \frac{1}{\varepsilon_r} \nabla \times \mathbf{H} = \frac{\omega^2}{c^2} \mathbf{H}, \quad (2.3b)$$

where $\mathbf{E}$ and $\mathbf{H}$ are now functions of space only. Alternatively, even treating the wave equation (Eq. (2.2)) by using a separation of variables technique, instead of time-harmonics, results in Eqs. (2.3a) and (2.3b).

These equations are the basic starting point to develop numerical algorithms for the electromagnetic simulation techniques, including plane wave expansion, plane wave with boundary conditions, and difference equation methods which will be implemented on several projects in this dissertation. But, the time-domain problems, such as the FDTD

method for investigating the field distribution, band spectrum, and waveguide modes, use Eqs (2.1a)-(2.1b) directly in order to develop the computing algorithms.

2.1.2 Analogy between Helmholtz and Schroedinger Problems

The Helmholtz equation for the electromagnetic problem is analogous to the Schroedinger equation for electronic systems. To illustrate this point more clearly, let us consider a finite 1D photonic crystal determined by the periodic dielectric function $\varepsilon_r(x)$. The electromagnetic propagation equation inside such a structure can be described by the 1D Helmholtz equation here, written explicitly using Eq. (2.3a), as

$$\partial_x^2 E(x) + \varepsilon_r(x) (\omega^2/c^2) E(x) = 0. \quad (2.4)$$

We can write Eq. (2.4) as

$$-\partial_x^2 E(x) - [\varepsilon_r(x) - 1] (\omega^2/c^2) E(x) = (\omega^2/c^2) E(x), \quad (2.5)$$

which has the same mathematical form as the Schroedinger equation for electron propagation in the 1D periodic potential $V(x)$:

$$-\partial_x^2 \psi(x) + (2m\hbar^{-2}) V(x) \psi(x) = (2m\hbar^{-2}) \epsilon \psi(x). \quad (2.6)$$

By comparison, it can be seen that the dielectric scatterers with $\varepsilon_r(x) > 1$ are analogous to regions of negative potential energy in a quantum problem [84]. This means that it is absolutely logical to apply the concepts of quantum mechanics to photonic crystal systems, but with a different frequency range.

We note here that the structures of Helmholtz equations written for any specific problem (e.g., homogeneous or non-homogeneous model equations) of photonic crystal systems may also be written in a form resembling the Schroedinger equation.

2.2 The Plane Wave Expansion for Band Structure

The PWE method is a frequency-domain eigenproblem for computing photonic band characteristics. It is the most popular method for photonic band structure computation. It was first implemented in 1990 [54] and was a breakthrough to the photonic band structure research at that time. There are many versions [34, 53, 54, 85–91] of this method. A Fourier series expansion is used to represent periodic functions of the system in this method. The terms in the Fourier series are the plane waves. Then the Helmholtz equation of the problem is expressed as a matrix eigenproblem and applied linear-algebra techniques are used to find the eigenvectors and eigenvalues. In our implementation, the Helmholtz Eqs. (2.3a)-(2.3b) can be cast as an eigenvalue problem,

$$\hat{\Theta}\mathbf{E} = (\omega^2/c^2)\varepsilon_r\mathbf{E}, \quad (2.7a)$$

$$\hat{\Theta}\mathbf{H} = (\omega^2/c^2)\mathbf{H}, \quad (2.7b)$$

with eigenvalue (ω^2/c^2) and eigen-operator $\hat{\Theta} = \nabla \times \nabla \times$ or $\nabla \times \frac{1}{\varepsilon_r} \nabla \times$ for harmonic modes, in analogy to the Schroedinger problem of quantum mechanics. Our goal here is to solve for energies in terms of ω and the electromagnetic fields at these energies. However, what we are given in the problem is the ε_r , which is a function of space. The ε_r is not constant in photonic crystal structures, it is periodic, meaning the position of the $\frac{1}{\varepsilon_r}$ term is important in the above operators.

Eq. (2.7a) describes a generalized $\mathbf{E}$ eigenproblem and Eq. (2.7b) the ordinary $\mathbf{H}$ eigenproblem. The question of which form of eigenproblem to solve depends mainly on the mathematical convenience. For example, the $\mathbf{E}$ form, as shown in Eq. (2.7a), is preferred for analytical calculation (Chapter 2 of Joannopoulos’s book, [81]), but this form

is undesirable for numerical computation, such as photonic band structure calculation, because the $\mathbf{E}$ eigen-operator $\nabla \times \nabla \times$ is not hermitian as the transversality requirement $\nabla \cdot \varepsilon \mathbf{E} = 0$ depends on ε .

The hermiticity is necessary in order for the eigenvalues to be real and, thus, have a physical meaning. To make the $\mathbf{E}$ eigen-operator hermitian, Eq. (2.7a) can be re-written as $\frac{1}{\varepsilon_r} \nabla \times \nabla \times \frac{1}{\varepsilon_r} (\varepsilon_r \mathbf{E}) = \frac{\omega^2}{c^2} \frac{1}{\varepsilon_r} (\varepsilon_r \mathbf{E})$, but the three factors of $\frac{1}{\varepsilon_r}$ appearing in this expression make the computation unnecessarily complicated. For this reason, the $\mathbf{H}$ form, as shown in Eq. (2.7b), where the operator $\Theta = \nabla \times \frac{1}{\varepsilon_r} \nabla \times$ is hermitian, is preferred for the band structure calculations and also the solution for the $\mathbf{H}$ field. The $\mathbf{E}$ field can then be recovered directly from Eq. (2.1a):

$$\mathbf{E} = i(\varepsilon_0 \varepsilon_r \omega)^{-1} \nabla \times \mathbf{H}. \quad (2.8)$$

This equation can be reduced to $E(x) = \eta_0[\varepsilon_r(x)]^{-\frac{1}{2}} H(x)$ for the 1D case for computing z -polarized x -directed propagating modes in the 1D problem in the dissertation.

The general terms used for developing the eigenproblem of the plane wave method and describing the fields of the finite-difference time-domain method, including the waveguiding modes of difference equation, are reviewed in the following subsections.

2.2.1 Bloch Function Application

The photonic crystal we consider is an infinite periodic dielectric structure. In order to solve the eigenproblem, e.g., Eq. (2.7b), in such structure, we should use a method that employs the periodicity of the dielectric distribution in the crystal structure. For a photonic crystal, Bloch's theorem is often used for representation of the eigenfunction

because the eigenfunction of an infinite periodic structure will be infinite and periodic. That is why Bloch's theorem is useful.

Bloch's theorem says that the eigenfunctions of an infinite periodic structure can be represented in the form of a plane wave multiplied by a periodic function with periodicity of the lattice. The magnetic field $\mathbf{H}$ can be expressed as

$$\mathbf{H}(\mathbf{r}) = \mathbf{u}_{\mathbf{k},n}(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}}, \quad (2.9)$$

where $\mathbf{u}_{\mathbf{k},n}(\mathbf{r})$ is the periodic function with periodicity described by the set of translational vectors $\{\mathbf{T}\}$ of the lattice, which corresponds to wave vector $\mathbf{k}$ and the state number n . Because of Bloch's theorem, both the periodic function $\mathbf{u}_{\mathbf{k},n}(\mathbf{r})$ and dielectric function $\varepsilon_r(\mathbf{r})$ satisfy the periodic property: $\mathbf{u}_{\mathbf{k},n}(\mathbf{r}) = \mathbf{u}_{\mathbf{k},n}(\mathbf{r} + \mathbf{T})$ and $\varepsilon_r(\mathbf{r}) = \varepsilon_r(\mathbf{r} + \mathbf{T})$. The eigenfunction, as shown in Eq. (2.9), should be used in the Helmholtz equation for band structure and dispersion analysis, which will be discussed in the following subsections.

Substituting the eigenfunction Eq. (2.9) in the Helmholtz Eq. (2.3b), we get

$$-\nabla \cdot \frac{1}{\varepsilon_r(\mathbf{r})} \nabla \mathbf{u}_{\mathbf{k},n}(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} = \frac{\omega^2}{c^2} \mathbf{u}_{\mathbf{k},n}(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}}. \quad (2.10)$$

Since the periodic and dielectric functions are not constants, they make the problem much more complex, and, consequently, the dispersion relation takes a more complex form, which can be solved numerically. However, if we consider uniform media where no modulation of the dielectric constant appears, the period of the dielectric function is infinite. The eigenfunction of the medium now can be represented in the form of a plane wave multiplied by a constant. Then, both periodic and dielectric functions are constants in the case of the uniform medium. In that condition, Eq. (2.10) results in $|\mathbf{k}| = \sqrt{\varepsilon_r}(\omega/c)$, which is a linear function, the dispersion relation of the radiation field inside the uniform medium.

2.2.2 Eigenproblem Analysis

We need a method for decomposing the periodic functions of the photonic crystal structure in order to develop the eigenproblem of the structure. The Fourier series provides the mathematical tool for decomposing the periodic functions involved in the problem. We cannot proceed with the computation of an infinite series, and, since $\mathbf{u}_{\mathbf{k},n}(\mathbf{r})$ has the same periodic property as $\varepsilon_r(\mathbf{r})$, we need to expand the function (Eq. (2.9)) in a Fourier series by reciprocal lattice vectors designated as $\mathbf{G}$:

$$\mathbf{H}(\mathbf{r}) = \sum_{\mathbf{G}} \mathbf{u}_{\mathbf{k},n}(\mathbf{G}) e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}}, \quad (2.11)$$

where $\mathbf{u}_{\mathbf{k},n}(\mathbf{G})$ is called the Fourier expansion coefficient of the periodic function.

Because of the spatial periodicity, the dielectric function should also be expanded into Fourier series. For convenience, we expand the inverted dielectric function as it is written down in Eq. (2.10):

$$[\varepsilon_r(\mathbf{r})]^{-1} = \sum_{\mathbf{G}} \kappa(\mathbf{G}) e^{i\mathbf{G}\cdot\mathbf{r}}, \quad (2.12)$$

where $\kappa(\mathbf{G})$ are Fourier expansion coefficients of the inverted dielectric function, which satisfy $\kappa(-\mathbf{G}) = \kappa(\mathbf{G})$ for real dielectric functions describing the photonic crystal structure. The information about the dielectric distribution inside the structure is now given in the form of the Fourier expansion coefficients. While treating the plane waves numerically, both Eqs. (2.11) and (2.12) are expanded to infinities in terms of the $\mathbf{G}$ in order to represent infinite periodic structure of the photonic crystal. For example, in the one dimensional case, $|\mathbf{G}| = 2\pi n/a_c$, where $n = 0, \pm 1, \pm 2, \dots, \pm\infty$ and a_c is the lattice constant.

The functions, Eqs. (2.11) and (2.12), in the expanded forms of Fourier series are substituted in Eq. (2.7b) by taking into account the translations of the reciprocal vectors appropriately:

$$\begin{aligned} & -\sum_{\mathbf{G}''} \nabla \cdot \kappa(\mathbf{G}'') e^{i\mathbf{G}'' \cdot \mathbf{r}} \nabla \sum_{\mathbf{G}'} \mathbf{u}_{\mathbf{k},n}(\mathbf{G}') e^{i(\mathbf{k}+\mathbf{G}') \cdot \mathbf{r}} = \frac{\omega^2}{c^2} \sum_{\mathbf{G}} \mathbf{u}_{\mathbf{k},n}(\mathbf{G}) e^{i(\mathbf{k}+\mathbf{G}) \cdot \mathbf{r}}, \quad \text{or} \\ & -\sum_{\mathbf{G}} \sum_{\mathbf{G}'} \nabla \cdot \kappa(\mathbf{G} - \mathbf{G}') e^{i(\mathbf{G}-\mathbf{G}') \cdot \mathbf{r}} \mathbf{u}_{\mathbf{k},n}(\mathbf{G}') \nabla e^{i(\mathbf{k}+\mathbf{G}') \cdot \mathbf{r}} = \frac{\omega^2}{c^2} \sum_{\mathbf{G}} \mathbf{u}_{\mathbf{k},n}(\mathbf{G}) e^{i(\mathbf{k}+\mathbf{G}) \cdot \mathbf{r}}, \end{aligned} \quad (2.13)$$

where $\mathbf{G} = \mathbf{G}' + \mathbf{G}''$ have been used to reduce the first summation to a common summation index. After a little algebra for taking derivatives, combining the exponents, and projecting to the basis $e^{i(\mathbf{k}+\mathbf{G}) \cdot \mathbf{r}}$, we get

$$\sum_{\mathbf{G}'} \kappa(\mathbf{G} - \mathbf{G}') \left((\mathbf{k} + \mathbf{G}') \cdot (\mathbf{k} + \mathbf{G}) \right) \mathbf{u}_{\mathbf{k},n}(\mathbf{G}') = \frac{\omega^2}{c^2} \mathbf{u}_{\mathbf{k},n}(\mathbf{G}) \quad (2.14)$$

which is known as the Master Equation. Since this equation has no coordinate dependence, all the variables depend on the reciprocal lattice vector only. In general, Eq. (2.14) can be symmetrized and diagonalized on a computer to determine the eigenvalues (frequencies) and eigenvectors (Fourier coefficients). Notice that instead of one differential equation containing the functions we have a system with an infinite number of linear equations and infinite number of unknowns in Eq. (2.14). Those linear equations can be restricted to quite a low number of equations depending on the accuracy required and other situations of the numerical treatments. A method of restricting the reciprocal lattice vectors for converting the problem into a finite number of equations is explained in [92].

The matrix differential operator in Eq. (2.14) can be expressed in the form:

$$\hat{M}_{\mathbf{G},\mathbf{G}'} = \kappa(\mathbf{G} - \mathbf{G}') \left((\mathbf{k} + \mathbf{G}') \cdot (\mathbf{k} + \mathbf{G}) \right) \quad (2.15)$$

whose elements appear as $\hat{M}_{\mathbf{G}_1, \mathbf{G}'_1}$, $\hat{M}_{\mathbf{G}_1, \mathbf{G}'_2}$, ..., $\hat{M}_{\mathbf{G}_1, \mathbf{G}'_m}$, etc. The set of reciprocal lattice vectors $\mathbf{G}$ is determined via the lattice vector of particular photonic crystals considered in the problem, where we use the method of reciprocal space from solid state crystals. In our treatment, we make the set of $\mathbf{G}'$ the same as $\mathbf{G}$ such that the matrix will be square for computation of the band structure.

The set of the reciprocal lattice vectors $\mathbf{G}$ should be selected appropriately to provide a correct Fourier expansion of the dielectric function and the wavefunctions. The selection is crucial, particularly for computing the band structure, because it is impossible to achieve the right result without correct numbers in the set of $\mathbf{G}$ in Eq. (2.15). For this reason, the reciprocal lattice vectors must be selected to form a zero-symmetric set. The details of such a selection method are given in [39].

In selecting the wave vectors $\mathbf{k}$, the speciality of the problem is taken into account. For instance, when finding impurity states of the photonic crystal (changing the dielectric constant or the thickness of one element causing light localization), one value of the wave vector is enough; however, while computation of a pure photonic crystal requires a set of wave vectors taken within the Brillouin zone. In the computation of more complex characteristics, such as photonic density of states, it is necessary to compute the eigenstates in all points of the Brillouin zone.

The matrix Eq. (2.15) is hermitian, i.e., it satisfies $\hat{M}_{\mathbf{G}, \mathbf{G}'} = \hat{M}_{\mathbf{G}', \mathbf{G}}^*$, which is necessary to have a real positive eigenvalue of the form ω^2/c^2 . We note here that this form of eigenvalue will be discussed again in Chapter IV for developing the difference equation theory using Green's function approach. While using the FDTD method, the

fields and dielectric functions are initialized periodically in the algorithms directly, and the eigenvalues are obtained through the Fourier analysis of the time response of the fields.

2.3 The Finite-Difference Time-Domain (FDTD) Simulation

FDTD is a time-domain simulation for electromagnetic problems. This technique uses finite-differences as approximations to the spatial and temporal derivatives of the electromagnetic fields, E and H , that appear in Maxwell's equations, as given in Eqs. (2.1a) and (2.1b) on page 14. In this simulation, we have assumed a linear, isotropic, and nondispersive photonic crystal media (properties independent of field, direction, and frequency) to simplify the explanation of the problem in this dissertation.

We reviewed the wave equation and Helmholtz equation in previous sections as a traditional method of introducing the electromagnetic problems, but, ultimately the FDTD method deals directly with Maxwell's equations. In order to treat Maxwell's equations numerically to finally develop the FDTD scheme, Ampere's and Faraday's laws can be written in component form as

$$\partial_\alpha H_\beta - \partial_\beta H_\alpha = \sigma E_\gamma + \varepsilon \partial_t E_\gamma, \quad (\alpha, \beta, \gamma = x, y, z), \quad (2.16a)$$

$$\partial_\alpha E_\gamma - \partial_\gamma E_\alpha = \mu \partial_t H_\beta, \quad (2.16b)$$

where $\partial_\alpha = \partial/\partial\alpha$, etc. These six first-order differential equations form a coupled system suitable for numerical computations, and they can be directly transformed into the FDTD algorithms that compute the propagating fields everywhere at a certain time or update the fields at a probe point in all times called the pulse response. In the equations above, the ε and μ are used as usual, as described on page 15.

The purpose of this section is to review the basic concepts of the FDTD method, considering the simplest case possible, so that we can use them later in the specific problems in this dissertation. For simplicity, and since the extension to 2D and 3D cases is straightforward, we continue by further assuming a 1D system with z -polarized x -directed propagation in lossless ($\sigma = 0$) medium. In this case, the propagation has no variations in the $\hat{y}$ and $\hat{z}$ directions, i.e., $\partial_x \neq 0$, $\partial_y = 0$, and $\partial_z = 0$. This allows us to write Eqs. (2.16a) and (2.16b) in the form

$$\partial_x H_y = \varepsilon \partial_t E_z \text{ and } \partial_x E_z = \mu \partial_t H_y \quad (2.17)$$

for existing fields E_z and H_y . The ∂_x operates on both fields at the rate of spatial offset on each temporal offset, that are described in the following.

By using the first order finite-differences of the derivatives and Figure 2.1 as a guide for discretization in space (Yee lattice) and time with a leapfrog algorithm (detailed in [93, 94]), the differentials in Eq. (2.17) can be implemented in the FDTD form. An often

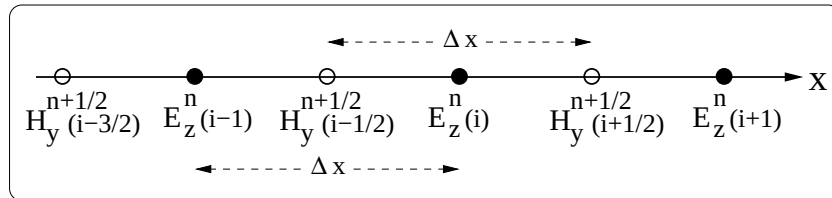


Figure 2.1: A typical 1D FDTD space chart of the Yee algorithm showing spatial offset between the electric and magnetic fields, E_z components symbolized as closed circles, and H_y components as open circles on the x -axis. The direction of the Poynting vector (flow of light energy) is along the positive x -axis. The integer i represents the spatial index with $x = i\Delta x$ and the n represents the time step with $t = n\Delta t$, where Δx and Δt , respectively, describe the spatial and temporal offsets.

used finite-difference (actually central-difference) approximation of the derivative of the function at x_0 is: $\partial_x f(x)|_{x_0} \approx [f(x_0 + \Delta x/2) - f(x_0 - \Delta x/2)](\Delta x)^{-1}$ with second-order accuracy, i.e., the error is $O[(\Delta x)^2]$. Here, the function (in the x -direction) representing

the fields is not actually sampled at x_0 . Instead, the function is sampled at the neighboring points $x_0 \pm \Delta x/2$. This idea was first used by Yee to develop the FDTD numerical algorithm for the fields in a computational grid scheme known as a Yee lattice [93]. A typical example of this for the 1D case is shown in Figure 2.1, where the difference of two adjacent E components are separated by Δx and located $\pm \Delta x/2$ on either side of an H component, and vice versa. Here the E and H components interleave in the space lattice at intervals of $\Delta x/2$. This condition yields a numerical approximation for the field derivative. For instance, the E field derivative, $\partial E/\partial x$, permits time stepping of the H component. Details of this scheme can be found in [94–96] or other texts.

Using the above idea of finite-differences in both space and time derivatives and following a few algebraic steps, including $\lambda = \Delta t/\varepsilon$ and $\Lambda = \Delta t/\mu$, we can arrive at an iterative algorithm for E_z and H_y fields as

$$E_z^{n+1}(i) = E_z^n(i) + \lambda \partial_x H_y^{n+\frac{1}{2}} \text{ and } H_y^{n+\frac{1}{2}}(i+1/2) = H_y^{n-\frac{1}{2}}(i+1/2) + \Lambda \partial_x E_z^n \quad (2.18)$$

which propagate in time steps. Notice that the computation is arranged in alternate layers in both space and time. For example, the new value of E_z at time step $n+1$ is computed from the previous value of E_z at n and the new values of H_y at $n+1/2$. This is the fundamental paradigm of the FDTD method. Note that the time indices n , $n+1$, $n+1/2$, and $n-1/2$ in the superscripts of Eq. (2.18) are dropped in the computer code because time is implicit in the FDTD method. They appear only in an iterative time loop propagating the fields. The wave equation as shown in Eq. (2.2) can be implemented directly for propagating the fields by taking the finite-difference approximations for the second-order derivatives [97,98]. However, the solution methods for the propagating fields,

as derived in Eq. (2.18), are considered robust methods because they involve both E and H fields in the algorithm.

The diagram in Figure 2.2 explains the FDTD process for a computer experiment of the algorithms in a computational space. After determination and discretization of

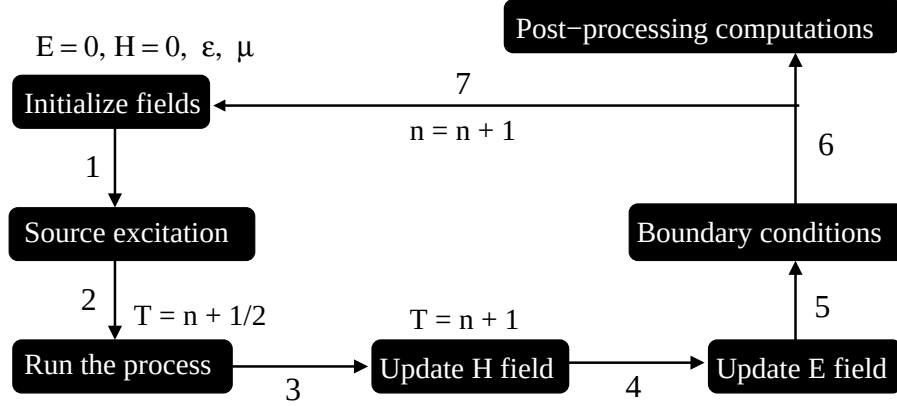


Figure 2.2: Diagram showing the FDTD process. The E and H fields are usually initialized to zero, and ϵ and μ are supplied in the problem. The n or T represents discrete time steps in which the factor $1/2$ denotes a time step corresponding to an H field mode.

the computational domain into FDTD nodes, the initial values of the E and H fields at the nodes should be assigned before starting the computation. Usually, the E and H fields are initialized at zero values. Therefore, initially there are two arrays filled with zeros in a 1D case. Likewise, four arrays occur in 2D and six arrays occur in 3D cases. These arrays are updated by propagating the fields in time steps, through the loop labelled 1–2–3–4–5–6–7 corresponding to terminology described in each of the black buttons in the figure, so that the arrays formed in the loop contain information of the field component values with corresponding coordinates.

After the initialization process, a radiation source should be introduced into an array element of one of the fields. The FDTD algorithm supports any types of source exci-

tations such as Gaussian, harmonic, etc. The radiation source varies in time so the source nodes should be initialized at each time step. Another most important consideration in the FDTD process is the implementation of boundary conditions. The main concept is that the boundary conditions allow us to consider a finite size of photonic crystal as an infinite system. A detailed study of FDTD boundary conditions is found in [93,94,99,100] or elsewhere. The boundary conditions and important FDTD terminologies used in this dissertation are reviewed in Appendix B.

2.4 The Difference Equation Method of Modeling

Another approach for electromagnetic simulation, probably the most important one for the main purpose of this dissertation, is the Difference Equation (DE) method. This approach is considered in several major projects in the dissertation, especially for investigating various transmission behaviors of the waveguide modes arising from the Kerr-type nonlinearity in a 2D photonic crystal. The difference equation method is an analytical approach which is particularly suitable in a photonic crystal system mediated by linear and/or Kerr nonlinear impurities. The guided modes of photonic crystal waveguides and results using this approach are presented in a number of publications [10,11,42,57,70,71,101–105]. The equations of the system are simple and can be quickly solved to demonstrate the wide and interesting varieties of behavior present in the system, including among others, optical bistability and induced transparency.

As in the case of the planewave expansion method, the difference equation approach uses the Helmholtz equation (2.3a). However, since this approach is based on using an analytical treatment for impurities in the photonic crystal waveguides, the dielectric function appearing in the Helmholtz equation is directly replaced by the total

dielectric function, $\varepsilon + \delta\varepsilon$, that describes the dielectric properties of the system. Here ε is a background dielectric and $\delta\varepsilon$ describes changes in the background which give rise to the periodic patterning of the photonic crystal structure. This replacement results in a non-homogeneous Helmholtz equation of the form:

$$\left(\nabla^2 + \varepsilon(\mathbf{r})\frac{\omega^2}{c^2}\right)\mathbf{E}(\mathbf{r},\omega) = -\delta\varepsilon(\mathbf{r})\frac{\omega^2}{c^2}\mathbf{E}(\mathbf{r},\omega), \quad (2.19)$$

where ε is the periodic part of the dielectric constant as usual and $\delta\varepsilon$ is the contribution due to the change in dielectric constant of the system. This equation can be solved for waveguide modes using Green's function techniques as given in Chapter IV. In this method, the waveguide impurity modes are written in integral form for $\delta\varepsilon$ nonzero of the photonic crystal [106]. Note that, for notational convenience, we have used ε instead of ε_r to denote the relative dielectric constant for the dielectric media in Eq. (2.19).

Assuming a condition of the field variation about the impurity material allows us to express the solutions of Eq. (2.19) in a generalized form of discrete algebraic equations, called difference equations that represent waveguide modes in the system. The solutions of the modes form recursively defined sequences that appear similar to the form of difference equations in linear algebra. However, because of dielectric non-homogeneity and nonlinear impurities introduced into the photonic crystal, even the difference equations for very simplified and idealized models result in complex linear and nonlinear expressions which require numerical treatment in order to obtain useful results. Use of computers is essential to solving such problems. This allows us to consider the difference equation treatment of photonic crystal waveguides as a computer simulation problem.

Details of difference equation formulation and its implementation on a square lattice photonic crystal waveguide with embedded Kerr impurities will be discussed in Chapter IV

and Chapter V. The chart in Figure 2.3 shows the implementation procedure of the difference equation method in general. Essentially, as in cases of the other simulation/modeling

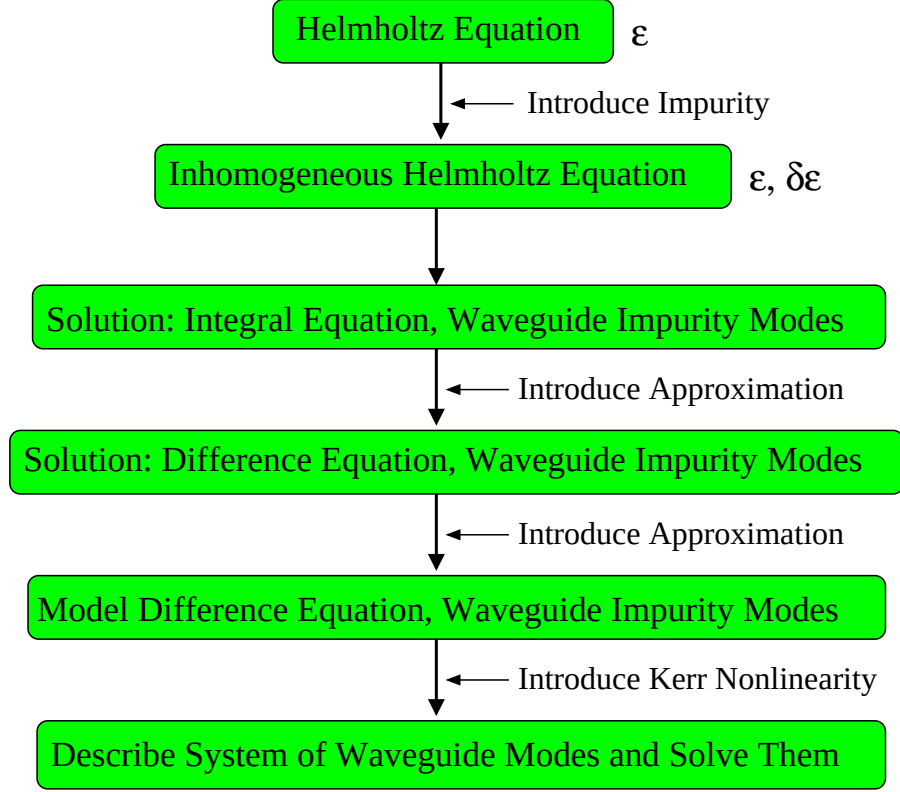


Figure 2.3: Diagram showing the development and implementation procedure of the Difference Equation method. ϵ represents the background dielectric constant of a pure photonic crystal in the Helmholtz equation and $\delta\epsilon$ represents the contribution due to the impurity into the crystal resulting in non-homogeneous Helmholtz equation.

approaches, the difference equation for photonic crystal waveguide modes is developed by considering several approximations over the non-homogeneous equation of the photonic crystal system. The important step in the difference equation implementation is that the equations of waveguide modes on each linear or nonlinear impurity lattice site should be coupled correctly to their nearest-neighbor sites in order for the system to be a useful model.

CHAPTER III

Fundamentals of Simulations of Photonic Crystal Structures

In this chapter, the concept of electromagnetic field distribution is applied to investigate the characteristics of the photonic crystal structures. Electromagnetic fields propagating in the photonic crystal give rise to complicated scattering problems. This complexity, naturally, leads us to think that the field distribution inside the structures is one of the fundamentals of the computation of photonic crystal characteristics. The fields can be used for computing the transmission spectra and band structure, including other properties which are often used for the design, simulation, and experiment of real specimens, such as photonic crystal filters, waveguides, resonators, multiplexers, and other photonic devices.

Considering the field distribution in a single layer of a 1D photonic crystal (or an optically layered system [107–109]), we developed an understanding of the underlying physical properties of periodic structures when they are excited by the radiation field. A typical field distribution using the analytical solution of an arbitrarily layered dielectric structure is shown in Figure 3.1. The waveguide in such a layer forms a starting point for the development of infinitely long (more complex) photonic crystal waveguides or photonic crystal fibers and integrated optical circuits. Actual photonic crystal waveguides are not infinitely long structures. The finite-size periodic structure, for instance, a distributed Bragg reflector [110, 111], with periodicity in an arbitrary direction can be formed by translating a group of two or more dielectric layers several times.

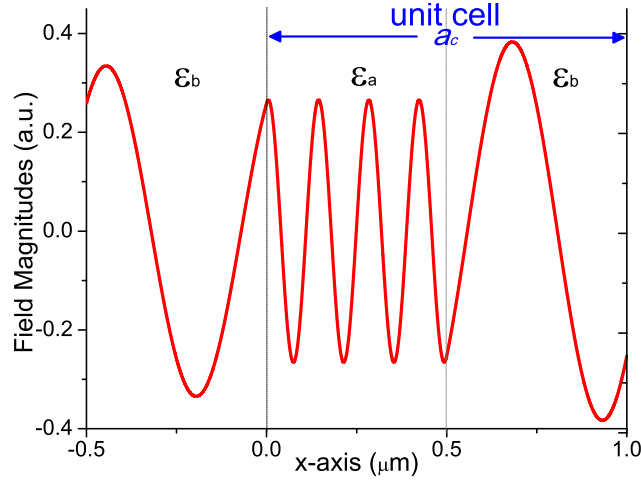


Figure 3.1: Field distribution inside a 1D periodic structure with one layer. The width of the period is 1 micron. The layer, $0.0 \leq x \leq 0.5\mu\text{m}$, with a high dielectric constant, $\epsilon_a = 12.85$, is surrounded by air with $\epsilon_b = 1$. The structure is the simplest form of waveguide that can support the localized modes of propagation. The unit cell will be taken as a super cell in the band structure analysis in Section 3.3 below.

Many of the desirable properties, including field distribution of 1D photonic crystal structures for potential applications, have been investigated using the various different solution methods [112–116]. The analytical solution is good for a simple optical structure and can be used to get the result quickly, in general, but it may not be an effective method for complex structures. Therefore, we want to develop a universal effective method of field distribution computation. One of our choices is the FDTD method because this method can be used to compute field distribution for structures of any type, which allows us to predict the behavior of electromagnetic scatterings inside the photonic crystal.

3.1 Field Distribution Computation using the FDTD Method

Our particular choice of FDTD simulation, as follow, is one of the extensively used methods for computation of the electromagnetic field distribution in optical structures. This method is based on discretization of Maxwell’s equations, meaning the computation area is discretized in terms of space and time parameters of Maxwell’s curl equations. The

fields are then defined in discrete nodes of the computation mesh. Boundary and initial conditions as well as dielectric constant, including other material parameters of interest within the computation domain, are defined as inputs for the computation.

For a procedural example here, we consider a computation domain of $1\mu\text{m}$ with discretization step $\Delta x = 0.1\mu\text{m}$ (totaling 11 nodes) in free-space and then compute the 1D field distribution of the E_z and H_y fields for five time steps in Tables 3.1-3.5, below. By

Table 3.1: Electric and magnetic fields in an array of a one-dimensional domain with 11 nodes at an arbitrary time n .

Field	Node										
	1	2	3	4	5	6	7	8	9	10	11
E_z magnitude	0	1	0	0	0	0	0	0	0	0	0
H_y magnitude	0	0	0	0	0	0	0	0	0	0	0

Table 3.2: Electric and magnetic fields in an array of a one-dimensional domain with 11 nodes after a second computation step at time $n + 1$.

Field	Node										
	1	2	3	4	5	6	7	8	9	10	11
E_z magnitude	0	0.75	0.25	0	0	0	0	0	0	0	0
H_y magnitude	0	-0.5	0	0	0	0	0	0	0	0	0

comparing the field distribution in Figure 3.2(b) with the one given in Figure 3.2(a), it is seen that the peak of the field starts to move towards the right. The electric (magnetic) field is a result of the difference between magnetic (electric) field values in the neighbouring elements, which can also be seen in Eqs. (3.1a)-(3.1b). The space is excited by a source of Dirac delta pulse of electric field with magnitude 1. For simplicity, a Dirichlet boundary condition is used in this example, but the FDTD treatments in later sections implement more accurate boundary conditions. The purpose here is to explain the FDTD field

distribution method that will be implemented in photonic crystals of electromagnetic scattering.

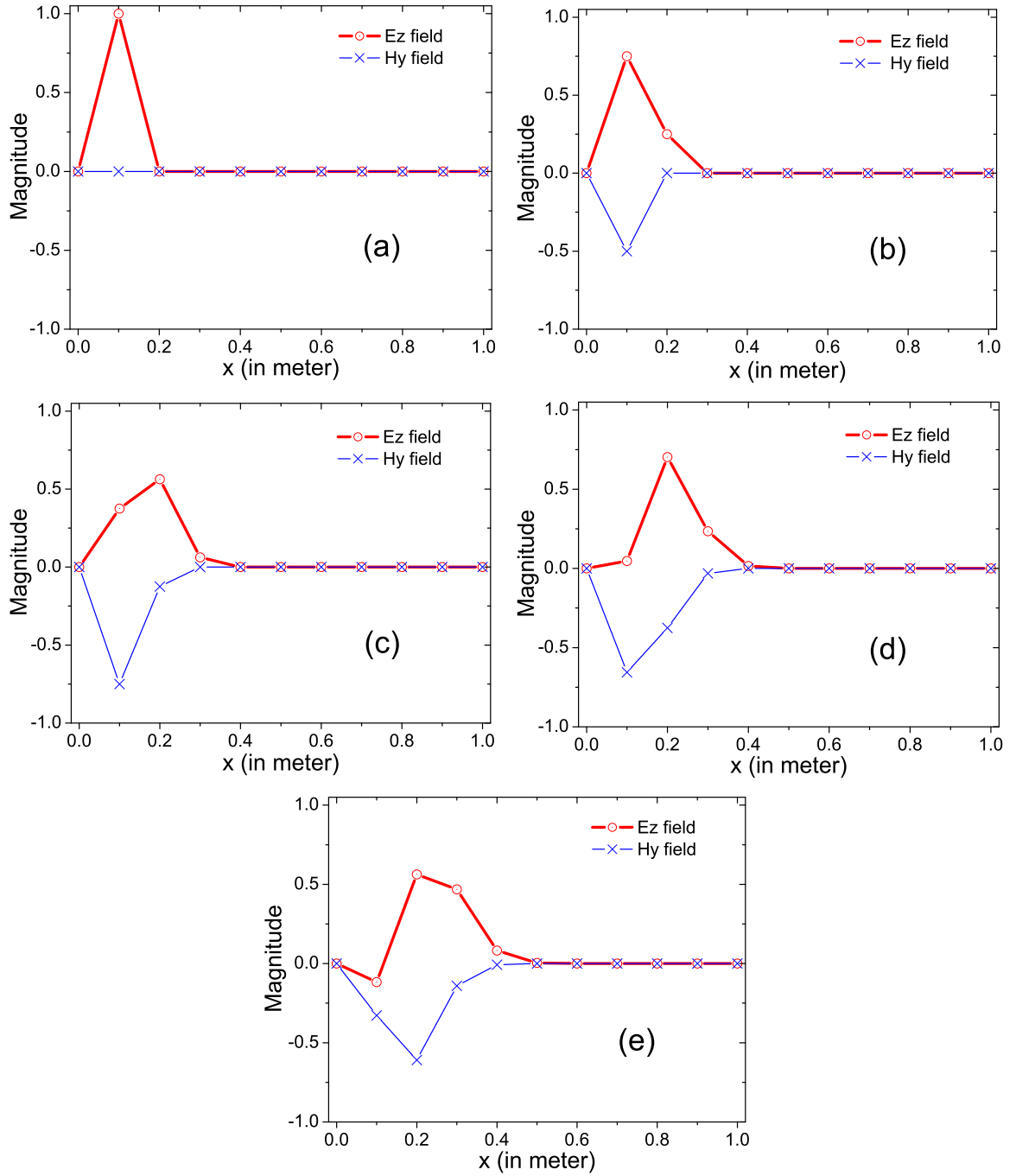


Figure 3.2: Electric and magnetic field distributions after (a) the initial step at time n , (b) the second step at time $n+1$, (c) the third step at time $n+2$, (d) the fourth step at time $n+3$, and (e) the fifth step at time $n+4$.

In order to simplify the treatment of the present problem, the E_z and H_y fields are normalized to ε_0 and μ_0 as in [95] by Sullivan and in [39] by Sukhoivanov *et al.* so that the differentials in Eq. (2.18) for the computer code take the following forms,

$$E_z(i) = E_z(i) + 0.5(H_y[i] - H_y[i-1]) \quad (3.1a)$$

$$\text{and } H_y(i) = H_y(i) + 0.5(E_z[i+1] - E_z[i]). \quad (3.1b)$$

The subscripts n , $n+1/2$, etc., for time steps are gone, because the time is implicit in the FDTD method. For computation, the initial values of the E_z and H_y fields in time step n are presented in Table 3.1, while the Figure 3.2(a) reproduces the corresponding initial field distribution. As seen in the table, one of the initial values of the E_z field is set to a Dirac delta pulse of magnitude 1 and all initial values of the H_y field are set to zero.

Table 3.3: Electric and magnetic fields in an array of a one-dimensional domain with 11 nodes after a third computation step at time $n+2$.

Field	Node										
	1	2	3	4	5	6	7	8	9	10	11
E_z magnitude	0	0.375	0.5625	0.0625	0	0	0	0	0	0	0
H_y magnitude	0	-0.75	-0.125	0	0	0	0	0	0	0	0

Table 3.4: Electric and magnetic fields in an array of a one-dimensional domain with 11 nodes after a fourth computation step at time $n+3$.

Field	Node										
	1	2	3	4	5	6	7	8	9	10	11
E_z magnitude	0	0.0469	0.7031	0.2344	0.0156	0	0	0	0	0	0
H_y magnitude	0	-0.6562	-0.375	-0.0312	0	0	0	0	0	0	0

Table 3.5: Electric and magnetic fields in an array of a one-dimensional domain with 11 nodes after a fifth computation step at time $n+4$.

Field	Node										
	1	2	3	4	5	6	7	8	9	10	11
E_z magnitude	0	-0.1172	0.5625	0.4687	0.082	0.004	0	0	0	0	0
H_y magnitude	0	-0.3282	-0.6094	-0.14	-0.0078	0	0	0	0	0	0

After the initialization of the problem, the fields are updated using Eqs. (3.1a)-(3.1b) in the next time step $n + 1$. In this case, first, Eq. (3.1b) is taken and the new H_y field is computed from previous (known) initial values of the H_y and E_z fields. Then, Eq. (3.1a) is taken and the new E_z field is computed from its previous initial value and the new values of the H_y field. The new E_z and H_y fields are now presented in Table 3.2 and their distribution is plotted in Figure 3.2(b). Notice that, in the tables, the first and last nodes are set to zero because of the Dirichlet boundary condition.

The field computation at the third, fourth, and fifth time steps is similar to the one at the second time step. Therefore, the updated field values at these time steps are presented directly in Tables 3.3 to 3.5 and the respective field distributions are shown in Figures 3.2(c) to (e). As can be seen in the plots at time sequence $(n, n + 1, \dots, n + 4)$, the pulse is reflected from the left boundary and then propagated to the right. The propagation behavior is similar to any type of wave propagating in any medium. In this example, we have used only a few nodes and few time steps for the clarity of explanation. However, standard FDTD simulation requires a large number of fine spatial nodes and time steps which will be implemented in the following treatments.

3.2 Modeling Kerr Nonlinear FDTD Modes in a 1D Photonic Crystal

Here, we continue our discussion of the field propagation by considering the polarization current in a nonlinear mediaum [117, 118]. This problem is interesting for understanding the nonlinear (impurity) modes in photonic crystal structures. Assuming the lossy, nondispersive Kerr-type nonlinear medium as formulated in Appendix B.1, we can derive a nonlinear FDTD of E_z and H_y field modes using polarization current density. For sim-

plicity, only lossless media will be treated in the simulation, which can be achieved by turning off the loss term in the algorithm.

We develop the algorithm using the two coupled equations, Faraday's law in the time domain and Ampere's law in the frequency domain, for mathematical convenience:

$$\nabla \times \vec{E} = -\mu \partial_t \vec{H} \text{ (Faraday), and } \nabla \times \vec{H} = \partial_t \vec{D} = j\omega \vec{D} \text{ (Ampere),} \quad (3.2)$$

where ω is frequency of the propagating mode. Faraday's law, as usual, results in Eq. (2.18). However, a numerical algorithm of Ampere's law, that involves $\vec{D}$, depends on the material properties of interest or the dielectric model. As we assumed in our model, Ampere's law can be written as

$$\nabla \times \vec{H} = \varepsilon_0 \varepsilon_r j\omega \vec{E}(\omega) + \frac{\sigma}{j\omega} \cdot j\omega \vec{E}(\omega) + \underbrace{j\omega \vec{P}_K^{NL}(\omega)}_{\vec{J}_K^{NL}(\omega)}. \quad (3.3a)$$

In a time domain, $\nabla \times \vec{H} = \varepsilon_0 \varepsilon_r \partial_t \vec{E}(t) + \sigma \vec{E}(t) + \vec{J}_K^{NL}(t)$ which, at time step $n+1/2$, can be written as $\nabla \times \vec{H}^{n+\frac{1}{2}} = \varepsilon_0 \varepsilon_r \partial_t E^{n+\frac{1}{2}} + \sigma E^{n+\frac{1}{2}} + J_K^{n+\frac{1}{2}}$. This implies

$$\nabla \times \vec{H}^{n+\frac{1}{2}} = \frac{\varepsilon_0 \varepsilon_r}{\Delta t} (E^{n+1} - E^n) + \frac{\sigma}{2} (E^{n+1} + E^n) + \frac{1}{2} (J_K^{n+1} + J_K^n). \quad (3.3b)$$

Now, substituting the J_K^{n+1} by using Eq. (B.5) and solving for E_z^{n+1} , we get

$$E_z^{n+1} = \gamma \left(1 - \frac{1}{2} \sigma \Delta x \lambda + 5\beta (E_z^p)^2 - 2\beta E_z^p E_z^n \right) E_z^n - 2\beta \gamma (E_z^p)^3 + \gamma \lambda \partial_x H_y^{n+\frac{1}{2}} \quad (3.4)$$

where $p = n-1$, $\lambda = \frac{\Delta t}{\varepsilon}$, $\beta = (3\alpha \chi_0^{(3)})/\varepsilon$, and $\gamma = \left(1 + \frac{1}{2} \sigma \Delta x \lambda + \beta (E_z^{n-1})^2 \right)^{-1}$, when α is a weight constant (see Appendix B.1) and $\chi_0^{(3)}$ is the nonlinear coefficient. Notice that Eq. (3.4) reduces to Eq. (2.18) for the $\sigma = 0$ and $\chi_0^{(3)} = 0$ (linear limit), which is expected in order to validate the nonlinear model for the present problem. Since only Kerr-type nonlinearity is considered in our treatment, the constant α is set equal to unity for simulation.

3.2.1 Numerical Analysis and Results

To apply the method of Kerr nonlinear FDTD, a simple case, a 1D photonic crystal formed of five periods, is considered. This structure can be achieved by repeating the unit cell, shown in Figure 3.1, for five times along the $\hat{x}$ -axis. The period has two layers composed of a lossless linear dielectric material with dielectric constants $\varepsilon_r = 9$ and $\varepsilon_r = 1$. But, by changing dielectric property of the center layer, this structure is also treated as a nonlinear waveguide comprising the linear dielectric material core with the same linear dielectric constant $\varepsilon_r = 9$, followed by a Kerr nonlinear part of the nonlinear dielectric constant containing the coefficient $\chi_0^{(3)}$ (see Eq. (B.1) in Appendix B), which is the field intensity dependent [59, 119–121].

The structure was excited using a cosine modulated Gaussian pulse $E_z(x_0, t) = E_0(x_0) \exp \left[-(t - t_c)^2 / t_w^2 \right] \cos [2\pi f_0(t - t_c)]$ where t_c is the time-delay of the Gaussian envelope function, t_w is its width, and f_0 is the modulation frequency. A particular frequency, $f_0 = 1 \times 10^{10} \text{ Hz}$, was chosen in order to provide an appropriate pulse width for structure response analysis. The pulse excitation only propagates in one direction (positive $\hat{x}$ -axis) due to the implementation of TF/SF boundary condition [94]. In addition, a differential-equation based absorbing boundary condition, e.g., Mur's ABC [94, 122], is implemented to terminate the FDTD grid at the boundary ends. Although the Mur ABC is not considered state-of-the-art, it provides a relatively simple way (much simpler compared with perfectly matched layer method [123]) to terminate the grid in the computation. Because of the boundary conditions here, the field simulates the computational domain as an infinite space. The fields are observed at ports in front and behind of the structure (five periods). The fields in the front contain the reflected field as well as the

incident field. Thus, the incident field is subtracted from this data in order to obtain just the reflected field. The fields are then analyzed by using Fourier transform technique for spectral information.

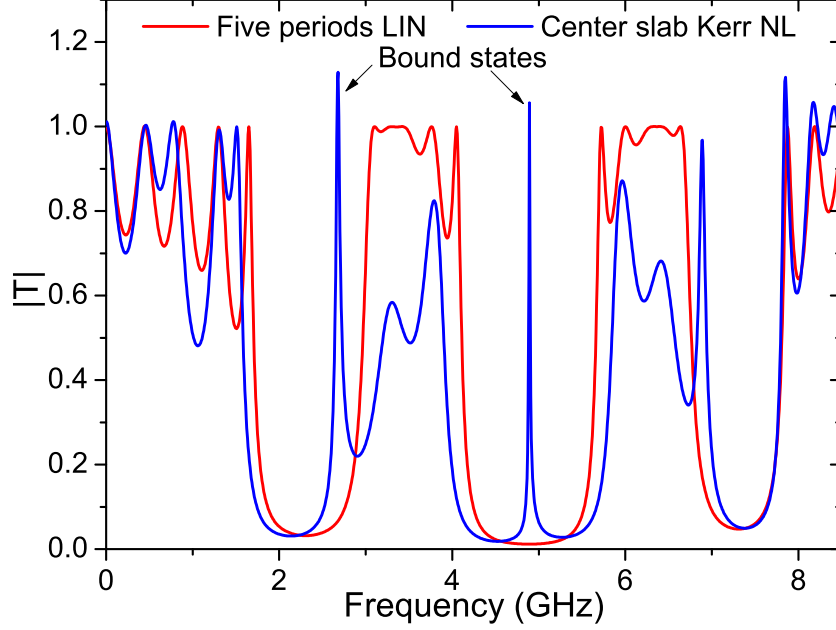


Figure 3.3: *Red curve:* Transmission spectrum of 1D photonic crystal of five periods at normal incidence. The period is formed of two layers with dielectric constants $\epsilon_r = 9$ and $\epsilon_r = 1$. *Blue curve:* Simulation of the bound modes arising from Kerr dielectric layer added at the center of the structure.

Transmission spectra reflect the band structure of the crystal, and they are often used for the design and characterization of real devices. The transmission spectra computed by using the time response FDTD fields at the ports are shown in Figure 3.3. As is seen in the figure, the transmittance is quite different at different frequencies. The result in red curve, because of the periodic lattices, exhibits a typical frequency band (stop band) of minimum transmittance falling at the frequency range 1.9 to 2.7 GHz or 4.0 to 5.5 GHz, etc. In the result of blue curve, the transmission properties of the system are altered due to the replacement of the central layer with Kerr nonlinear impurity char-

acterized by the nonlinear coefficient of the third-order susceptibility $\chi_0^{(3)} = 0.01$ (a.u.). By comparison with solution in the red curve, it can be seen that the bound modes have been created inside the band gaps of the perfectly periodic structure. As an example, a typical narrow perfect transmission peak of the bound mode can be seen to occur at around 4.9 GHz frequency in the figure. Such a modal peak can be described by its Q-factor, a measure of the width of the peak, defined as $Q = \omega_0/\Delta\omega_0$, where ω_0 is the modal frequency of the peak and $\Delta\omega_0$ is the full width half maximum (FWHM) of the peak. The Q-value of this peak is estimated to be about 1,300, which quantifies that the peak is very narrow (the value was calculated by using an example for the line shape analysis in [124]). As seen in the figure, the magnitude of the transmission coefficient for nonlinear transmission increases, which can be explained with the self-phase modulation like effect [125, 126]. The structures of bound modes can be used as the resonant cavities.

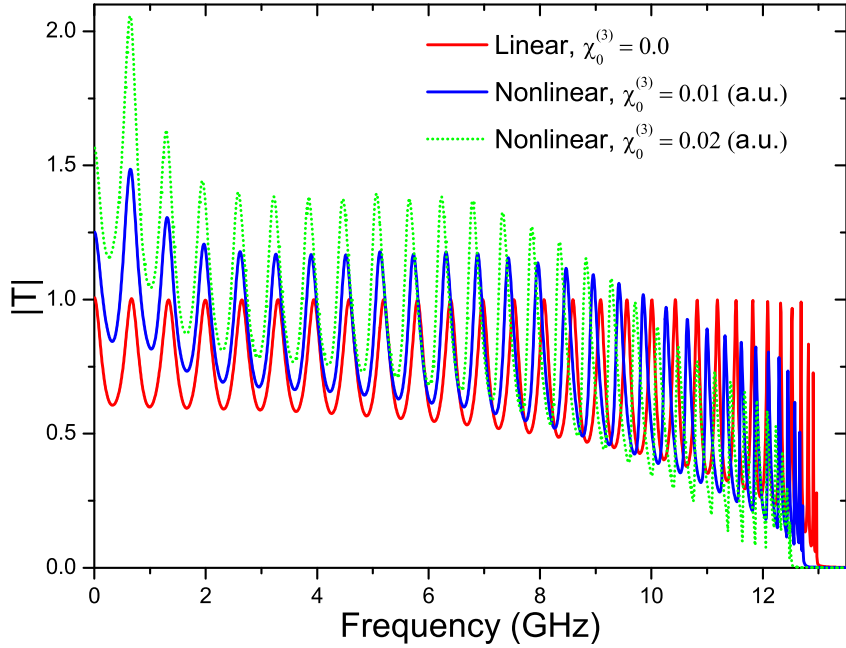


Figure 3.4: Self-phase modulation like effects of a nonlinear slab with the Kerr coefficients $\chi_0^{(3)} = 0.00$, $\chi_0^{(3)} = 0.01$ (a.u.), and $\chi_0^{(3)} = 0.02$ (a.u.).

In order to further explain the self-phase modulation effect, we studied the structure shown in Figure 3.1 by considering the slab region composed of Kerr-type nonlinear dielectrics. Figure 3.4 shows the effects as the transmission peaks vary in the curves for the $\chi_0^{(3)} = 0.01$ (a.u.) and $\chi_0^{(3)} = 0.02$ (a.u.). Such a type of nonlinear effects as the self-phase modulation is useful in the applications in which light controls light through the modulation of the Kerr dielectric constant.

3.3 Band Structure Techniques

The computation of transmittance spectra, as computed in the previous section, allows us to obtain the basic structure characteristics of a photonic crystal. The method is good for simple structures of photonic crystal; however, it cannot provide the most general idea of photonic crystal characteristics as well as effectively design photonic crystal devices. The computation of band structures allows us to extract full information of the field propagation within the specific direction inside the photonic crystal. This shows the significance of the band structure computation of photonic crystals. In this section, a general overview of the FDTD technique for band structure computation is explained briefly and the result of the computation will be compared using the PWE method. The concept of band structure can be extended to dispersion characteristics, photonic density of states maps or band gap maps, etc., which are required for design and simulation for photonic crystal devices.

The FDTD requires discretization of computational domain. But photonic crystal is an infinite structure and the computation over such infinite structure takes an infinite time period, which makes the computation impossible to complete. A solution of this situation is the consideration of unit cell and the implementation of the periodic boundary

condition (PBC) over the cell. The unit cell contains the information about the whole structure, which allows us to consider the single unit cell as the computational domain. The PBC essentially translates the phase of the source radiation from one side of the unit cell to another. This boundary condition also allows computation of the field distribution with different wave vectors. We assume the computation time to be infinite in order to achieve accuracy of the method. Since we have limited computer resources, the computation time is taken to be finite but parameterized with significantly large number.

For the simplicity of presenting the concept of photonic band structure, we consider the unit cell for the 1D case, above, in which $d = 0.3a_c$, d is *GaAs* layer width and a_c is the lattice constant or the cell size. A detailed mathematical background of this consideration is found in [127]. The unit cell here becomes a super cell due to the periodic boundary condition. The pulse or time response of the structure is obtained through computation of the field distribution. The fields are then analyzed by employing the Fourier transform that gives the response spectrum or eigen-states of the photonic crystal under our investigation. Eigen-states of the photonic crystal correspond to local maxima of the spectrum since the eigen-state is the resonant frequency of the structure. The spectrum is scanned and local maxima are found for each value of the wave vector. Since the eigen-states are found for different wave vectors, we obtain the band structure of the system. Note that, for each wave vector, there are more than one local maxima (spurious data are ignored) which give rise to the band frequencies at different states.

The FDTD band result (blue scatter plots) is shown in Figure 3.5, and it is compared with the PWE result (red curve plots) [28] computed using the sum of 99 plane waves in Eq. (2.14) as the initial condition. All other parameters for the unit cell are

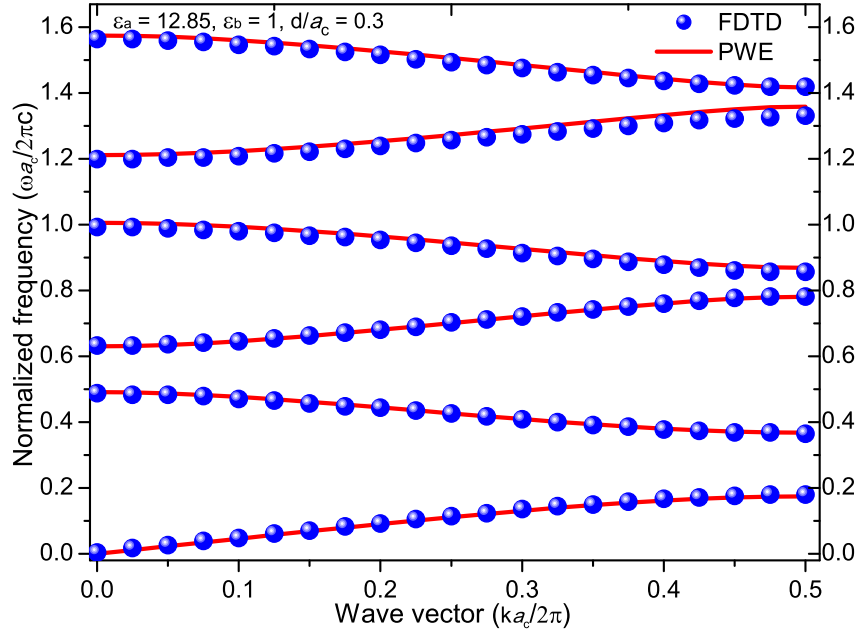


Figure 3.5: Band structure of 1D photonic crystal using a unit cell consisting of GaAs ($\epsilon_a = 12.85$) and air ($\epsilon_b = 1$). The solutions for solid blue scatter plots are due to the FDTD results, and those for solid red curve plots are due to the PWE results.

taken exactly the same as used in the FDTD result. The results of both methods agree at least in the lower frequencies. As can be seen in the result, the k -vectors are sampled uniformly along the edge of the irreducible Brillouin zone, and the bands are found open along certain frequency ranges. For example, with this calculation, as seen in the result, above, the first stop band falls in the range $0.17 - 0.37$.

Figure 3.6 shows the impurity bands arising from defect/impurity dielectric layer of thickness $0.4a_c$ and dielectric constant $\epsilon_{im} = 13$, as they are introduced into the unit cell. The impurity caused the average dielectric constant to increase. Thus, the resulting impurity bands (red curve plots) dropped into the stop band and created the donor like impurity bands as we predicted using the solid-state theoretical approach.

In Figure 3.7 the frequencies of various impurity modes are plotted as a function of the impurity dielectric constant. We created the modal region by adding a layer at the

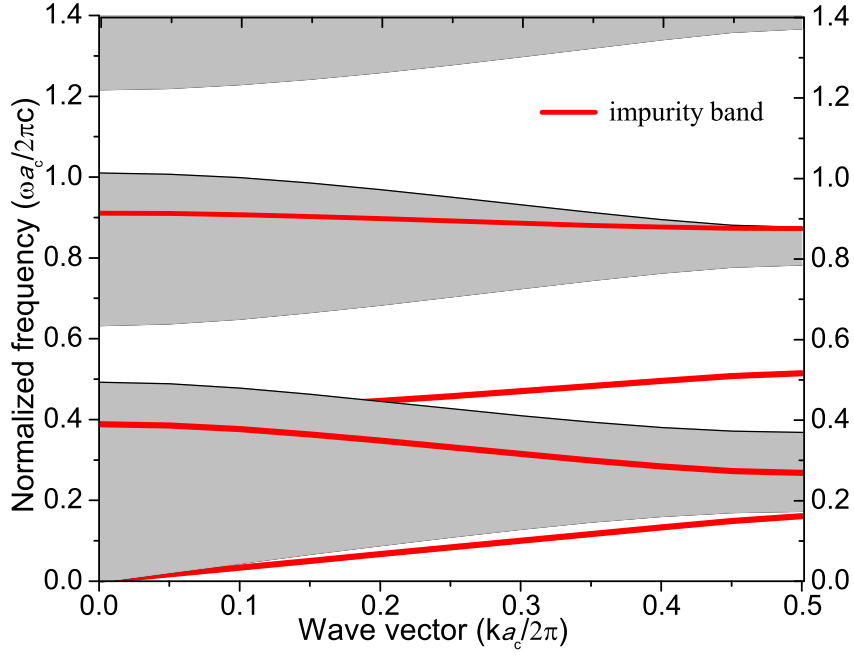


Figure 3.6: Impurity bands (solid red curves) with respect to the bands computed in the previous results in Figure 3.5, above. The impurity bands arise from inserting impurity dielectric layer at the center of the unit cell. The thickness and dielectric constant for the impurity were $0.4a_c$ and $\varepsilon_{im} = 13$.

center of the unit cell with a material with a dielectric constant ε_{im} , as shown in the inset. In this case, the Fourier transform scans the impurity frequencies and reconstructs the impurity modes from the corresponding eigen-vectors. In the figure, the frequency modes calculated from FDTD are compared with corresponding calculations using PWE super-cell calculations [28, 33]. Notice that the first stop band gap was at around frequency 0.17 to 0.37. From the plot it shows that the bigger the impurity dielectric constant the greater quantity of defect modes occurred.

The impurity frequency mode analysis, as shown in Figure 3.7, allows us to determine the characteristics for a particular resonant (or cavity) mode with frequency ω in a resonator (or cavity) created by the impurity ε_{im} . As an example, based on the results in this figure, the field distribution for the cavity mode with frequency $\omega = 0.4 \times 2\pi c/a_c$

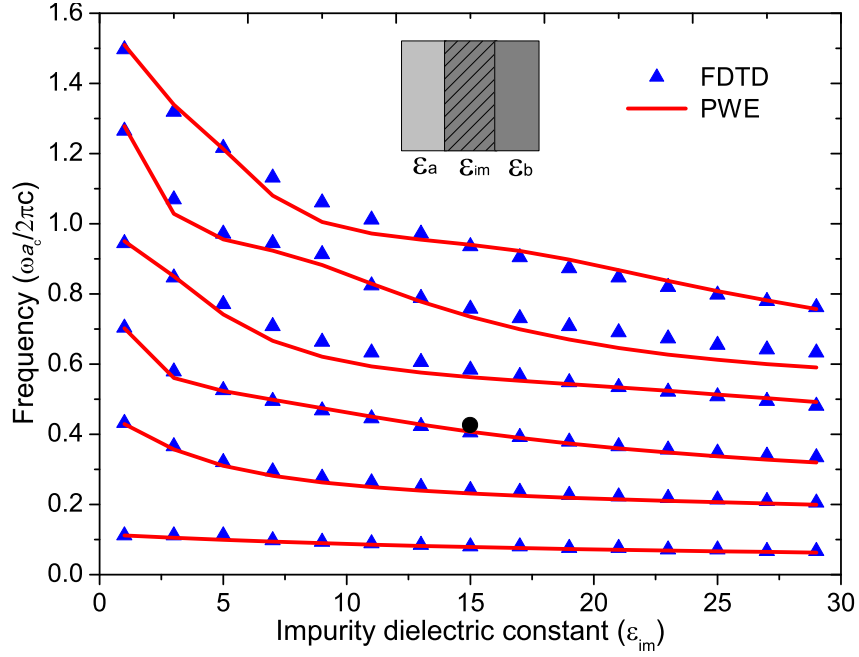


Figure 3.7: Impurity frequency modes associated with a dielectric impurity in 1D photonic crystal structure. The frequencies changed as the values of the impurity dielectric constant (ϵ_{im}) were changed. Inset shows an impurity layer of thickness $0.4a_c$ inserted at the center of the unit cell. All other parameters of the underlying photonic crystal are the same as in Figure 3.5. The particular wave vector taken for this result is $k = (0.5)\pi/a_c$.

(see black circle on the plot) can be excited by creating the resonator with an impurity dielectric constant $\epsilon_{im} = 15$. Also, it is found that the impurity frequency sweeps continuously across the stop band as the ϵ_{im} is varied. That means we can tune the impurity frequency or resonant frequency to any value within the stop band with a judicious choice of ϵ_{im} , which is an important feature of the photonic crystals.

3.4 Simulation of Impurity Structures in 2D Photonic Crystals

We design impurity structures in a photonic crystal system originally proposed by McCall *et al.* [55]. Line of single site impurities forms a photonic crystal waveguide, and only a single site impurity forms a photonic crystal microcavity. These structures are of great interest because of their applications as components of an integrated optical circuit [128].

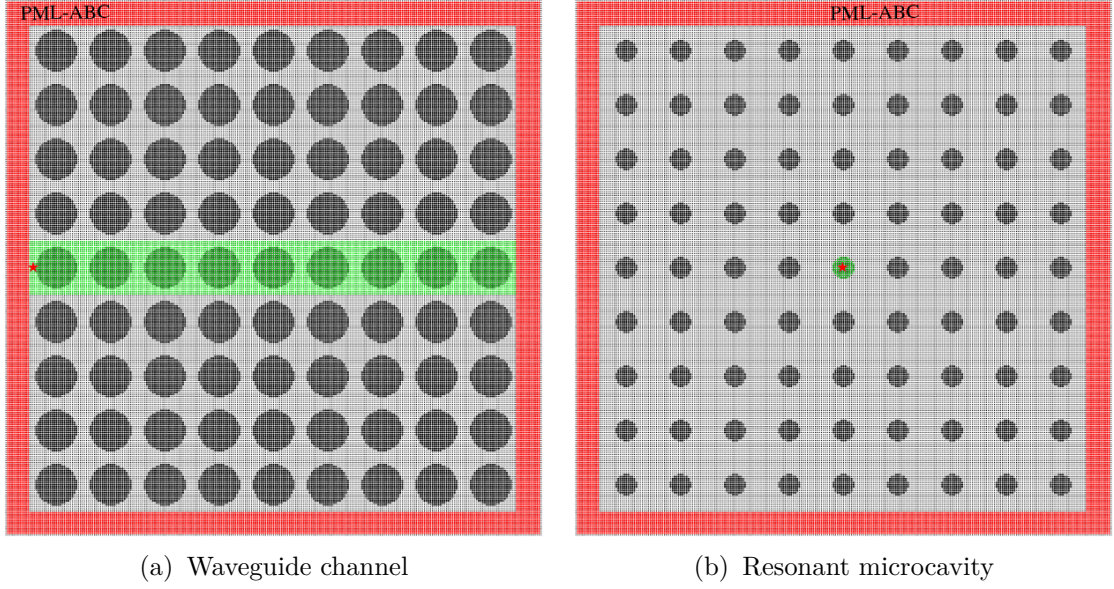


Figure 3.8: Geometrical setup for calculation of the confined modes in photonic crystal (a) waveguide channel (green area) and (b) resonant microcavity (green cylinder), both using the FDTD simulation grids of size 267×267 . Each grid point is represented by small cross or small solid circle that are also illustrated in magnification in Figure 3.9 for visualization ease. The red areas represent the PML boundaries, and the stars indicate the source locations. On both geometries the lattice constant is the same, i.e., $a_c = 1.27\text{cm}$, but the radii of cylinders are taken as $R = 0.48\text{cm}$ in (a) and $R = 0.24\text{cm}$ in (b).

Figures 3.8(a) and (b) display the linear and single site impurities introduced into the period lattice of a 2D photonic crystal containing dielectric cylinders at the lattice sites [129]. Actually, the linear impurity (waveguide channel in (a)) and the single site impurity (microcavity in (b)) were created by removing the cylinders, as indicated by the green area of the 2D lattice in each part of the figure. We developed PostScript commands with “% !PS” [130, 131] for this figure in order to convey information about an FDTD simulation where the fields are described on every grid point. Figure 3.9 is a magnified corner section of a dielectric cylinder from Figure 3.8(b). In this figure, each point is designated by either a gray cross or dark dot, which represent the FDTD fields.

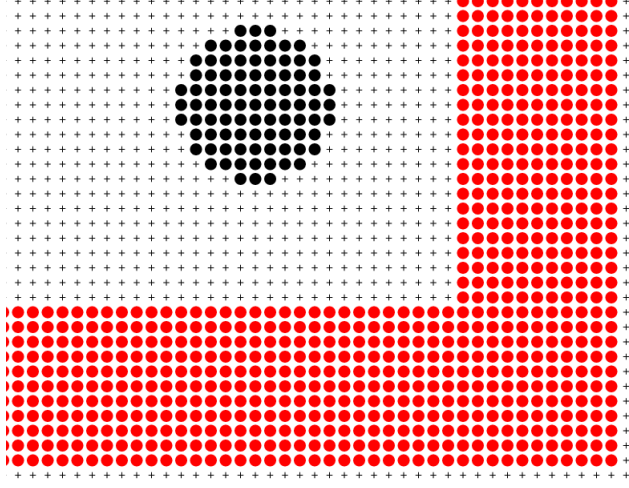


Figure 3.9: Enlarged version of small crosses and dots in a magnified section of the right-bottom corner of Figure 3.8(b). Each small gray cross or dark solid dot represents a computational node or grid of the fields. The circular region formed by the solid black dots represents a dielectric cylinder of the photonic crystal.

Maxwell's equations for the fields, for instance, the $E_z(x, y)$, $H_x(x, y)$, and $H_y(x, y)$ fields can be reduced to the 2D FDTD algorithms by implementing differentials $\partial_x \neq 0$, $\partial_y \neq 0$, and $\partial_z = 0$ in Eqs. (2.16a) and (2.16b). The algorithms then propagate the fields on each grid point in Figure 3.8. The working FDTD algorithms derived from differential implementations are shown in Appendix B.3 or the similar algorithms can be found in [93, 94, 99, 100]. The other references used for developing our FDTD programming codes are found in [129, 132–136]. In order to accurately simulate the structures, the PML boundary, including fine discretization of the computational mesh, small time step with long period of simulation, proper excitation source, etc., are all considered carefully in the following results.

The fields are simulated along the waveguide channel of about 11.43cm length in which the simulation parameters are chosen for all the analyses to be $\Delta x = \Delta y = 0.047\text{cm}$ (spatial discretization), $\Delta t = 1.1\text{ps}$ (time step), and $\varepsilon = 9$ including the source excitation

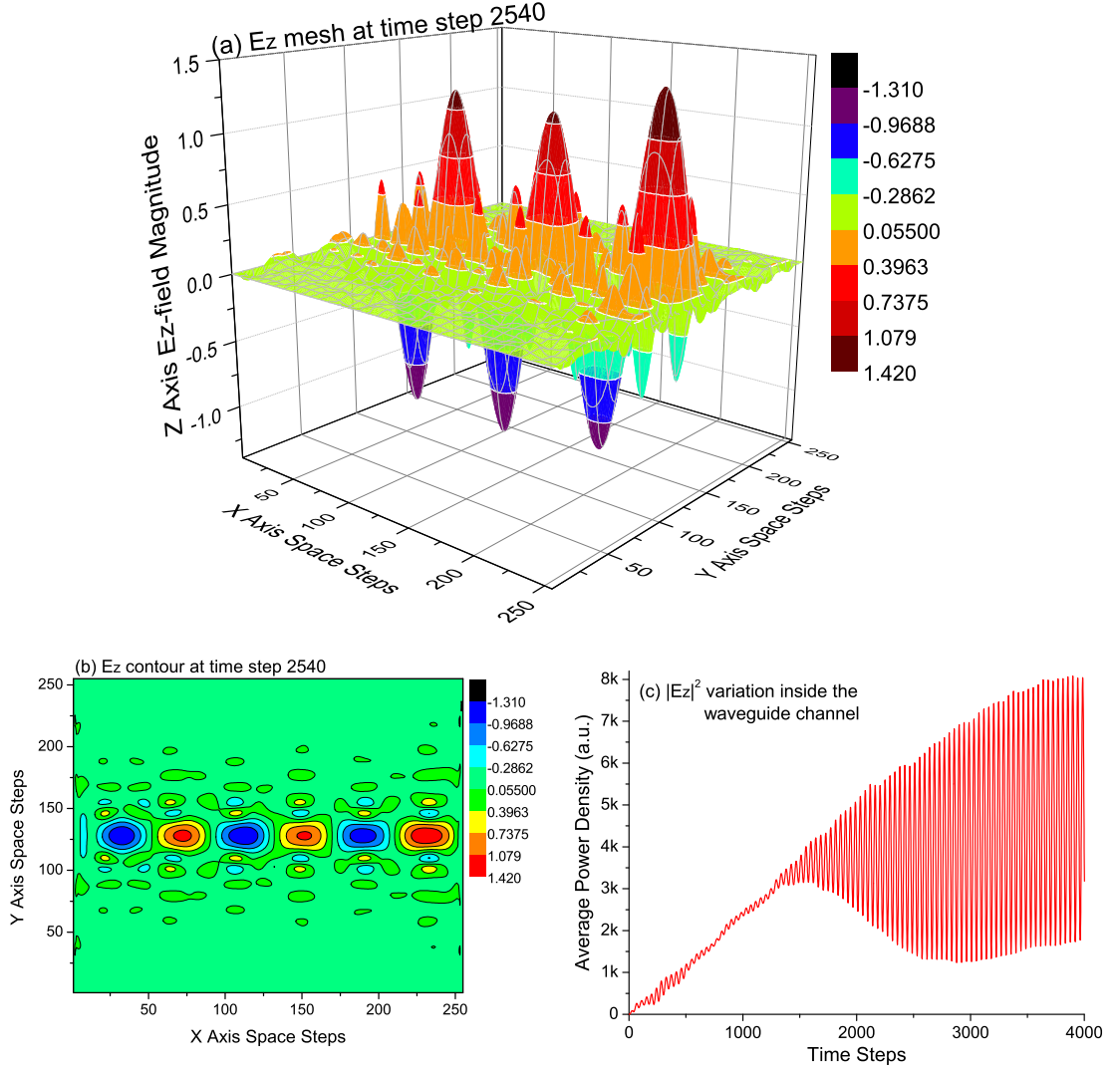


Figure 3.10: E_z component of the planewave modes localized along the waveguide channel. (a) Mesh representation of the E_z field mode, (b) Contour representation of the E_z field mode, and (c) Average power density variation inside the waveguide channel. Note: 1 space step = 0.047cm, 1 time step = 1.1ns.

at frequency $\omega a_c / 2\pi c = 0.440$. The dielectric loss of the cylinders of photonic crystal was neglected. Details about these parameters and the source codes for the simulation are shown in Appendix C.1. Figure 3.10 shows mesh and contour plots for the $E_z(x, y)$ field component of the propagating waveguide mode at the time 3.8ns (or equivalently time step 2540). As seen in the detailed results, the moving waveguide mode appears as strong

red and blue peaks (on the plot (a)), which are also visualized as red and blue contours (on the plot (b)) along the waveguide channel. The power flow estimated using the Poynting vector for a plane wave inside the waveguide region is shown in the plot (c). The power remains stable and oscillates strongly because of the confinement of the mode within the waveguide channel. The Poynting method for the power flow estimation here can be applied in the analysis of the power transmission and cross talk in a DEMUX/MUX device.

Figure 3.11 shows implementation of color/contour maps for all three components of cavity-like modes at time 2.0ns (time step 1860) found in a design of the microcavity

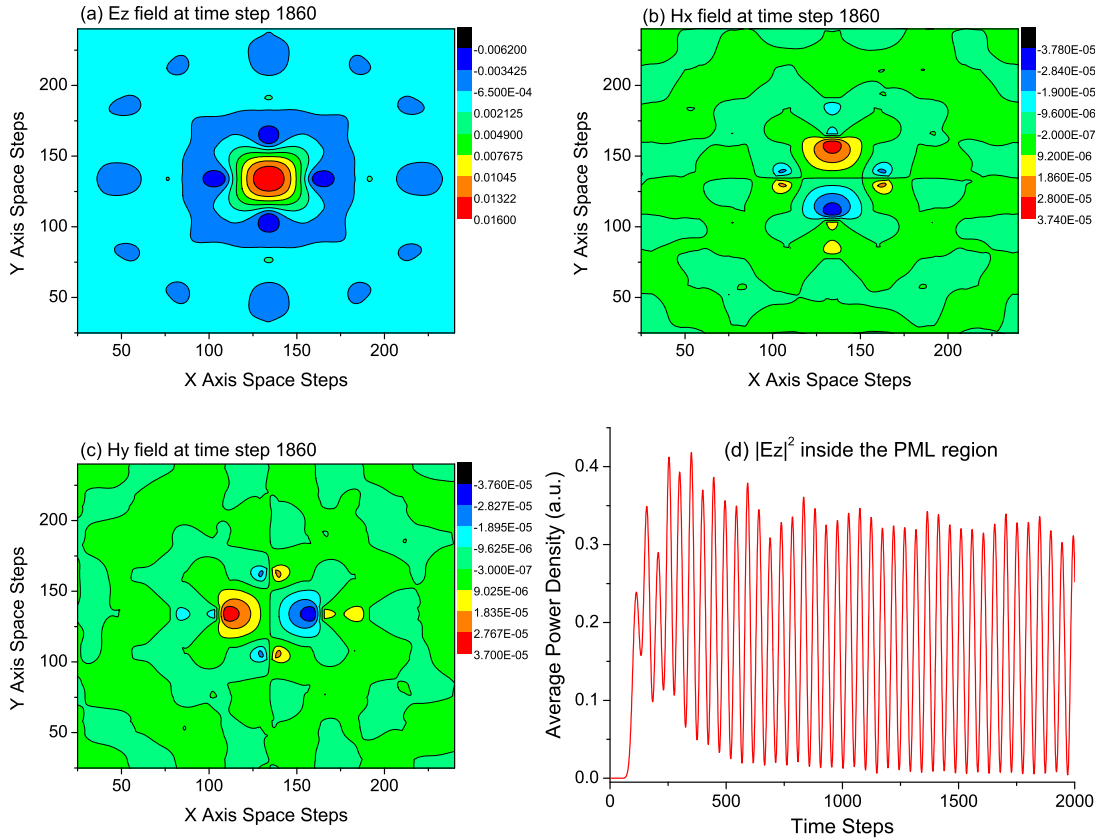


Figure 3.11: TMz components of the resonantly excited Gaussian pulse modes confined about the single site impurity or microcavity. (a) E_z field mode, (b) H_x field mode, and (c) H_y field mode at time step 1860. (d) The power variation inside the PML boundary.

in Figure 3.8(b). In this case, a Gaussian pulse source with pulse width 30ps was excited at the center of the cavity. The other computational parameters were taken the same as in the case of waveguide except the radius of the cylinders of photonic crystal was reduced to half. Consequently, the resonantly excited cavity modes are supported by the impurity or defect of the microcavity. As seen in the plots (a)-(c), the E_z field mode exhibits rotational symmetry, H_x exhibits odd symmetry about the x -axis, and H_y exhibits odd symmetry about the y -axis with respect to the point of source excitation. The symmetry is important because the coupling between resonant mode of an optical cavity and localizing mode in a waveguide depends on types of the modal symmetries. It is possible that a mode of one symmetry will not couple at all to a waveguide or an excitation with a different symmetry [81]. The power confined inside the PML boundary as a function of time step is shown on the plot (d). As is clearly seen in Figures 3.10 and 3.11, the field amplitudes are confined to the region of single site impurities due to the presence of stop band introduced by the surrounding periodic lattices.

The physical system and computation process shown for the results in this chapter are fairly simple. However, they may have a wide range of applications. Using the FDTD in photonic crystal, it is possible to design different passive optical devices such as high-efficiency reflectors, anti reflection films, distributed Bragg reflectors for vertical-cavity surface-emitting lasers [137, 138], wavelength division mux/demux on the basis of fiber gratings, mirrors of tunable lasers, etc. The main advantage of this approach is that it allows us to consider dispersions, nonlinearities, and losses that can not be ignored when modeling the active devices, e.g., laser resonators. Additionally, our approach can be extended to investigate Debye, Lorentz, and Drude models of material by using the

auxiliary differential equation method of FDTD [94, 95, 139]. Some disadvantages of the FDTD method are the spurious solutions and very large computation time.

The FDTD technique is a general purpose method. Although this technique has been used overwhelmingly for theoretical investigations of impurities in the photonic crystals, it cannot provide all information about the underlying impurities, which may limit us in gaining physical insight into the impurity modes of the structures. Thus, the focus on the following chapters will remain suggesting a novel approach, based on Difference Equation Waveguide, for describing many of the properties of the photonic crystal waveguide modes.

CHAPTER IV

Difference Equation Method for Waveguide Modes

Difference equation formalism for waveguide modes is reviewed by considering a 2D photonic crystal formed of identical dielectric cylinders embedded in vacuum and aligned parallel to the z -axis (Figure 4.1). The dielectric cylinders are characterized by a dielectric constant ε relative to air. The position vectors in the x - y plane (i.e., the real-space two-dimensional Bravais lattice) are represented by $\vec{r}_{\parallel} = x\hat{i} + y\hat{j}$ [32, 140]. With this, we

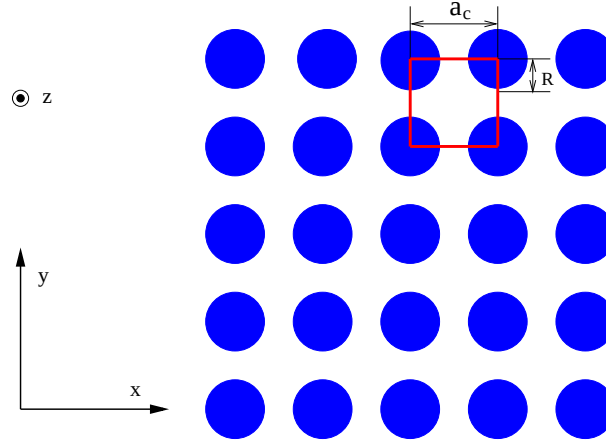


Figure 4.1: Schematic drawing of 2D photonic crystal square lattice of infinitely long dielectric cylinders in the x - y plane of real space. The solid blue circles represent the top view of the cylinders at the square crystal lattice sites with lattice constant a_c . The cylinders are arranged parallel to the z -direction, and each cylinder has radius R .

now define the periodic dielectric constant of the 2D photonic crystal as

$$\varepsilon(\vec{r}_{\parallel}) = \begin{cases} \varepsilon, & |\vec{r}_{\parallel} - \vec{T}| \leq R < a_c/2 \\ 1, & \text{otherwise (vacuum)} \end{cases} \quad (4.1)$$

where $\vec{T} = s_1\vec{a}_1 + s_2\vec{a}_2$ are the lattice translation vectors that are generated by primitive lattice vectors $\vec{a}_1 = (a_c, 0)$ and $\vec{a}_2 = (0, a_c)$ for integers s_1 and s_2 , and a_c is the lattice

constant of the square lattice of photonic crystal shown in Figure 4.1. The integers s_1 and s_2 define the direction of a waveguide channel in the two-dimensional photonic crystal. For example, $s_2 = 0$ describes a row of cylinders on the x -axis.

A waveguide is formed in the 2D photonic crystal of Eq. (4.1) by adding impurity dielectric materials to a row of cylinders in the $[1,0]$ direction or to a column in the $[0,1]$ direction of the square lattice. A waveguide can also be achieved by replacing a row or column of the cylinders with cylinders containing impurity dielectric media. Such a row of replacement cylinders form a directed path of light called the waveguide channel, and the light passing down the channel at stop band frequency constitutes the guided mode.

The waveguide may have different lengths, for example, infinite or finite, depending on how many dielectric cylinders in a row of the photonic crystal lattice are replaced by impurity dielectric cylinders. In an infinitely long waveguide, an infinite number of sites in a row of the photonic crystal lattice are replaced by impurity cylinders. In other words, such a waveguide is formed with impurity cylinders at $\{(nt_1a_c, nt_2a_c)\}$, where t_1 and t_2 are fixed integers and n runs over all integers from $-\infty$ to $+\infty$. In a finite-length waveguide, a finite number of cylinders in a row of the photonic crystal lattice are replaced by impurity cylinders at $\{(nt_1a_c, nt_2a_c)\}$, where t_1 and t_2 are fixed integers again and $n = 0, 1, 2, \dots, m$ with m an integer.

In order to model a waveguide, the dielectric constants of the row of cylinders forming the waveguide channel needs to be specified. The dielectric function of the waveguide channel, $\varepsilon_T(\vec{r}_{\parallel})$, can be written as $\varepsilon_T(\vec{r}_{\parallel}) = \varepsilon(\vec{r}_{\parallel}) + \delta\varepsilon(\vec{r}_{\parallel})$ where the $\varepsilon(\vec{r}_{\parallel})$ is given in Eq. (4.1) and $\delta\varepsilon(\vec{r}_{\parallel})$ is the change in dielectric constant of the waveguide channel sites from the photonic crystal. Therefore, the dielectric constant of the 2D photonic crystal

waveguide system of interest can be expressed as

$$\varepsilon_T(\vec{r}_{\parallel}) = \varepsilon(r_{\parallel}) + \delta\varepsilon(\vec{r}_{\parallel}), \quad (4.2)$$

where we will treat a particular type of impurity obtained by changing the waveguide channel cylinders by

$$\delta\varepsilon(\vec{r}_{\parallel}) = \begin{cases} \delta\varepsilon, & |x - nt_1a_c|, \text{ or } |y - nt_2a_c| \leq \tau, \text{ for } \{n\} \text{ integers} \\ 0, & \text{otherwise (i.e., absence of dielectric impurities),} \end{cases} \quad (4.3)$$

where $2\tau (<< R)$ is the length of a side of one of the single-site impurity medium, and $\{n\}$ is the range of the consecutive integers describing the length of waveguide segment [57, 58, 106]. This gives a small change in dielectric along the axis of each cylinder of the waveguide channel.

4.1 Green's Function Theory for Impurity Modes

The modes in the 2D photonic crystal and waveguide are described in classical electromagnetic theory by the Helmholtz equation

$$\left[\nabla^2 + \varepsilon_T(\vec{r}_{\parallel}) \frac{\omega^2}{c^2} \right] \vec{E}(\vec{r}_{\parallel}, \omega) = 0 \quad (4.4)$$

where $\nabla^2 = \partial_x^2 + \partial_y^2$ is the 2D Laplacian. Substituting the dielectric function (4.2) into Helmholtz Eq. (4.4) results in a inhomogeneous Helmholtz equation:

$$\left[\nabla^2 + \varepsilon(\vec{r}_{\parallel}) \frac{\omega^2}{c^2} \right] \vec{E}(\vec{r}_{\parallel}, \omega) = -\delta\varepsilon(\vec{r}_{\parallel}) \frac{\omega^2}{c^2} \vec{E}(\vec{r}_{\parallel}, \omega). \quad (4.5)$$

Such an equation is generally solved using the Green's function method. Denoting the Green's function of Eq. (4.5) by $G(\vec{r}_{\parallel}, \vec{r}'_{\parallel})$, we study

$$\left[\nabla^2 + \varepsilon(\vec{r}_{\parallel}) \frac{\omega^2}{c^2} \right] G(\vec{r}_{\parallel}, \vec{r}'_{\parallel}) = \delta(\vec{r}_{\parallel} - \vec{r}'_{\parallel}) \quad (4.6)$$

where $\delta(\vec{r}_{\parallel} - \vec{r}'_{\parallel})$ is the delta function of the problem.

In the Green's function method, we transform Eq. (4.5) into an equivalent integral equation [141, 142]. Then, the formal solution of Eq. (4.5) is given by

$$E(\vec{r}_{\parallel}, \omega) = \int_{all\ sites} d^2 r'_{\parallel} G(\vec{r}_{\parallel}, \vec{r}'_{\parallel} | \omega) \delta\epsilon(\vec{r}'_{\parallel}) \frac{\omega^2}{c^2} E(\vec{r}'_{\parallel}, \omega). \quad (4.7)$$

In this, the Green's function $G(\vec{r}_{\parallel}, \vec{r}'_{\parallel})$ can be expressed in terms of the eigenvalues and eigenfunctions of Eq. (4.4) as

$$G(\vec{r}_{\parallel}, \vec{r}'_{\parallel}) = \sum_n \int_{BZ} d^2 k_{\parallel} \psi_{n\vec{k}_{\parallel}}^*(\vec{r}_{\parallel}) \frac{\lambda_n(\vec{k}_{\parallel})}{\lambda_n(\vec{k}_{\parallel}) - \frac{\omega^2}{c^2}} \psi_{n\vec{k}_{\parallel}}(\vec{r}'_{\parallel}), \quad (4.8)$$

where $\{\lambda_n(\vec{k}_{\parallel})\}$ and $\{\psi_{n\vec{k}_{\parallel}}(\vec{r}_{\parallel})\}$, respectively, represent the eigenvalues and eigenfunctions of Eq. (4.5) [34]. Eq. (4.7) gives all of the modes of the photonic crystal and, in particular, the waveguide modes for ω in the stop gap of the photonic crystal.

4.2 Impurity Modes via Difference Equations

An appropriate geometrical consideration is necessary to discretize the integral equation derived in Eqs. (4.7) and (4.8). For this, the square cross-sectional area (area = $4\tau^2 \ll \pi R^2$) of the impurity material in each dielectric cylinder in the x - y plane of photonic crystal forming the waveguide is assumed to be small enough so that the field, $E(\vec{r}_{\parallel}, \omega)$, varies slowly over $\delta\epsilon(\vec{r}_{\parallel})$ at each impurity site; therefore, the electromagnetic field now can be considered as constant over the small area of impurity material at each cylinder and taken outside the integral [37, 69, 75, 106]. This criteria allows us to reduce the integral form of the waveguide equation into a difference (or discrete) equation. This is done by evaluating $E(\vec{r}_{\parallel}, \omega)$ on the left hand side of Eq. (4.7) at the centers of the cylinders forming the waveguide channel in the crystal lattice. The same is done for the $E(\vec{r}'_{\parallel}, \omega)$ on the right hand side of Eq. (4.7).

To obtain a discrete waveguide mode from Eq. (4.3) and Eq. (4.7), the field in the impurity material (at the center of the impurity material) is denoted by E_{nt_1,nt_2} , $E_{nt_1,nt_2} = E[n(t_1\hat{i} + t_2\hat{j}), \omega]$, with t_1 and t_2 are fixed integers and $n = 0, 1, 2, \dots, m$ with m an integer. The resulting difference equation for the modes becomes

$$E_{nt_1,nt_2} = \sum_m B_{nt_1,nt_2;mt_1,mt_2} \delta\varepsilon(m(t_1\hat{i} + t_2\hat{j})a_c) E_{mt_1,mt_2}, \quad (4.9)$$

where the factor $B_{nt_1,nt_2;mt_1,mt_2}$ is described in terms of Green's function as

$$B_{nt_1,nt_2;mt_1,mt_2} = \frac{\omega^2}{c^2} \int_{(mt_1,mt_2)^{thimpurity}} d^2r_{\parallel} G[n(t_1\hat{i} + t_2\hat{j})a_c, \vec{r}_{\parallel} | \omega]. \quad (4.10)$$

The new integer m introduced in Eq. (4.9) or (4.10) runs over the integers denoting the waveguide channel sites, and ω is the frequency of the impurity mode that will be chosen to be within a stop band of the photonic crystal described by Eq. (4.1). Then, the bound fields about the impurity cylinders in the waveguide channel can be written by using Eqs. (4.9) or (4.10):

$$E_{nt_1,nt_2} = \delta\varepsilon \sum_{(mt_1,mt_2)^{thimpurity}} B_{nt_1,nt_2;mt_1,mt_2} E_{mt_1,mt_2}, \quad (4.11)$$

where $\delta\varepsilon(\vec{r}_{\parallel})$ characterizes the linear and/or nonlinear response to the fields.

Our interest in this dissertation is on Kerr nonlinear impurity media with a dielectric constant of the form: $\varepsilon_T = \varepsilon_0 + \delta\varepsilon_0(1 + \lambda|E|^2)$. Here E is the electric field at the site of the impurity and λ is a constant called Kerr nonlinearity parameter. Using this type of change in the dielectric constant in Eq. (4.2) leads to

$$\varepsilon_T(\vec{r}_{\parallel}) = \varepsilon(\vec{r}_{\parallel}) + \delta\varepsilon_0(\vec{r}_{\parallel})(1 + \lambda|E|^2), \quad (4.12)$$

which describes the total dielectric constant for Kerr nonlinear media at the relevant lattice sites of the photonic crystal. The general form of the change in the dielectric

constant for the difference equation can now be expressed as

$$\delta\varepsilon[m(t_1\hat{i} + t_2\hat{j})a_c] = \delta\varepsilon_0(1 + \lambda|E_{mt_1,mt_2}|^2) \quad (4.13)$$

where $\delta\varepsilon_0$ is independent of the sites [11]. Here, the dielectric property of the Kerr impurity media depends on the intensity of the applied electric field.

Substituting Eq. (4.13) into Eq. (4.11) results in a waveguide mode equation in the form of a recursion relation that can be written as

$$E_{nt_1,nt_2} = \delta\varepsilon_0 \sum_m B_{nt_1,nt_2;mt_1,mt_2} (1 + \lambda|E_{mt_1,mt_2}|^2) E_{mt_1,mt_2}. \quad (4.14)$$

Considering only the same site and nearest neighbor site couplings in the system, the equation further reduces to

$$\begin{aligned} E_{nt_1,nt_2} = \delta\varepsilon_0 & [\alpha E_{nt_1,nt_2} + \beta(E_{(n+1)t_1,(n+1)t_2} + E_{(n-1)t_1,(n-1)t_2}) \\ & + \beta_0 E_{nt_1,nt_2}^3 + \beta_1(E_{(n+1)t_1,(n+1)t_2}^3 + E_{(n-1)t_1,(n-1)t_2}^3)], \end{aligned} \quad (4.15)$$

where

$$\begin{cases} \gamma = 4\tau^2 \delta\varepsilon_0, & \alpha = B_{nt_1,nt_2;nt_1,nt_2}/4\tau^2, & \beta = B_{nt_1,nt_2;(n+1)t_1,(n+1)t_2}/4\tau^2, \\ \beta_0 = \lambda\alpha, & \text{and} & \beta_1 = \lambda\beta. \end{cases} \quad (4.16)$$

Here, the γ , α , and β are generally described in integral form as

$$\begin{cases} \gamma = \int d^2r_{\parallel} \delta\varepsilon(\vec{r}_{\parallel}), & \text{but the small area} = \int d^2r_{\parallel} = 4\tau^2, \\ \alpha = \frac{\omega^2}{c^2} \int d^2r_{\parallel} G(0, \vec{r}_{\parallel}|\omega) \delta\varepsilon(\vec{r}_{\parallel}) / \gamma, & \text{onsite coupling, and} \\ \beta = \frac{\omega^2}{c^2} \int d^2r_{\parallel} G[(t_1\hat{i} + t_2\hat{j})a_c, \vec{r}_{\parallel}|\omega] \delta\varepsilon(\vec{r}_{\parallel}) / \gamma, & \text{nearest-neighbor coupling,} \end{cases} \quad (4.17)$$

where the integrals are taken over a primitive lattice cell of the waveguide structure formed in the photonic crystal and a_c is the lattice constant of the waveguide structure.

Notice that Eq. (4.10) is substituted in Eq. (4.16) in order to describe the γ , α , and β in the integral forms as shown in Eq. (4.17). As seen in the equation, the α and β are

related to the Green's function (G), eigenvalue $\left(\frac{\omega^2}{c^2}\right)$, and the dielectric change ($\delta\epsilon$) of the non-homogeneous Helmholtz Eq. (4.5).

Now, in order to express the difference Eq. (4.15) to a simple linear form, we may set the nonlinear coupling terms to zero such that $\beta_0 = 0$ and $\beta_1 = 0$. This results in a generalized difference equation for the waveguide mode in the linear media:

$$E_{nt_1,nt_2} = \gamma \left[\alpha E_{nt_1,nt_2} + \beta (E_{(n+1)t_1,(n+1)t_2} + E_{(n-1)t_1,(n-1)t_2}) \right]. \quad (4.18)$$

Since $\beta_0 = \lambda\alpha$ and $\beta_1 = \lambda\beta$ as described in Eq. (4.16), the nonlinear form of the differential shown in Eq. (4.15) can be recovered by introducing the Kerr factor of the form $(1 + \lambda|E|^2)$ into the linear differential Eq. (4.18). By changing suffix notations this equation can be reduced to a familiar form as

$$E_{n,m} = \gamma [\alpha E_{n,m} + \beta (E_{n+1,m+1} + E_{n-1,m-1})], \quad (4.19)$$

where n, m are integers. Essentially, this algorithm forms recursively defined sequences (a recursion relation similar to the form of difference equations in linear algebra) which can be used in numerical simulation for investigating possible waveguide modes in various geometries of the photonic crystal waveguide. Additionally, the model Eq. (4.19) may be very useful as a means of outlining the basic physical properties of the optical guiding systems based on the photonic crystal geometry. The structure of Eq. (4.19) was originally proposed by McGurn in [57, 58] for characterizing the intrinsic localized modes in photonic crystals. The similar discrete equations used in our approach were also studied by authors in [37, 75, 143, 144] for the light modes in the photonic crystals.

As the rule for generating a sequence of difference equations, the modes of Eq. (4.19) for each lattice site of impurities interact with their nearest-neighbor sites. This technique

may be described graphically through the computational molecule of Figure 4.2 where the sites at $n - 1$, n , and $n + 1$ are the lattice points on the waveguide channel coupled with an off-channel impurity feature at $m + 1$. In this molecule, the open circles are used

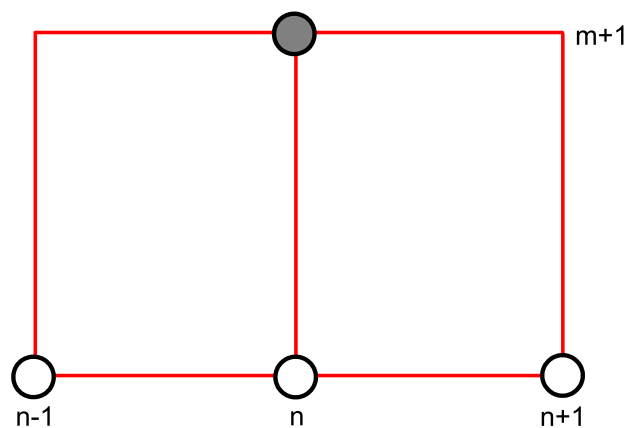


Figure 4.2: A graphic way showing the computational molecule for the difference equation waveguide for a typical off-channel feature. The open circles represent the lattice points where E -modes are presumed known, and the filled circle represents an off-channel site where the mode is unknown.

to represent the sites where the modes are presumed known and the filled circle (usually formed of nonlinear impurity in our model) where the mode is unknown.

CHAPTER V

Transmission Characteristics of Kerr Media Photonic Crystal Waveguides

5.1 Introduction

The goal in this chapter is to study the interaction of single and/or two different frequency guided modes in a linear medium photonic crystal waveguide arising from in- and/or off-channel Kerr nonlinear features. The self interaction of the mode, or the resonant scattering properties between two modes, mediated by the Kerr nonlinear medium, is treated and compared with results of the scattering of the modes in the linear limit of the Kerr medium, i.e., in the absence of the $|E|^2$ term in the Kerr dielectrics. The guided modes are investigated using an analytical approach (the difference equation method) applied to a model of the photonic crystal waveguide that has been used in a number of previous publications [42, 70, 71, 101, 102, 145–147].

Recently photonic crystal waveguides have been the focus of a number of experimental and theoretical efforts [32, 44, 148–153]. The objective of these studies is to develop photonic crystal waveguides as an alternative to fiber optics technologies and for possible applications in nanoscience. Photonic crystal waveguides have a potential to fulfill many of the present functions of fiber optics, and it is hoped by many researchers that they will realize improvements over fiber optics functions.

One focus of particular recent interest has been on the interaction of photonic waveguide modes with in- and off-channel features [11, 42, 70]. These types of systems have potential applications in switching and multiplexing designs which may be of impor-

tance in routing and uploading and downloading information carried in optical networks. Though the bulk of the work has been done on linear dielectric media systems, systems formed of nonlinear optical media may provide potentially more important applications.

In- and off-channel features formed of Kerr nonlinear media provide a means for waveguide modes to self-interact or to interact with other modes in the system. Physical representations of such typical problems are illustrated in Figure 5.1. Self-interaction

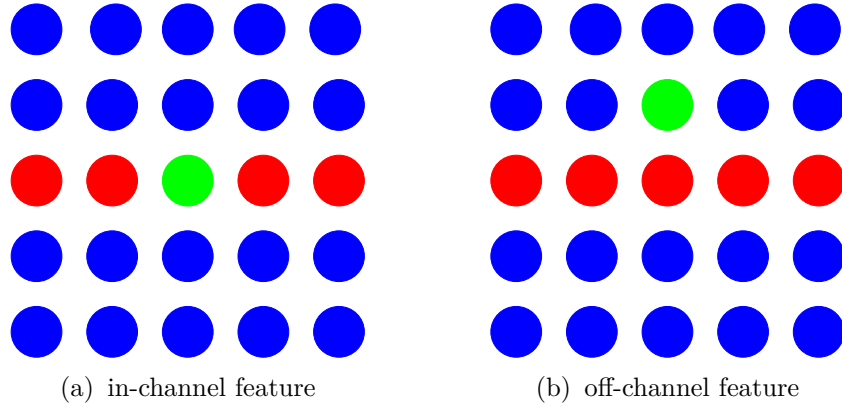


Figure 5.1: Schematic drawings of 2D photonic crystal waveguides. On both geometries, the line of solid red circles represents impurity dielectric cylinders of the waveguide channel in $[1,0]$ direction. The solid green circles depict single site Kerr nonlinear media for in- and off-channel features.

allows the transmission properties of the waveguides to depend on the mode amplitude whereas Kerr mediated interactions between two different waveguide modes permit one mode to change the transmission characteristics of the other within the system. In our presentation, the focus will be on the investigation of the transmission characteristics of two different frequency guided modes interacting with each other through Kerr nonlinear media features in a 2D photonic crystal.

The 2D photonic crystal we consider is a regular array of infinitely long, parallel, circular cylinders of linear dielectric media in a vacuum [38, 55, 81]. The concept of such

a structure is illustrated in Figure 4.1 on page 52. Waveguides are introduced into the 2D photonic crystal lattice by replacement of a row of cylinders in the photonic crystal with cylinders composed of a different linear dielectric medium (see Figure 5.1, the row of solid red circles representing such replaced cylinders). By choosing the media forming the waveguide correctly, it is possible to bind electromagnetic modes to the channel and cause them to propagate along the length of the channel. Due to the linear dielectric properties of the media of the waveguide, guided modes of the system do not interact with themselves or other guided modes. However, upon addition of features formed of nonlinear (field dependent) dielectric media to the system, guided modes can be made to interact at the nonlinear media with themselves and with other guided modes. As a consequence, the nonlinear features will exhibit a field dependent scattering of the guided modes which can be tuned to display transmission resonances and/or various features of optical bistability.

Important programming source codes developed for nonlinear difference equations of the photonic crystal waveguides are listed in Appendix D. The standard programming language in difference equation analysis of the nonlinear modes is still Fortran. Thus, for the results of our investigation in this chapter, we will make use of a more conservative approach, in order to keep the programming transparent, and use the Fortran 77 version in the calculations. The listed source codes illustrate key issues in programming and initial conditions for simulating the transmissivity of the waveguide modes. The main programs or subroutines are made as short as possible.

5.2 Single Frequency Mode onto In-Channel Features

The straight waveguide is taken along the x -axis with a Kerr nonlinear site in the waveguide channel, and the guided mode at stop band frequency ω is incident from the far left into the waveguide channel formed of the linear dielectric media. The schematic of such a system of the in-channel feature is shown in Figure 5.1(a). The fields, $E_{n,m}$, $(n, m) \in \{Z\}$ indexing lattice sites, at the waveguide channel lattice sites will be described in the planewave solution form. At the Kerr nonlinear sites there is a nonlinear dielectric, $\delta\varepsilon = \delta\varepsilon_0(1 + \lambda|E_{n,m}|^2)$, so that the fields at these sites will be described in terms of the Kerr nonlinearity parameter λ as $(1 + \lambda|E_{n,m}|^2)E_{n,m}$, which occurs recursively in the difference equation specifying the fields [Chapter IV].

In the lattice of the problem in Figure 5.1(a) the Kerr site is assumed at $(0, 0)$, so the waveguide difference equations at $(0, 0)$, $(1, 0)$, and $(-1, 0)$ with the corresponding modes $E_{0,0}$, $E_{1,0}$, and $E_{-1,0}$, respectively, are expressed as

$$E_{0,0} = \gamma' \alpha (1 + \lambda|E_{0,0}|^2) E_{0,0} + \gamma \beta (E_{1,0} + E_{-1,0}), \quad (5.1a)$$

$$E_{1,0} = \gamma (\alpha E_{1,0} + \beta E_{2,0}) + \gamma' \beta (1 + \lambda|E_{0,0}|^2) E_{0,0}, \quad (5.1b)$$

$$E_{-1,0} = \gamma (\alpha E_{-1,0} + \beta E_{-2,0}) + \gamma' \beta (1 + \lambda|E_{0,0}|^2) E_{0,0}, \quad (5.1c)$$

$$\text{and for } |n| > 1, \quad E_{n,0} = \gamma [\alpha E_{n,0} + \beta (E_{n+1,0} + E_{n-1,0})]. \quad (5.1d)$$

Here, $\gamma' \propto \delta\varepsilon_0$ at Kerr impurity site $(0, 0)$, $\gamma \propto \delta\varepsilon_l$ on the linear media waveguide channel sites, and α and β , respectively, are on-site and nearest-neighbor couplings that are described in Eq. (4.17) on page 57. The schematic of such a coupling process is illustrated

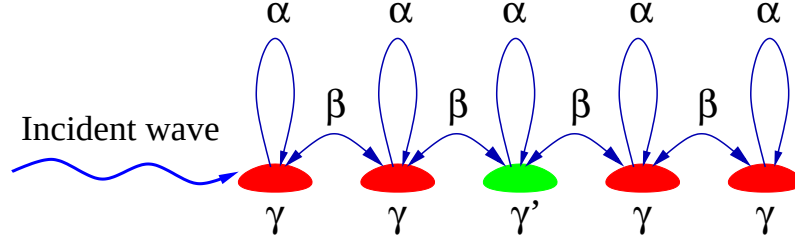


Figure 5.2: Schematic illustration for on-site coupling, α ; the nearest-neighbor sites coupling, β ; γ' denoting the single Kerr impurity; and γ describing the linear media waveguide sites. Here, only the waveguide channel lattice sites (solid red oval shapes) and Kerr impurity lattice site (solid green oval shape) are shown.

in Figure 5.2. In this, the α and β are the functions of incident waveguide mode at a stop band frequency ω of the photonic crystal.

We now take the general solution of the waveguide mode Eqs. (5.1a) - (5.1c) in the plane wave form

$$E_{n,0} = \begin{cases} u e^{ikn} + v e^{-ikn}, & n < 0, \\ (xt) e^{ikn}, & n > 0, \end{cases} \quad (5.2)$$

where u , v , and (xt) have the meaning of the incident, reflected and transmitted field amplitudes respectively with the x real. Here k is the wave number of the guided mode of the plane wave form $E_{n,0} \propto e^{ikn}$ in the linear media waveguide channel. A further explanation of the term (xt) will be given in Subsection 5.2.1 below.

In order to obtain the dispersion relation of the waveguide modes in the linear media waveguide channel, we substitute Eq. (5.2) into Eq. (5.1d). This gives a waveguide dispersion relation of the form

$$1 = \gamma(\alpha + 2\beta \cos(k)) \quad (5.3)$$

relating γ and k . This relation will be a basic condition to be satisfied in any numerical formulation of waveguide modes in the subsequent equations. Similarly, we substitute the

plane wave forms in Eq. (5.2) into the Eqs. (5.1a) - (5.1c) obtaining a solution for u and v in terms of xt . Using these solutions, the resulting transmission and reflection coefficients for scattering into the waveguide channel are obtained as

$$T = \frac{\sin^2(k)}{1 + Q^2/4 - Q \cos(k)} \quad \text{and} \quad R = \frac{(\cos(k) - Q/2)^2}{1 + Q^2/4 - Q \cos(k)} \quad (5.4)$$

respectively with $Q = \frac{1}{\gamma\beta}(E_{0,0} - \gamma\alpha)$ and $R + T = 1$. The substitution also gives a nonlinear equation for $E_{0,0}$ of the form

$$\eta \left(1 + \lambda(xt)^2 |E_{0,0}|^2\right) E_{0,0} = 1. \quad (5.5)$$

Here, $\eta = \gamma'/\gamma$. In Eq. (5.4), $E_{0,0}$ is real, and it is the solution of Eq. 5.5. For the linear impurity ($\lambda x^2 = 0$), Eq. 5.5 reduces to $E_{0,0} = 1/\eta$.

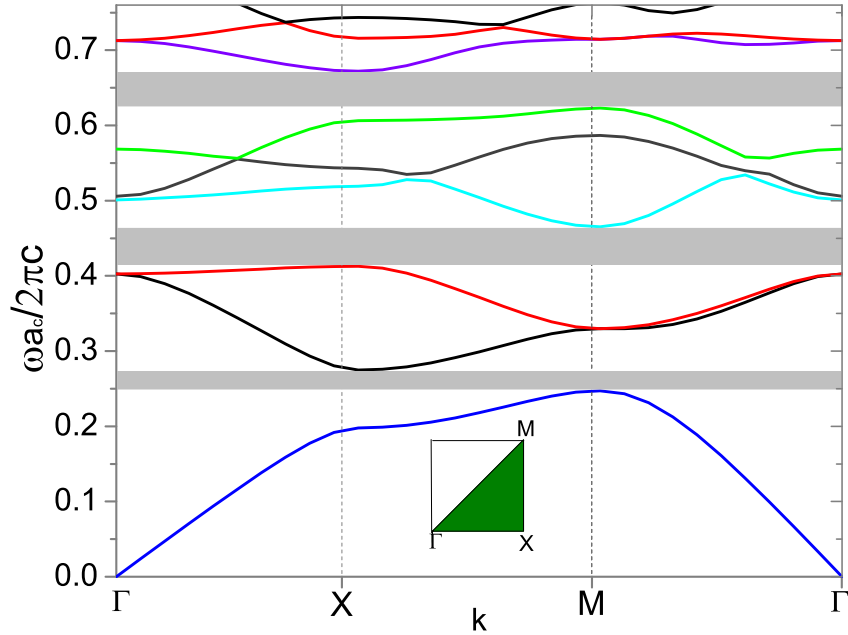


Figure 5.3: 2D photonic crystal band structure calculated by using the same parameters for the experimental data of McCall *et al.* Here, $R = 0.48\text{cm}$ and $\varepsilon = 9.0$ for the alumina composite rods. Stop gaps of the system appear near $\omega a_c/2\pi c = 0.26$, 0.44 , and 0.65 which are indicated by the rectangular shaded areas. The inset shows first-quarter of Brillouin zone for the 2D square lattice. The points in the Brillouin zone Γ , X , and M are $k = \pi/a_c$ times $[0,0]$, $[0,1]$, and $[1,1]$, respectively.

The parameters α , β , and λ in the above equations have been shown in Chapter IV to depend on the geometry, composition, and frequencies of the guided modes. In the following discussions our results will be presented in terms of the ratio β/α . The results are for a square lattice photonic crystal (as shown in Figure 4.1 schematically) that was originally studied experimentally by McCall *et al.* [55]. The system consists of aluminium composite rods with $\varepsilon = 9.0$ in an air background. The cylindrical rods of the system were such that the ratio of their radii, R , to the lattice constant, a_c , was $R/a_c = 0.37$. Here, in Figure 5.3, using the same parameters in [55], we present a plot of the band structure of the photonic crystal. For the single mode system of in-channel feature, we initially consider a guided mode of frequency $\omega a_c/2\pi c = 0.440$ which occurs at the center of the second lowest stop band of the photonic crystal [11, 55, 57, 58].

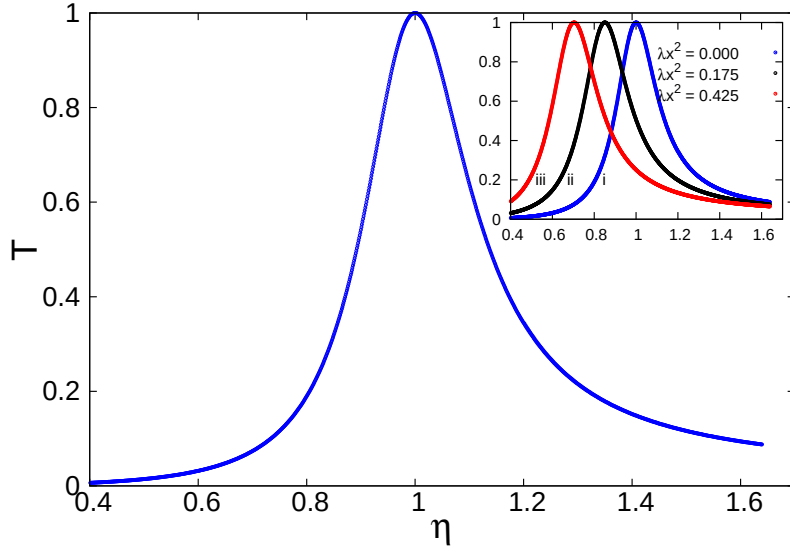


Figure 5.4: Plot of transmissivity T versus $\eta = \gamma'/\gamma$ for the waveguide mode for $\lambda x^2 = 0.0$ (linear limit). The transmission peak is normalized to occur at unity. The interaction of the mode with an in-channelled Kerr feature is shown in the inset where the curves i, ii, and iii show the transmission resonances at $\eta = 1.0$, 0.8513 , and 0.7036 , respectively, corresponding to the nonlinearity $\lambda x^2 = 0.0$, 0.175 , and 0.421 .

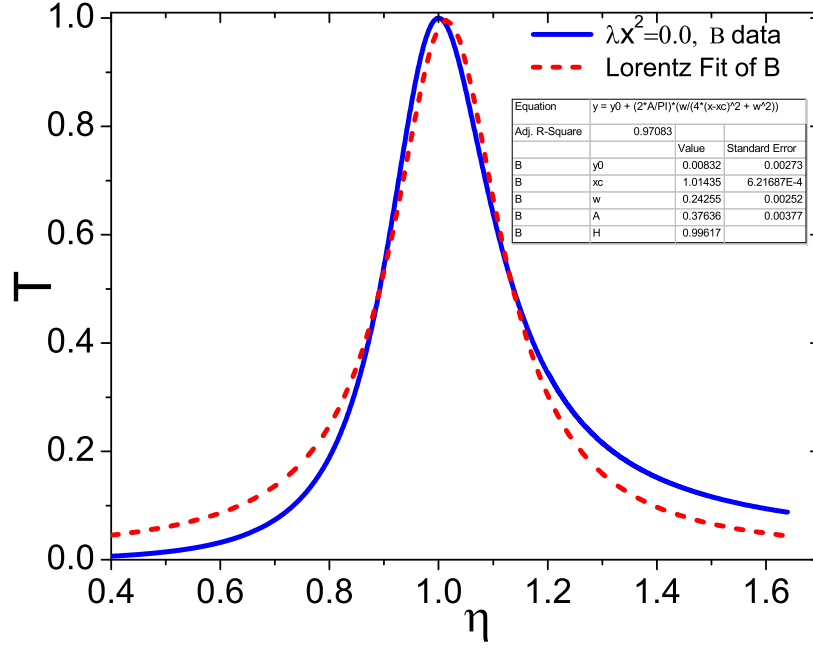


Figure 5.5: Lorentz Fit of the plot of transmissivity T versus η for the waveguide mode at the linear limit $\lambda x^2 = 0$. The original Fit parameters generated by Origin Lab is shown on a table inside the plot. The Fits for the plots in the nonlinear limits (not shown) can be satisfied similarly because of the identical nature of transmission profiles.

To illustrate the effects of nonlinearity on the system, Figure 5.4 presents the results of simulated transmission coefficient for the waveguide mode $\omega a_c / 2\pi c = 0.440$ as a function of $\eta = \gamma' / \gamma$ for the linear (i.e., $\lambda x^2 = 0.0$) and Kerr nonlinear (e.g., $\lambda x^2 = 0.175$ and 0.425) regimes for $t = 1$. The strength of the nonlinearity λx^2 is then proportional to the intensity of the electric field of the guided mode. As seen in the figure, a resonant transmission profile for the linear case has a transmission maximum at $\eta \approx 1$.

The resonances for Kerr values $\lambda x^2 = 0.175$ and 0.425 have maxima that occur at $\eta = 0.8513$ and 0.7036 , respectively. These are shown in the inset of the figure. The downshifted transmission profiles of the waveguide mode ω at the given Kerr parameters show the effect of the nonlinear response to the waveguide mode incident into the waveguide channel of the system. As can be seen clearly in the inset, all three resonant curves

are identical in shape, and the resonant curves ii and iii downshift from the linear limit due to the imposition of the Kerr nonlinearity in the waveguide channel. In general, the stronger the nonlinearity the farther the downward shift of resonant transmission from the linear media resonant transmission regime. This type of system in photonic crystal has also been studied by Banerjee in [48] using beam propagation method.

A notable feature of the result in Figure 5.4 is that the present model allows us to describe the resonant light propagation as a Fano-type resonance, i.e., a non Lorentzian, asymmetric, form of the resonant transmission in the nonlinear waveguide. For a comparison, a Lorentz Fit of the resonant transmission in the linear limit is shown in Figure 5.5 below. In obtaining this, an analysis tool for nonlinear curve fit of Origin Lab was used with no change in any of the original fit parameters. It is found that the asymmetry arises both in the linear and nonlinear impurities.

5.2.1 Transmission Through a Kerr Barrier

The problem posed in Section 5.2, above, can be considered as a nonlinear barrier and the difference equations, Eqs. (5.1a)-(5.1d), as the model equations for this barrier problem. The solutions of these equations using the boundary conditions in Eq. (5.2) allow us to express the transmission coefficient, $T = |(xt)/u|^2$, as a function of η and t for fixed λx^2 , which can be written explicitly as in Eq. (5.4). The T depends on the nonlinearity characterized by the Kerr parameter, λ , and transmitted field amplitude, xt , through the parameter $\lambda x^2 t^2$ in Eq. 5.5 where both the fixed λx^2 and the variable t^2 are dimensionless parameters. In the results presented below, taking λx^2 to be a fixed dimensionless parameter, t is a dimensionless parameter which changes the intensity of the field and, consequently, the nonlinearity affecting the system. In this subsection, by computing the

T for fixed λx^2 , the transmission maxima as a function of the parameter, t , characterizing the nonlinearity of the barrier material is studied.

The T computed as a function of η and t for fixed λx^2 , in general, is found to have basically a series of resonant transmission maxima at different (t, η) . The results shown in Figure 5.4 have peaks as functions of η at fixed $t = 1$. In the limit $\lambda x^2 = 0$, the barrier is linear dielectric media, and the nonlinearity of the barrier media increases as λx^2 increases from zero. Initially, of particular interest to us will be the positions of the transmission maxima found in the (t, η) parameter space for various fixed λx^2 .

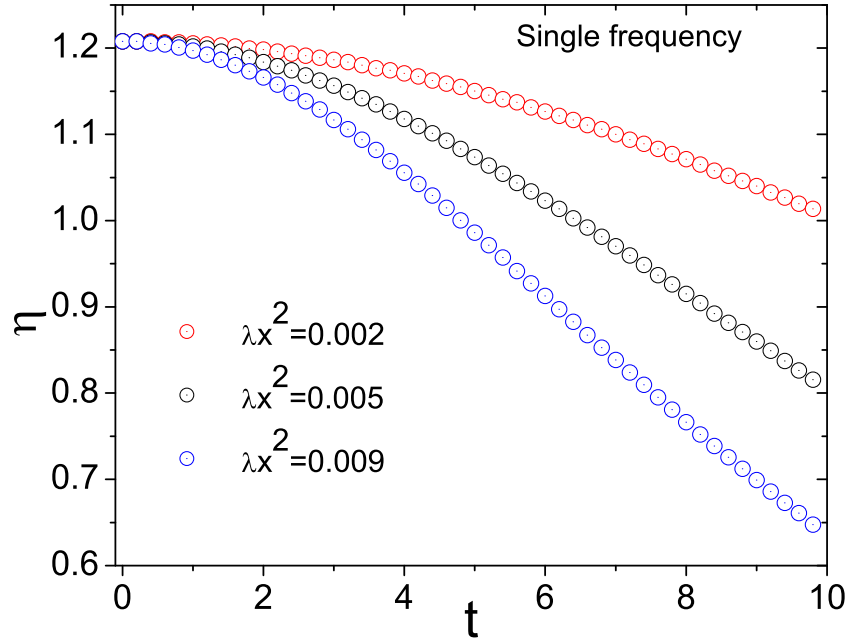


Figure 5.6: The plot of positions of the maxima of the transmission coefficient for a single barrier in the (t, η) space at three different Kerr nonlinearities: $\lambda x^2 = 0.002, 0.005$, and 0.009 . In the limit $t = 0$, as seen in the plot, all three transmission maxima meet at a point indicating the absence of nonlinear effect because the system has only the linear solution, $E_{0,0} = 1/\eta$, at $t = 0$. At other values of t the nonlinearity causes the separation of the transmission maxima for each λx^2 .

Figure 5.6 shows the plot of transmission maxima for three different fixed λx^2 in (t, η) space. The λx^2 were chosen consistent with values found in the literature [102, 154].

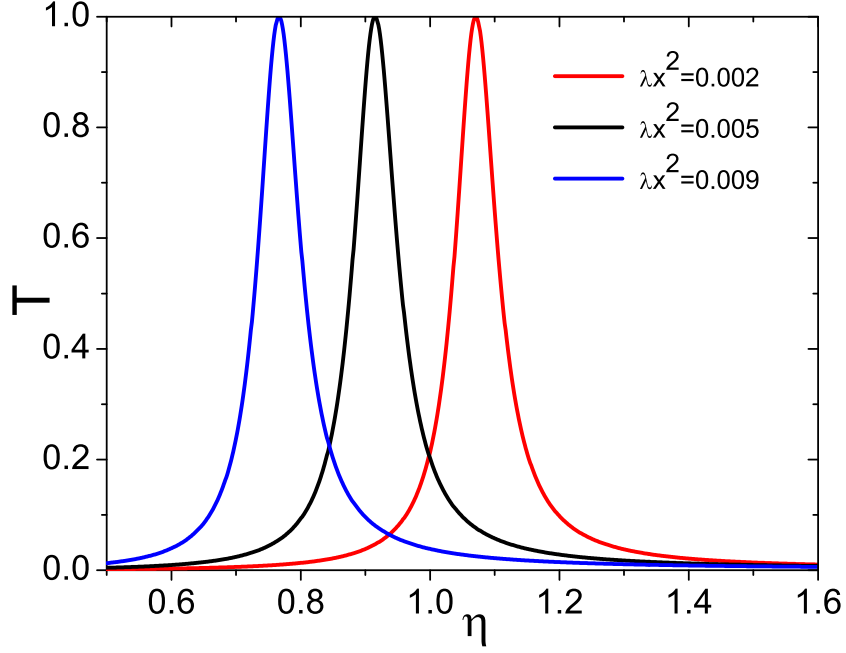


Figure 5.7: Resonant transmission profiles at $t = 8$. The three resonances at around $\eta = 1.0711, 0.9151, 0.7663$ match with the location of the transmission maxima in the (t, η) space shown in Figure 5.6.

The plot is made by using the difference equation parameters including wave vector $k = 2.5$ specified on page 66 and the λx^2 values labelled on the plot itself. With that, the transmission coefficient as a function of η for each t is computed and the corresponding maxima of each transmission profile is scanned out and recorded numerically. In this analysis, the transmission maxima in the $t \rightarrow 0$ limit for each fixed λx^2 approach $\eta \approx 1.2079$ which corresponds to the resonance in the case of linear dielectric media. This is reasonable as $t \rightarrow 0$ is the zero field limit of the system, which is apparent mathematically from Eq. (5.5) as well. For $\lambda x^2 \neq 0$ and t increasing from zero, the system gradually turns into that of the nonlinear media. As a result, the transmission maxima for each fixed λx^2 begin to separate from each other in η .

Figure 5.7 shows the transmission coefficient profiles at $t = 8$ for each λx^2 under investigation. It can be seen in the figure that the positions of the transmission peaks

on η -axis are found at $\eta = 1.0711$, 0.9151 , and 0.7663 and these recover the results of the corresponding transmission maxima found in (t, η) space in Figure 5.6. This result can be considered as supplementary computation for transmission maxima and validates our numerical routines that can be employed later for computing transmission maxima arising from multiple/complex Kerr nonlinear sites.

5.2.2 Optical Bistability - a Background Concept with an Example

In this subsection, we will illustrate the concept of optical bistability. Optical bistable systems are similar to magnetic systems which exhibit hysteresis effects. In particular, they are systems that exhibit multiple stable solutions. In our present system in Eqs. (5.1a)-(5.1d), the bistability enters the system when $\lambda x^2 < 0$.

Interest in optical bistability comes from its potential application as a switch for use in optical networks. The problem illustrated in Figure 5.1(a), with its difference equation formulation, (as described in Section 5.2), may be the simplest photonic crystal waveguide structure that exhibits optical bistability. The structure is a case of the linear dielectric waveguide that contains a single Kerr nonlinear site representing a nonlinear barrier. This was originally treated by McGurn in [11] using the difference equation approach and was later extended to a case of the junction barrier of three identical waveguides [70]. If the electromagnetic energy of a waveguide mode is incident on such a barrier from its left infinity, part of the mode will be reflected and part of the mode will be transmitted through the barrier. We shall search the bistability of this system in the following by analyzing the solvability of model equations.

To treat this problem properly, we assume $\eta = 1.1084$ in model Eq. (5.5) so that only the Kerr parameter λ determines the difference in the dielectric properties of the linear channel sites and the nonlinear barrier site. Here, bistability, specifically, arises from the multiple solutions of Eq. (5.5) for $E_{0,0}$. It is important to note, however, that due to the factor of $|E_{0,0}|^2$, Eq. (5.5) has regions in (λ, xt) with two kinds of solutions. Firsts are single solutions (no bistability) over a certain range of input parameter; and, then there are multiple solutions (bistability) over an appreciable range of the input parameter. In our case, the input is either the Kerr constant λx^2 or the transmitted power $\lambda(xt)^2$ and the output is the transmission coefficient through the barrier site.

In Figure 5.8, a plot of the transmission coefficient versus the λx^2 is given for the same wave vector $k = 2.5$ and stop band frequency $\omega a_c / 2\pi c = 0.440$, as used in the previous discussions. However, the waveguide impurity property now is characterized by fixed $\eta = 1.1084$, and the ratio of the nearest-neighbor to the on-site couplings is chosen to be larger, i.e., $\beta/\alpha = 0.1738$, twice the strength 0.0869 used in the previous simulations. This new ratio of β/α causes perturbation of the transmission profile smearing out downwards that results in an increased area of the bistable region. For the region $\lambda x^2 < -0.3003$ and $\lambda x^2 > 0.0$ (corresponding to a positive Kerr parameter), the system displays only the single solutions, and no bistability is observed over these regions. However, for a negative Kerr parameter in the region $-0.3003 \leq \lambda x^2 \leq 0.0$, bistability is observed. This is shown by a shaded region of the plot in the figure, above.

In the same plot, the four open circles at points b , c , d , and f may be called the jump points, where the system switches its solutions rapidly. These points, including the launching point a and the final point e , are considered in the discussion to explain the

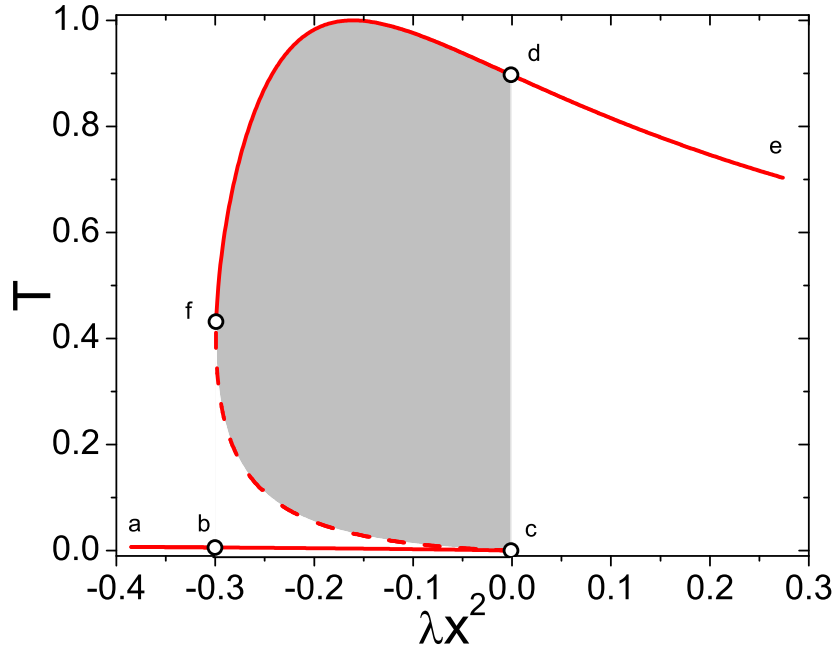


Figure 5.8: Plot of transmissivity, T , versus λx^2 for a photonic crystal waveguide with a barrier of a single Kerr nonlinear site. The parameter λx^2 is a measure of both the nonlinearity and the transmitted power. The shaded area of the plot in the range $-0.3003 < \lambda x^2 < 0.0$ shows the region of optical bistability (multiple solutions). Dashed curve $f - c$ represents the unstable solution.

method of how the system displays bistability in the following sense. We imagine the input power is initially set to a fixed value $\lambda x^2 = -0.3845$ and is slowly increased. As λx^2 begins to increase, the solutions are given by the curve segment $a - c$. At $\lambda x^2 = 0$, the system makes a transition to point d and traces out the solution curve $d - e$. If λx^2 is now slowly decreased (reversed) from $\lambda x^2 = 0.2739$, the system will remain on the upper branch and the solutions will be given by the curve segments $e - d - f$. As λx^2 passes through $\lambda x^2 = -0.3003$, the system makes a transition to point b and traces out the curve $b - a$. Thus, both forward and reversed biases of the transmission coefficients result in a loop of stable solutions about the shaded region. The solution of the curve $f - c$, shown by a dashed line, is unstable, and if the system is initially in this state, it will rapidly switch to one of the stable solutions through the stability property of the equations of the

system. The bistability process of the system shown above is much the same as found in the study of the nonlinear cases in [45, 155, 156], or the cases similar in [157, 158].

5.3 Two Different Frequency Modes onto In-Channel Features

Here, the system of interest is the two different frequencies, both incoming from left infinity onto a Kerr nonlinear site located in the waveguide channel that is formed of the linear media in a 2D photonic crystal, as shown in Figure 5.9. In this, we expect the

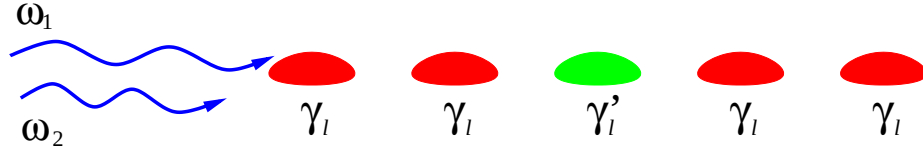


Figure 5.9: Schematic illustration of two different frequencies, ω_1 and ω_2 , interacting through Kerr nonlinear dielectrics in the 2D photonic crystal lattice. The γ_l represents the dielectric property of the waveguide channel, and the γ'_l denotes γ_l for the Kerr site with $l \in (1, 2)$. Here, only the waveguide channel lattice sites (solid red shapes) and Kerr impurity lattice site (solid green shape) are shown.

light-light interactions to occur and such interactions may affect the transmission of each of the guided modes in the waveguide channel in $[1, 0]$ direction. Here, the propagation of the one frequency mode could turn on and off the resonant transmission of the other along the waveguide channel.

We adopt the notations for the fields as $E_{n,m}^l$, and other relevant parameters such as γ_l , γ'_l , a_l , and b_l , which are each functions of the guided modes, ω_l , for $(n, m) \in \{Z\}$, and $l \in (1, 2)$ indexes the two different frequency modes. Here γ_l is related to dielectric constant of the linear media forming the waveguide channel, and γ'_l is the γ_l for the Kerr nonlinear site. The a_l and b_l , respectively, represent the on-site and nearest-neighbor site coupling coefficients that are determined from the Green's function and the stop band frequency of the guided mode, as explained in Chapter IV.

Using these general notations and the concept of the difference equation formalism given in Chapter IV, the set of discrete waveguide equations for the two guided modes in the $[1, 0]$ direction can be expressed as

$$E_{0,0}^l = \gamma_{l'}' a_l \{1 + \lambda \delta\} E_{0,0}^l + \gamma_l b_l (E_{1,0}^l + E_{-1,0}^l) \text{ for a Kerr site at } (0,0), \quad (5.6a)$$

$$E_{n,0}^l = \gamma_l \{a_l E_{n,0}^l + b_l E_{2n,0}^l\} + \gamma_{l'}' b_l \{1 + \lambda \delta\} E_{0,0}^l \text{ for } |n| = 1, \quad (5.6b)$$

$$\text{and } E_{n,0}^l = \gamma_l \{a_l E_{n,0}^l + b_l (E_{n+1,0}^l + E_{n-1,0}^l)\} \text{ for } |n| \geq 2, \quad (5.6c)$$

where $\delta = \left(d_l |E_{0,0}^l|^2 + e_l |E_{0,0}^{l'}|^2\right)$ and (l, l') implies $(1, 2)$ or $(2, 1)$. The constants d_l and e_l are coefficients of the Kerr effect arising from each of the two different frequency guided modes, ω_1 and ω_2 , interacting with each other. Notice that we have introduced the two-frequency dielectric model of the form $\varepsilon = \varepsilon_0 \left[1 + \lambda \left(d_l |E^l|^2 + e_l |E^{l'}|^2\right)\right]$ where d_l and e_l appear as the cubic susceptibilities in the nonlinear polarization. In the opinion of some of the committee members, but not the chair of the committee: The model presented here may not be suitable for describing the propagation of two modes in the absence of higher-order effects. For instance, Agrawal [46] derives two coupled, non-linear differential equations with coupling coefficients about which he states “ ... f_{11} , f_{12} , f_{22} differ from each other because of the frequency dependence of the modal distribution ... The difference is small, however, and can be neglected in practice.” In this case, our two-frequency model may find its significance in the medium that may exist under time-reversal symmetry [159, 160] in strong magnetic fields. It is important to note that, besides the standard definition, the structure of the d_l and e_l in our system causes the perturbation which is the fundamental concept in nonlinear science, and, we simply use this concept to model the two-frequency modes. Actually, the coefficients d_l and e_l account

for the variation of the relative field intensities and the relative coupling values. The unit analysis of the field solution later can be used to describe the coefficients as dimensionless parameters which allow us to vary the absolute intensities of the fields and the values of the nonlinear couplings. This will be looked into elsewhere.

The field solutions for the modes in the problem are naturally taken in planewave form,

$$E_{n,0}^l = \begin{cases} u_l e^{ik_l n} + v_l e^{-ik_l n}, & n < 0, \\ (xt_l) e^{ik_l n}, & n > 0, \end{cases} \quad (5.7a)$$

as explained in Eq. (5.2) on page 64, and the solution at the Kerr site is

$$E_{0,0}^l = s_l e^{i\theta_l} = s_l, \quad \because \theta_l = 0, \quad (5.7b)$$

where u_l , v_l , and (xt_l) , respectively, are the amplitudes of the incident, reflected, and transmitted fields, for $l = 1$ or 2 corresponding to ω_1 or ω_2 . The $E_{0,0}^l$ is complex in general, so it has a magnitude s_l and phase $e^{i\theta_l}$ as shown in Eq. (5.7b). Substituting Eqs. (5.7a) and (5.7b) into the waveguide mode Eqs. (5.6a)-(5.6c) results in a set of distinct equations (linear and nonlinear), relating to each other and describing the propagation of two different frequency modes along the waveguide channel of the linear media as

$$\gamma_l' (1 + d_l(\lambda x^2)|t_l|^2|r_l|^2 + e_l(\lambda x^2)|t_{l'}|^2|r_{l'}|^2) r_l - \gamma_l = 0, \quad (5.8a)$$

$$u_l + v_l = xt_l, \quad \text{and} \quad u_l e^{-ik_l} + v_l e^{ik_l} = xt_l (r_l - \gamma_l a_l - \gamma_l b_l e^{ik_l}) / \gamma_l b_l. \quad (5.8b)$$

Here, the field solutions at the Kerr nonlinear site are labelled as $r_l = s_l/t_l$ and $r_{l'} = s_{l'}/t_{l'}$, again for $(l, l') = (1, 2)$ or $(2, 1)$. The amplitudes of the incident, reflected, and transmitted

fields, respectively, u_l , v_l , and xt_l can be arranged in the form

$$\begin{pmatrix} 1 & 1 \\ e^{-ik_l} & e^{ik_l} \end{pmatrix} \begin{pmatrix} u_l/xt_l \\ v_l/xt_l \end{pmatrix} = \begin{pmatrix} 1 \\ (r_l - \gamma_l a_l - \gamma_l b_l e^{ik_l})/\gamma_l b_l \end{pmatrix}, \quad (5.9)$$

where r_l are the field solutions at the Kerr nonlinear site, and a_l , b_l , γ_l , and k_l have their usual meanings corresponding to ω_l , again for $l \in (1, 2)$.

This, after some algebra, results in transmission in terms of the incident field amplitudes as $T_l = |(xt_l)/u_l|^2$ for the modes ω_l :

$$T_l = \left\{ 1 + \left(\cot k_l - \frac{1}{2\gamma_l b_l \sin k_l} (r_l - \gamma_l a_l) \right)^2 \right\}^{-1}, \quad (5.10)$$

with the relation $|(xt_l)/u_l|^2 + |v_l/u_l|^2$, the sum of the transmission and reflection coefficients for each guided mode, satisfying unity. To simulate transmissivity for the modes, the fields r_l or $r_{l'}$ can be numerically calculated from the nonlinear Eqs. (5.8a):

$$\eta_l \left(1 + d_l(\lambda x^2) |t_l|^2 |r_l|^2 + e_l(\lambda x^2) |t_{l'}|^2 |r_{l'}|^2 \right) r_l = 1, \quad (5.11)$$

for $(l, l') \in (1, 2)$ or $(2, 1)$, $\eta_l = \gamma_{l'}/\gamma_l$, and $\gamma_{l'}$ representing γ_l of the Kerr nonlinear site. Here, the Kerr parameter (λx^2) and the constant coefficients (d_l, e_l) are treated as numerical factors for modeling the transmission behaviors of the guided modes because the frequencies of the nonlinear bound modes generated by the Kerr impurity now depend on the linear combination of the $|r_l|^2$ and $|r_{l'}|^2$.

Eq. (5.11) essentially consists of two simultaneous cubic nonlinear equations forming a complicated relationship of the field solutions r_1 and r_2 . In this situation, our choice of the numerical tools for computing the field solutions was the Newton-Raphson method for nonlinear system of equations, which allowed us to transform the nonlinear equations into a two-dimensional Jacobian matrix. The matrix was then solved for the fields using

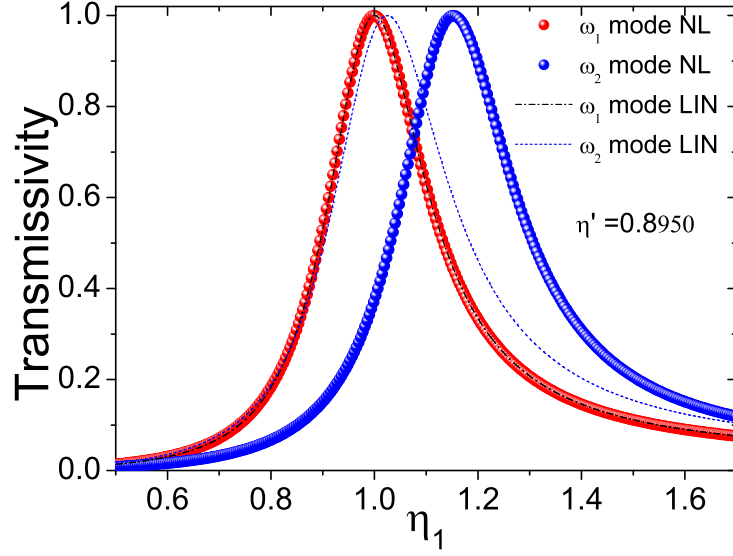
the available numerical routines [161, 162] or by manipulating the elements of the matrix developed in the source code.

Here, we argue, based on the formalism developed in the above discussion, that the two modes, ω_l for $l \in (1, 2)$, propagating along the waveguide channel of the linear media, interact with each other through the field excitations of the Kerr nonlinear site. For example, in the nonlinear Eq. (5.11), the field solutions r_1 and r_2 , representing the excitations of the Kerr site, interact with each other through the linear combinations of the constants (d_1, e_1) and (d_2, e_2) . The r_1 exchange information with r_2 through e_2 , and r_2 with r_1 through e_1 , as given in the last term inside the parenthesis on the left-hand side of Eq. (5.11). Here the fields r_1 and r_2 correspond to the modes ω_1 and ω_2 , respectively. Therefore, we expect the transmission states of the ω_2 mode can affect the transmission of the ω_1 mode, or vice-versa through nonlinear enhancement of the bound modes at the Kerr impurity site.

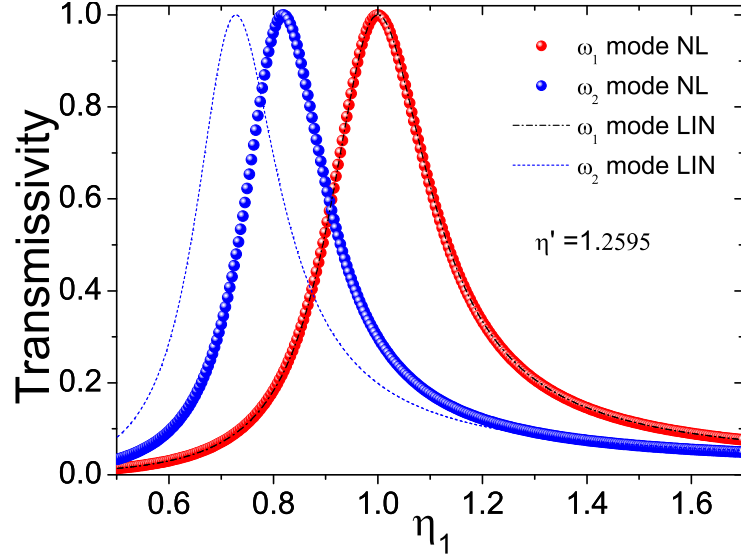
In what follows, we will do numerical calculations to simulate the transmissivity of the guided modes of interest. The important point for the simulation here is finding the transmission coefficients using Eq. (5.10), which is straightforward in the present case, but the transmission coefficients largely depend on both the field solutions r_1 and r_2 contained in Eq. (5.11). In addition, the field solutions are the initial value problem. Therefore, the constants of the equations are described such that the system, through the interplay of variables in Eq. (5.10) and Eq. (5.11), can exhibit the transmittal of the modes. For this, the constant parameters as adopted by McGurn in [71] are described as the coupling ratios of $a_2/a_1 = 0.8952$, $b_1/a_1 = 0.0852$, and $b_2/a_1 = 0.0701$. The two frequencies within the same stop band of photonic crystal are $\omega_1 a_c / 2\pi c = 0.440$

and $\omega_2 a_c / 2\pi c = 0.431$ with wave numbers $k_1 = 2.5$ and $k_2 = 2.0$, respectively, at fixed Kerr nonlinearity parameter of $\lambda x^2 = 0.00025$ (i.e., $\lambda x^2 > 0$ case) and $t_1 = t_2 = 1$, unless stated a different value. The $\gamma_1 a_1$ and $\gamma_2 a_1$, respectively, are calculated from the linear dispersion relations $\gamma_1 (a_1 + 2 b_1 \cos k_1) = 1$ and $\gamma_2 (a_2 + 2 b_2 \cos k_2) = 1$, that are obtained from the linear difference equations ($\lambda x^2 = 0$ case) for the modes. Notice that we write the numerical constants in terms of a_1 to simplify the calculations. The other constants are taken such that $e_l = d_l = 1$, $l \in [1, 2]$. We expect e_l and d_l to be of the same order of magnitude as the two frequency modes, ω_l , are within the same stop band of the photonic crystal.

In this form, the results are presented in Figure 5.10(a) and (b) for the in-channel feature. In this feature, the guided modes along the waveguide channel of the linear media are incident into the single Kerr nonlinear site, so part of the modes will be reflected and part of the modes will be transmitted by the Kerr site. The results show asymmetric resonant transmissions for the modes, ω_1 and ω_2 , on the plot of the transmissivity versus η_1 for the ratios of $\eta' = \gamma'_2 / \gamma'_1 = 0.8950$ in plot (a) and 1.2595 in plot (b). These ratios, particularly, perturb the dielectric properties of the in-channel feature, and the effects are seen on the transmission resonances of the modes. In the present case only the two typical cases of the η' are chosen; however, the resonances for a whole range of η' will be investigated along with the transmission maxima later in this chapter. The resonant transmission arises due to the fact that the bound impurity (linear or nonlinear) states are localized about the Kerr impurity site. These interact with the guided modes at stop band frequencies resulting in resonances in the system. At peaks of the curves, the transmissivity is found unity, meaning impurity dielectric properties led to the possibility



(a) ω_2 mode (blue) up-shifted from ω_1 mode (red)



(b) ω_2 mode (blue) down-shifted from ω_1 mode (red)

Figure 5.10: In-channel feature for $\lambda x^2 > 0$ (i.e., the nonlinear (NL) case with fixed $\lambda x^2 = 0.00025$), and $\lambda x^2 = 0$ (i.e., the linear (LIN) case). Transmissivity versus $\eta_1 = \gamma'_1/\gamma_1$ for the waveguide modes ω_1 and ω_2 at numerical ratios of $\eta' = \gamma'_2/\gamma'_1 =$ (a) 0.8950, and (b) 1.2595. On both plots the linear limits of the resonances with respect to the nonlinear resonances are shown.

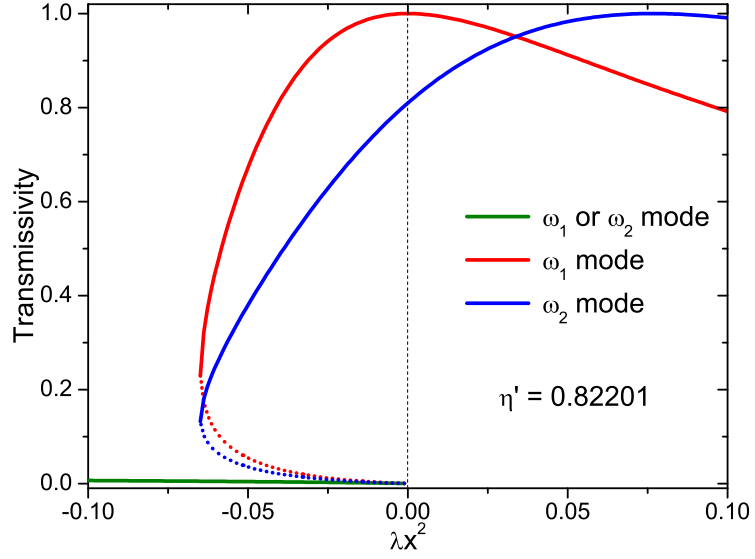
that, within the stop band, the material may become completely transparent. Also, as can be seen in plots (a) and (b), the resonant transmission profile of the ω_2 mode down-shifts from the resonance of the ω_1 mode found at $\eta_1 \approx 1$ on both plots as the ratio of

η' increases from 0.8950 to 1.2595. This shows that the nonlinearity led the light-light interaction so that one frequency component can switch on and off the transmission of the other along the waveguide. Notice that the nonlinearity causes the resonances of the ω_2 mode to move upwards on each plot; however, in the case of the ω_1 mode, both linear and nonlinear resonances occur at the same position ($\eta_1 \approx 1$) because the transmissions were normalized with respect to the parameter space of the ω_1 mode.

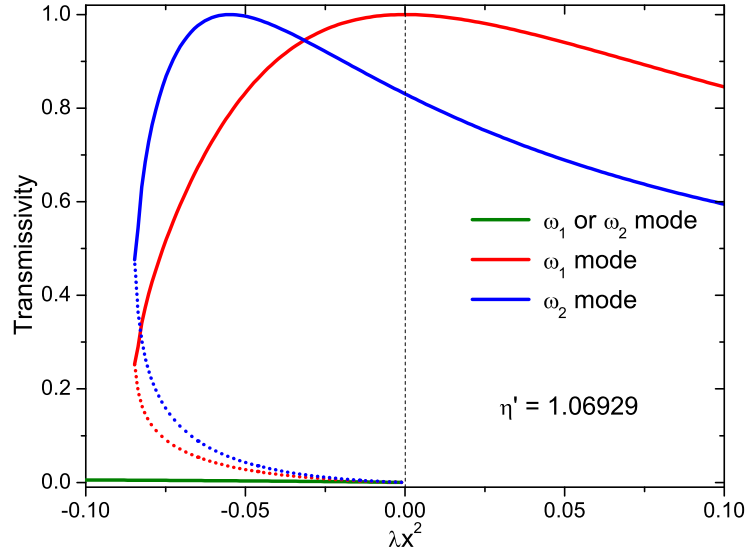
The in-channel feature with the excitations of the two different modes can exhibit optical bistability phenomenon under certain conditions with negative Kerr nonlinearity, i.e., $\lambda < 0$. This phenomenon is shown in the result presented in Figure 5.11(a) and (b).

The result uses the same constant parameters used in Figure 5.10, except λx^2 is now varied for the range of negative as well as positive values characterizing the Kerr nonlinearities at the fixed value of $\eta_1 = \gamma'_1/\gamma_1 = 1$. The plots show the transmissions of the modes through the Kerr site as a function of λx^2 where λ is the Kerr parameter. On both plots, the resonant transmission curves corresponding to the ω_1 and ω_2 modes show the possibilities of the existence of two transmission states for the same input or initial value for a range of the Kerr parameter. The plot (a) shows multiple states on the range $-0.07 \lesssim \lambda x^2 < 0$, and the plot (b) shows such states on the range $-0.08 \lesssim \lambda x^2 < 0$. These are the regions of the optical bistabilities occurring with the same concept used in Subsection 5.2.2 on page 71. For $\lambda x^2 \lesssim -0.07$ (or -0.08) and $\lambda x^2 > 0$, the transmissions of the modes are the single-valued functions of λx^2 . Here, the region of optical bistability can be varied by choosing numerical parameters characterizing the system.

Furthermore, the results show the transmission of the one mode affected by another mode. One can see in Figure 5.11(a) how the resonant transmission of the ω_1 mode occurs



(a) ω_2 up-shifted from ω_1



(b) ω_2 down-shifted from ω_1

Figure 5.11: In-channel feature for $\lambda x^2 < 0$ and fixed η_1 -space at $\eta_1 = \gamma'_1/\gamma_1 = 1$. Transmissivity versus λx^2 for the waveguide modes ω_1 and ω_2 at numerical ratios of $\eta' = \gamma'_2/\gamma'_1 =$ (a) 0.82201, and (b) 1.06929. On both plots, the resonant curve corresponding to ω_1 is shown with red color and ω_2 mode with blue color.

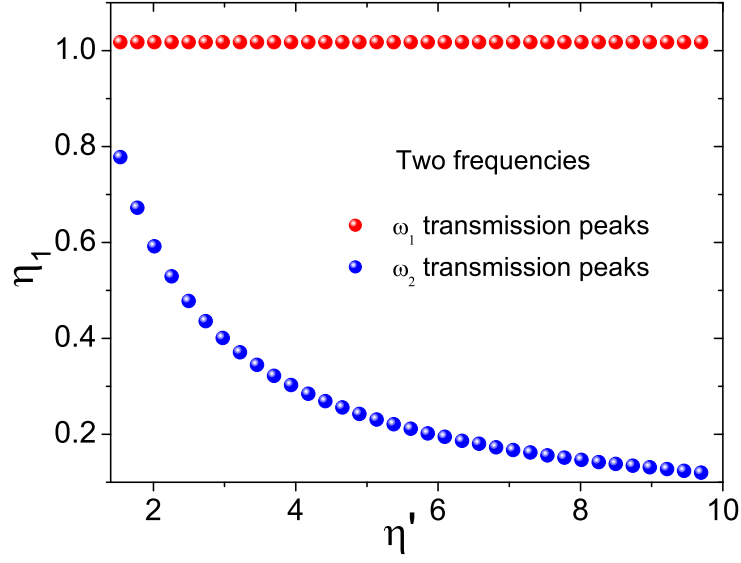
at $\lambda x^2 = 0.0$ and that of the ω_2 mode occurs at $\lambda x^2 \approx 0.077$ for the ratio of $\eta' = 0.82201$.

By increasing this ratio to 1.06929, the ω_2 mode resonance down-shifts to $\lambda x^2 \approx -0.055$,

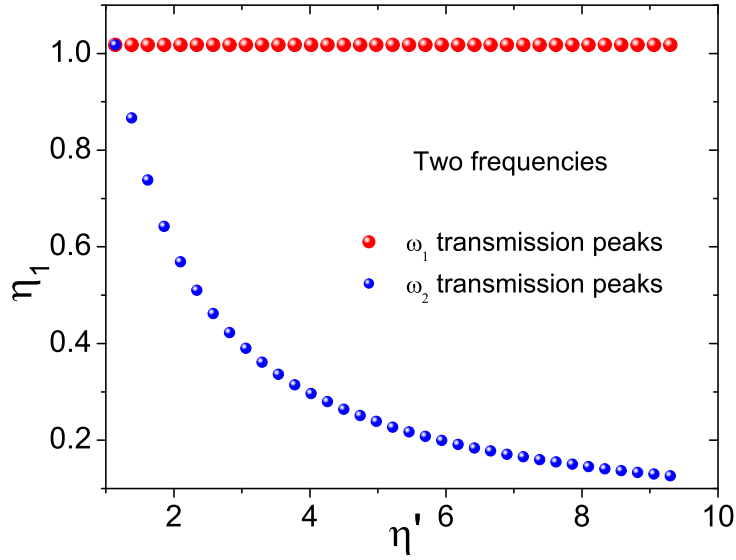
as seen in Figure 5.11(b). Clearly, the effect of downshifting the ω_2 mode from the ω_1

mode results from the alteration of nonlinearity in the system. This may allow us to propose a method of switching on and off the bistable transmission of the one guided mode in the waveguide channel of the linear media by another mode moving within the same channel mediated by a negative Kerr nonlinearity.

Dynamical behavior of ω_2 mode, with respect to ω_1 mode studied in Figures 5.10 or 5.11 for fixed ratios of $\eta' = \gamma'_2/\gamma'_1$, is re-stated here in the more generalized form by determining locations of the transmission peaks of both modes in the parameter space (η', η_1) with $\eta_1 = \gamma'_1/\gamma_1$, as described in Figure 5.10. The results of this generalization of the ω_2 mode with respect to the ω_1 mode is presented in Figure 5.12. In order to compute the transmission peaks, the transmission coefficient as a function of η' is computed by taking the same values of the constant parameters used for the result in Figure 5.10 for the modes. Both plots, (a) and (b), in Figure 5.12 here, show the similar behavior except the scanning of the peaks in plot (a) begins with an initial offset of $\Delta\eta_1 \approx 0.24$ for the modes, while the initial offset is zero in plot (b). The zero initial offset in plot (b) is visualized by coinciding the first data points of both ω_1 and ω_2 modes. Essentially, we forced perturbation in the system by using two different initial conditions of γ'_2 ($= 1.4750$ or 1.0775) in Eq. (5.11), which allowed us to calculate the field modes. In this case, we expected the system can display the new transmission profiles of the modes. The effect is seen as the offsets in the η_1 -space, but the general behavior of the transmission on η' -space remains the same for both conditions. It is found that given the parameter space characterizing the system of two different frequency modes interacting with a single Kerr site on the waveguide channel, the nonlinear effect of the one mode can be controlled by using another mode in the system.



(a) Initial offset: $\Delta\eta_1 \approx 0.24$ at $\lambda x^2 = 0.00025$



(b) Initial offset: $\Delta\eta_1 \approx 0$ at $\lambda x^2 = 0.00025$

Figure 5.12: Positions of the peaks of the resonant transmission coefficient ($T = 1$) for the ω_1 and ω_2 modes interacting through a single barrier in the (η', η_1) plane. In plot (a) the initial offset between the ω_1 and ω_2 modes in the η_1 -space is found to be $\Delta\eta_1 \approx 1.018(\text{red}) - 0.778(\text{blue}) \approx 0.24$, and in (b) $\Delta\eta_1 \approx 0$.

Now, discussions are given of the transmission maxima (peaks) found in the (t_1, η_1) space for the ω_1 and ω_2 modes by using the same concepts for investigating the transmission maxima of the single frequency mode in the previous section on page 69. The

transmission maxima in the (t_1, η_1) space are associated with barrier excitations of the ω_1 and ω_2 modes, which can be treated again by using the model given in Eqs. (5.10) and (5.11). Then, based on these nonlinear equations, the solutions in this discussion are made for the constant parameters used previously for the result in Figure 5.10. Specifically, $a_2/a_1 = 0.8952$, $b_1/a_1 = 0.0852$, $b_2/a_1 = 0.0701$, $k_1 = 2.5$, $k_2 = 2.0$, $\lambda x^2 = 0.00025$, $t_2 = 1$, $\gamma_l = 1/(a_l + 2 b_l \cos k_l)$, and $e_l = d_l = 1$, with $l \in [1, 2]$.

In Figure 5.13, the position of the maxima of the transmission coefficient in the (t_1, η_1) space for the ω_1 (red) and ω_2 (blue) modes are plotted. The plot was made by computing the transmission coefficient, $T_l = |(xt_l)/u_l|^2$ for the modes ω_l for $l \in (1, 2)$, as a function of $\eta_1 = \gamma'_1/\gamma_1$ and then scanning out the maxima in T_l . The expression for T_l is described explicitly in Eq. (5.10). As seen in the plot, the nonlinear response

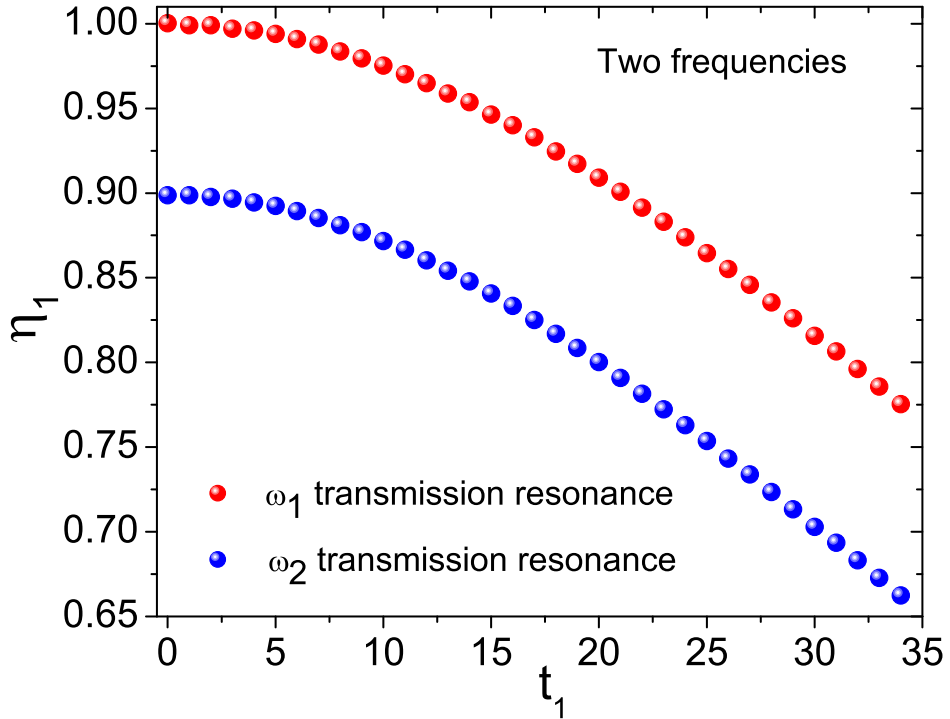


Figure 5.13: Plot of the maxima of the transmission coefficient, T , in the (t_1, η_1) plane for the ω_1 and ω_2 waveguide modes interacting with each other through the single on-channel feature. The on-channel feature is formed of the Kerr nonlinear impurity with $\lambda x^2 = 0.00025$.

for the fixed λx^2 with t_1 variation causes the transmission maxima of both the modes shifting together with an offset of $\Delta\eta_1$ between the modes in the system. It is clearly seen in the plot that such a vertical offset always exists between the ω_1 and ω_2 modes for each data point on the t_1 -axis of the present model. The initial offset at $t_1 = 0$ is found as $\Delta\eta_1 \approx 1.0002296 - 0.89868373 \approx 0.10155$ and the final offset at $t_1 = 34$ as $\Delta\eta_1 \approx 0.77537799 - 0.66243416 \approx 0.11294$, which is about 11% larger than the initial offset. Although both λ and t_1 appear to contribute the same term (i.e., the nonlinear term pertaining to the solution r_l in model Eq. (5.11)), the variation of the t_1 also induces the nonlinearity of the solution $r_{l'}$, $(l, l') \in (1, 2)$ or $(2, 1)$. This process occurs through the use of the constant parameters of the model equation such that the ω_2 mode transmission maxima follow similar behaviors of the ω_1 mode transmission maxima or vice-versa in the (t_1, η_1) plane. It is important to note that the t_1 -parameter space may be used to switch on or off both the modes in the system of the photonic crystal waveguide.

5.4 Off-Channel Features

In this section, the problem of a waveguide interacting with the linear or Kerr nonlinear impurities embedded into the off-channel (out-of-channel) site of a waveguide channel is discussed. Such a structure may allow the waveguide mode to interact with localized impurity modes bound on one or more off-channel Kerr sites which can exhibit new waveguide transmission effects. This type of optical problem has increased our interests to the photonic crystal waveguides of off-channel features in the discussion.

5.4.1 Single Frequency Waveguide Mode into Off-Channel Features

We consider a straight infinitely long photonic crystal waveguide of linear dielectric media interacting with a single off-channel site of Kerr nonlinear dielectric medium [42, 163]. The schematic plot of such a problem is given in Figure 5.1(b) on page 61. The waveguide channel is along the x -axis at lattice sites $(n, 0)$ where n are integers, and the off-channel Kerr nonlinear site is located on the y -axis at $(0, m)$ for $m > 0$ an integer. The coupling of the waveguide mode to the off-channel site is assumed to be weak so that the guided mode with frequency other than the resonance is not affected by the bound mode of the off-channel site. In the lattice, the coupling strength can be varied by changing the separation of the waveguide channel and the off-channel site, or by using dielectrics of different optical properties and changing the geometry of the Kerr impurity site.

By using the formalism in Chapter IV, the set of difference equations describing the waveguide modes of this system is

$$E_{n,0} = \gamma \{aE_{n,0} + b(E_{n+1,0} + E_{n-1,0})\}, \quad \text{with } |n| \geq 1, \quad (5.12a)$$

$$E_{0,0} = \gamma \{aE_{0,0} + b(E_{1,0} + E_{-1,0})\} + \gamma' c (1 + \lambda |E_{0,m}|^2) E_{0,m}, \quad (5.12b)$$

$$\text{and } E_{0,m} = \gamma' a (1 + \lambda |E_{0,m}|^2) E_{0,m} + \gamma c E_{0,0}, \quad (5.12c)$$

where γ' denotes γ of the off-channel Kerr site at $(0, m) = (0, 1)$, and c denotes a coupling between the $(0, 0)$ site of the waveguide channel and the off-channel site at $(0, 1)$. In this form, the transmissivity for moving waveguide modes incident onto the channel from left infinity $(-\infty, 0)$ is calculated from Eqs. (5.12a)-(5.12c). The solutions of the waveguide modes for $n < 0$ and $n > 0$ are of the form given in Eq. (5.2). Substituting these forms

into Eqs. (5.12a)-(5.12c) gives

$$\begin{pmatrix} 1 & 1 \\ e^{-ik} & e^{ik} \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} (xt) \\ (xt) e^{-ik} - \frac{\gamma' c}{\gamma b} (1 + \lambda |E_{0,1}|^2) E_{0,1} \end{pmatrix}, \quad (5.13)$$

$$\text{and } E_{0,1} - \gamma' a (1 + \lambda |E_{0,1}|^2) E_{0,1} - (xt) \gamma c = 0, \quad (5.14)$$

where the notations have their usual meaning as used in the previous section. Along with these equations, the dispersion condition, $\gamma(a + 2b \cos k) = 1$, is also obtained in the solution process.

Transmission coefficient in terms of the incident field amplitude is given by $T = |(xt)/u|^2$ so that using Eq. (5.13), we get,

$$T = \left\{ 1 + \frac{1}{4 \sin^2 k} \left(\frac{\gamma' c}{\gamma b} \right)^2 \left((1 + \lambda (xt)^2 |E_{0,1}|^2) E_{0,1} \right)^2 \right\}^{-1}, \quad (5.15)$$

with $(1 + \lambda (xt)^2 |E_{0,1}|^2) E_{0,1} = \{E_{0,1} - \gamma c\} / \gamma' a$, where the field solution, $E_{0,1}$, at the off-channel Kerr site is now expressed in terms of transmitted field amplitude. It is then computed by solving the cubic nonlinear Eq. (5.14) numerically. In the numerical treatment of the transmission coefficient, we first consider the case in which the off-channel site is made from linear dielectric impurity media, i.e., $\lambda x^2 = 0$. In this case, Eq. (5.14) reduces to $E_{0,1} = \gamma c / (1 - \gamma' a)$ so that a maximum of the $E_{0,1}$ occurs at $\gamma' a \approx 1$. Here, the maximum arises from the existence of a bound state of the single-site impurity at $\gamma' a = 1$. The transmission coefficient exhibits unusual behavior with resonant scattering from this bound state.

Figure 5.14 shows a plot of the results for a system of the linear impurity media (the case $\lambda x^2 = 0$) at the off-channel site. For this plot, we have taken nearest-neighbor

coupling $b/a = 0.0869$ from the photonic crystal waveguide system studied in the previous section or elsewhere, and with $k = 2.8$ representing the wave vector. The weak coupling $c/a = 0.02$ is chosen to be significantly smaller than the nearest-neighbor coupling to give a typical solution in the plot. To analyze the plot for the linear case, the linear mode

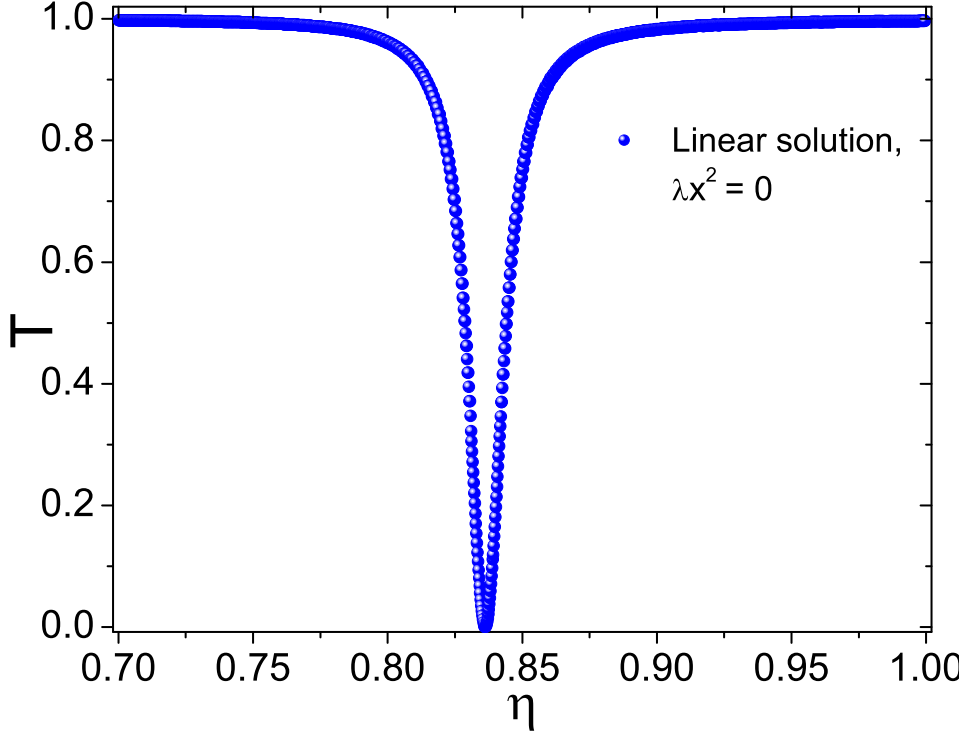


Figure 5.14: Plot of the transmission coefficient of the guided mode versus $\eta = \gamma'/\gamma$ for the system in Figure 5.1(b) of a waveguide weakly interacting with a single off-channel site composed of the linear impurity, i.e., the case $\lambda x^2 = 0$.

$E_{0,1} = \gamma c / (1 - \gamma' a)$ predicts a bound state at $\gamma'/\gamma = 1/\gamma a \approx 0.83624$, with γa evaluated at $b/a = 0.0869$ and $k = 2.8$ from the linear dispersion condition $\gamma a = \left(1 + 2\left(\frac{b}{a}\right) \cos(k)\right)^{-1}$. The corresponding numerically computed scattering resonance is shown in the plot at $\eta = \gamma'/\gamma \approx 0.83627$ (see Figure 5.14). The result of the transmission coefficient for the linear case, here, is similar to the analytical solution by McGurn in [42] for an off-channel problem. Experimental and simulation investigations of Noda *et al.* and Yakahane *et*

al. in [5, 21, 22, 73] report similar results for a different form of the off-channel impurity problem.

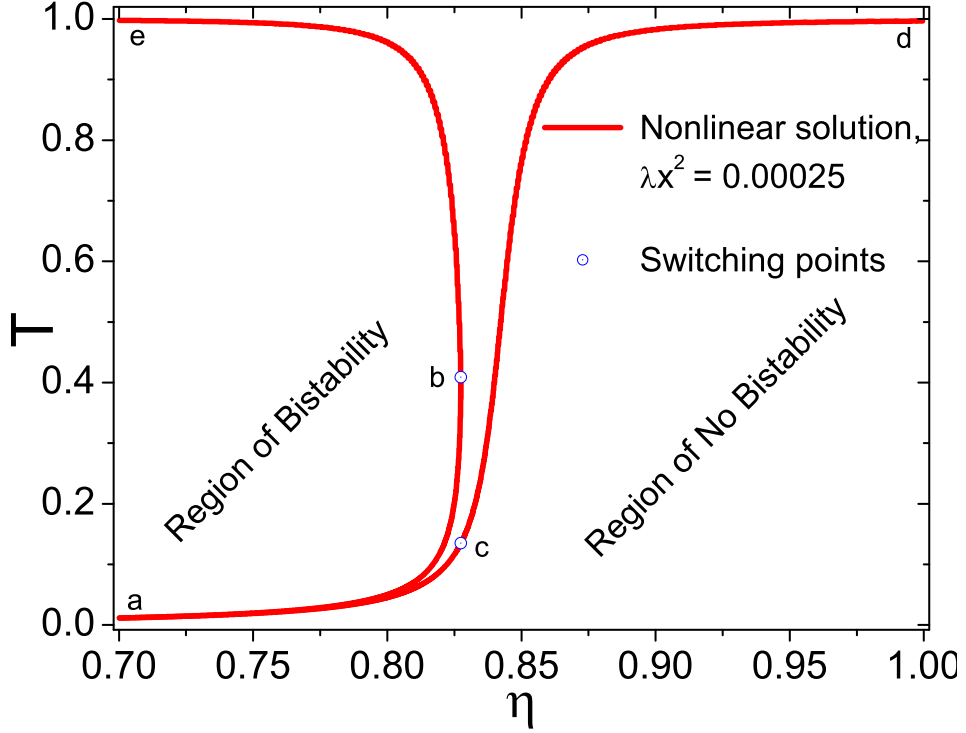


Figure 5.15: Solutions of Eq. (5.15) for the transmission coefficient of the guided mode versus $\eta = \gamma'/\gamma$ for the system in Figure 5.1(b) of a waveguide weakly interacting with a single off-channel site formed of the Kerr nonlinear impurity, i.e., the case $\lambda x^2 = 0.00025$.

Interest in the off-channel problem of Kerr nonlinear excitations comes from its specific ability to support multiple solutions exhibiting the concept of optical bistability. Such a nonlinear property on an off-channel problem is studied in Figure 5.15 by plotting the solutions of the transmission coefficient (Eq. (5.15)) through the off-channel impurity site, now of the Kerr nonlinearity parameter described by $\lambda x^2 = 0.00025$. All other constant parameters for the present problem, here, are taken from the linear case above, because the physical situation of the problem remains the same except the Kerr nonlinearity is present on the off-channel site now.

The plot in Figure 5.15 exhibits regions of multiple solutions for $\eta \leq 0.8273$. In this region, the initial state of the system is determined by the boundary condition to be either near $T \approx 1$ or $T \approx 0$. As η increases from zero, one solution for $T \approx 0$ transmission travels continuously on the lowest branch of the solutions. Another, near $T \approx 1$, switches branches near $\eta \approx 0.8273$ to continue the solution with increasing η back to $T \approx 1$.

5.4.2 Single Frequency Mode into Multiple Off-Channel Features

Here, extension of the single off-channel feature of the waveguide mode is made by considering the feature of two neighboring off-channel sites of different Kerr nonlinear impurity media. The two off-channel features support two localized bound state modes at different frequencies. Basically, we want to investigate how the presence of the impurity mode on the $(0, m+1)$ site affects the nonlinear resonance of the mode on the $(0, m)$ site modifying the behavior of the transmission coefficient. The waveguide channel is along the x -axis

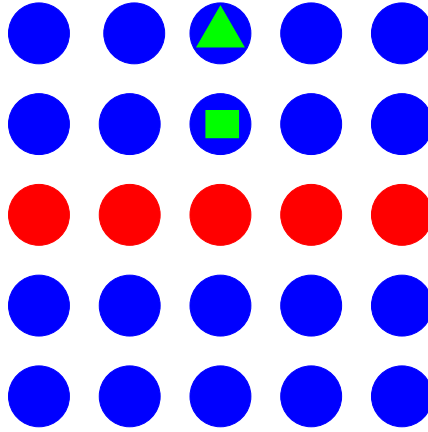


Figure 5.16: Schematic plot of a straight infinitely long waveguide of linear dielectric media (solid red circles) and a cluster of two off-channel Kerr impurity sites of different media. Here, *solid green square* represents off-channel Kerr media at the $(0, m)$ site characterized by γ' and Kerr parameter λ , and *solid green triangle* represents off-channel Kerr media at the $(0, m+1)$ site characterized by γ'' and Kerr parameter λ'' .

and the off-channel sites are located on the y -axis. The schematic of this system is drawn in Figure 5.16 in which the waveguide channel is shown by the line of solid red circles, and the two off-channel impurity media are depicted by the solid green square and triangle.

The set of difference equations for the waveguide modes of this system is obtained from Chapter IV. We find

$$E_{n,0} = \gamma \{aE_{n,0} + b(E_{n+1,0} + E_{n-1,0})\}, \quad \text{with } |n| \geq 1, \quad (5.16a)$$

$$E_{0,0} = \gamma \{aE_{0,0} + b(E_{1,0} + E_{-1,0})\} + \gamma' c (1 + \lambda |E_{0,m}|^2) E_{0,m}, \quad (5.16b)$$

$$E_{0,m} = \gamma' a (1 + \lambda |E_{0,m}|^2) E_{0,m} + \gamma'' b (1 + \lambda'' |E_{0,m+1}|^2) E_{0,m+1} + \gamma c E_{0,0}, \quad (5.16c)$$

$$E_{0,m+1} = \gamma'' a (1 + \lambda'' |E_{0,m+1}|^2) E_{0,m+1} + \gamma' b (1 + \lambda |E_{0,m}|^2) E_{0,m}, \quad (5.16d)$$

where c is the measure of the coupling strength, usually a weak interaction, between the field mode at the $(0,0)$ site on the waveguide channel and the off-channel impurity mode at the $(0,m)$ site. The γ' and Kerr parameter λ characterize the impurity media at the $(0,m)$ site as usual, and the γ'' and Kerr parameter λ'' characterize the impurity media at the $(0,m+1)$ site. The off-channel parameters, particularly γ'' and λ'' , will be the main subject of discussions in the following paragraphs.

Solving Eqs. (5.16a) through (5.16d) for the guided mode incident from infinity onto the off-channel feature, the transmission coefficient of the mode and the nonlinear equations involving both $E_{0,m}$ and $E_{0,m+1}$ field modes are obtained as

$$T = \left\{ 1 + \frac{1}{4 \sin^2 k} \left(\frac{\gamma' c}{\gamma b} \right)^2 \left((1 + \Lambda_{0,m}) E_{0,m} \right)^2 \right\}^{-1}, \quad (5.17a)$$

$$E_{0,m} \left\{ 1 - \gamma' a (1 + \Lambda_{0,m}) \right\} - \gamma'' b (1 + \lambda'' |E_{0,m+1}|^2) E_{0,m+1} - \gamma c = 0, \quad (5.17b)$$

$$E_{0,m+1} \left\{ 1 - \gamma'' a (1 + \lambda''(xt)^2 |E_{0,m+1}|^2) \right\} - \gamma' b (1 + \Lambda_{0,m}) E_{0,m} = 0, \quad (5.17c)$$

with the factor $(1 + \lambda(xt)^2 |E_{0,m}|^2) E_{0,m}$ in Eq. (5.17a) is now expressed as

$$(1 + \Lambda_{0,m}) E_{0,m} = \left\{ E_{0,m} - \gamma c - \gamma'' b (1 + \lambda''(xt)^2 |E_{0,m+1}|^2) E_{0,m+1} \right\} / \gamma' a \quad (5.18)$$

in contrast to simply $(1 + \Lambda_{0,m}) E_{0,m} = \{E_{0,m} - \gamma c\} / \gamma' a$ as given in the single site case in Eq. (5.15). The $\Lambda_{0,m}$ written in the above expressions is a shorthand notation for $\lambda(xt)^2 |E_{0,m}|^2$ in that the x and t enter through a transmitted amplitude of the field solution. Notice that in the limits $\lambda'' x^2 = 0$ and $\gamma'' = 0$, the problem of the two-sites model in Eqs. (5.17a) through (5.18) reduces to exactly the single off-channel site limit discussed in the previous Subsection 5.4.1. Also notice that Eqs. (5.17b) and (5.17c) are nonlinear in $E_{0,m}$ and $E_{0,m+1}$ and can be solved simultaneously for $E_{0,m}$ and $E_{0,m+1}$, both real, using the standard numerical routines (e.g., Newton-Raphson method) of nonlinear equations. Unlike the single off-channel case where T depends on only one solution of the $E_{0,m}$ field, the T of the two sites problem generally depends on both $E_{0,m}$ and $E_{0,m+1}$, because the solutions of them are interdependent through Eqs. (5.17b) and (5.17c).

The two off-channel sites model can be simplified by taking the limit $\lambda'' x^2 = 0$. This removes the nonlinearity effect from the $(0, m+1)$ site while retaining the nonlinearity on the $(0, m)$ site through the λ . However, the linear effect in the $(0, m+1)$ site still remains. In this limit, the nonlinear Eqs. (5.17b) and (5.17c) can be combined into a single nonlinear equation in terms of only the $E_{0,m}$ mode:

$$E_{0,m} \left\{ 1 - \gamma' a f (1 + \lambda(xt)^2 |E_{0,m}|^2) \right\} = \gamma c \quad \text{with } f = 1 + \gamma'' b / (1 - \gamma'' a), \quad (5.19)$$

where f appears as a factor describing the dielectric response in the $(0, m+1)$ site.

In Figure 5.17 the transmission coefficient, T , as a function of $\eta = \gamma'/\gamma$ is plotted for three different ratios of $\eta'' = \gamma''/\gamma = 1.0, 0.0$, and 0.50505 . The plot, then, consists of three sets (blue, black, and red) of the curves corresponding to the three η'' values, including a dashed curve for the $\eta'' = 0.6$. This shows the behavior of T in the presence of the modes modified by the dielectric impurity on the $(0, m+1)$ site as studied in [146]. The results in the plot are presented for $b/a = 0.1738$, $c/a = 0.04$, $k = 2.5$, $\lambda x^2 = 0.00125$,

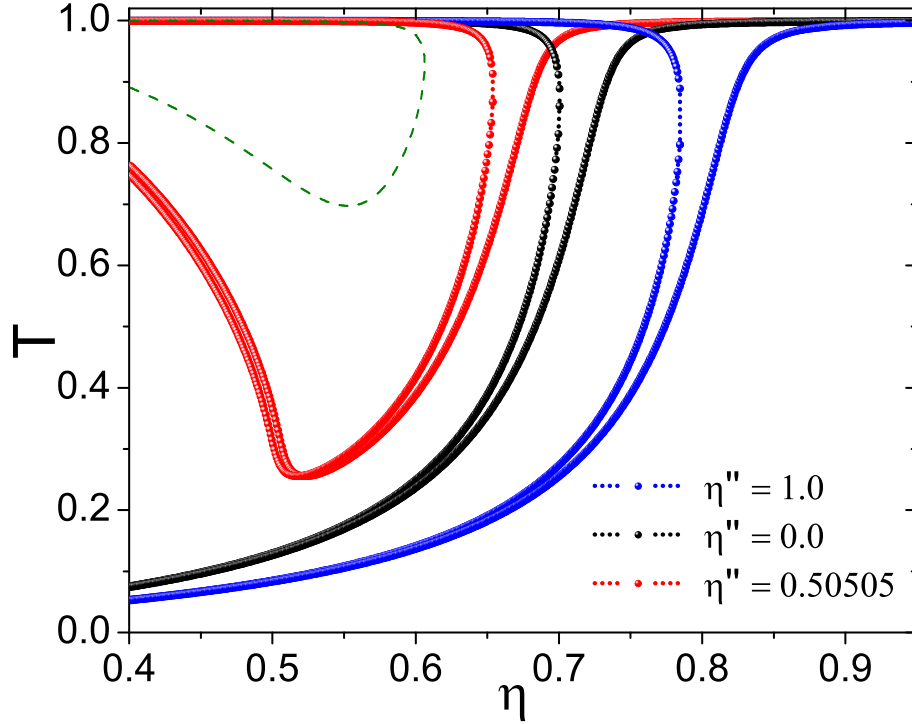


Figure 5.17: Plot of the transmission coefficient of the guided mode versus $\eta = \gamma'/\gamma$ for the system in Figure 5.16 where Kerr value at the $(0, m)$ site is $\lambda x^2 = 0.00125$ and at the $(0, m+1)$ site is $\lambda'' x^2 = 0.0$. The plot is made at three different ratios of $\eta'' = \gamma''/\gamma$: Center (black) curve is for the $\eta'' = 0$, Right (blue) curve is for the $\eta'' = 1$, and Left (red) curve is for the $\eta'' = 0.50505$. Dashed curve shows only the bistable part of the transmission profile for the $\eta'' = 0.6$.

and $\lambda'' x^2 = 0.0$ at different ratios of η'' labelled inside the plot. The set of the curves in the center (black) with $\eta'' = 0.0$ is the result for the transmission of the guided mode when assuming there is no second off-channel site. The results as seen in the black curves are

similar to those in Figure 5.15 for only one out-of-channel site, i.e., only the $(0, m)$ site. The set of the curves on the right are for the case in which there is a second out-of-channel site present with the $\eta'' = 1$, and the set of the red curves on the left are for the case of the second out-of-channel site with the $\eta'' \approx 0.50505$. The presence of the second site is found to shift the resonance upward for the $\eta'' = 1.0$ and downward for the $\eta'' = 0.50505$ with respect to the resonance corresponding to the $\eta'' = 0$ (the case of only the single site). As seen in the plot, the η'' not only caused the shifting-effect, but also strongly perturbed the transmissions near the $T \approx 0$, which resulted in a lifting-effect and displayed the valley like features for $\eta'' = 0.50505$ and $\eta'' = 0.6$. The composite effect of the λ'' and η'' or γ'' on the resonant transmission profile of the guided mode is complicated, but by taking $\lambda''x^2 = 0.0$, the effect of the η'' simplifies. Such a simplification was also done in studies by McGurn in [146].

Another interesting characteristics of the two sites model is the self-steepening-like behavior in the transmission coefficient. This is studied by setting the ratio of η'' to a fixed number and introducing nonlinearity into the system only through various combinations of λx^2 and $\lambda''x^2$. Figure 5.18 shows a plot for the transmission coefficient versus $\eta = \gamma'/\gamma$ for three different combinations of $(\lambda x^2, \lambda''x^2)$: $(1.25 \times 10^{-4}, 1.25 \times 10^{-3})$, $(1.75 \times 10^{-3}, 1.75 \times 10^{-3})$, and $(3.75 \times 10^{-3}, 1.25 \times 10^{-3})$ at a fixed ratio of the $\eta'' = \gamma''/\gamma = 1$. Other constant parameters for this result are adopted from the previous result in Figure 5.17. The effect of the given combinations of $(\lambda x^2, \lambda''x^2)$ to the two sites of the present problem is seen to steepen the resonant transmission profiles of the guided mode to the left.

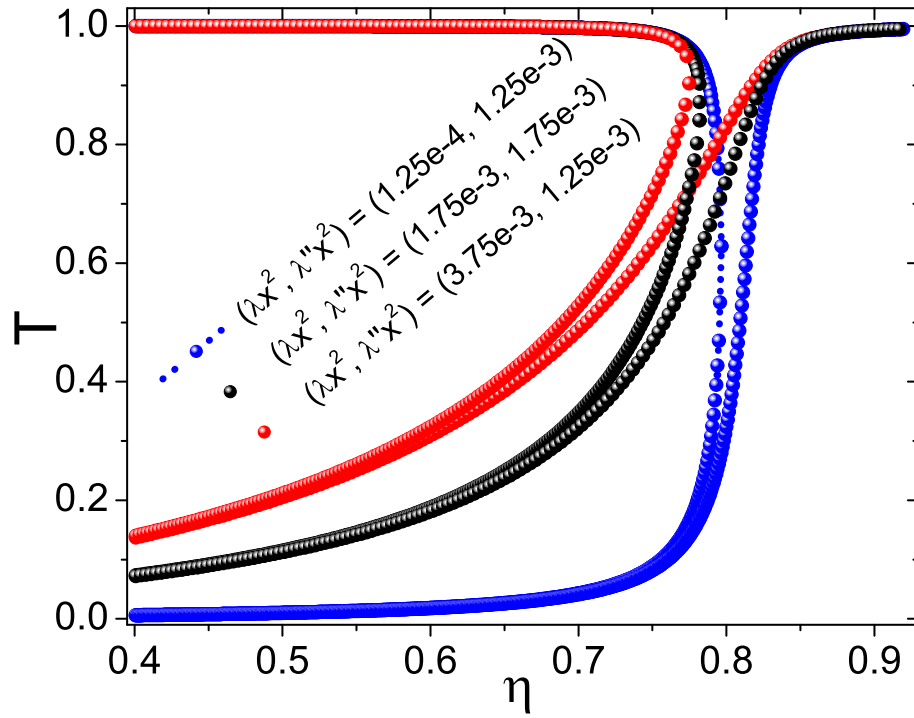


Figure 5.18: Plot of the transmission coefficient of the guided mode versus $\eta = \gamma'/\gamma$ for the guided mode for three different combinations of $(\lambda x^2, \lambda'' x^2)$. *Right (blue) curve* is for the $(1.25 \times 10^{-4}, 1.25 \times 10^{-3})$, *Center (black) curve* is for the $(1.75 \times 10^{-3}, 1.75 \times 10^{-3})$, and *Left (red) curve* is for the $(3.75 \times 10^{-3}, 1.25 \times 10^{-3})$. The plot illustrates self steepening like nonlinear effect.

CHAPTER VI

Two Different Frequencies into the Single Off-Channel Features

We now treat waveguide modes of two different frequencies, $\{\omega_l\}$, $l \in [1, 2]$, both within the same stop band of a photonic crystal, and both are incident from infinity down the waveguide channel formed in a photonic crystal, similar to the problem in the previous Chapter V Section 5.3. However, the waveguide modes in this case are scattered by a single off-channel site of the Kerr nonlinear media located at $(0, m)$ for $m > 0$ of the photonic crystal square lattice (Figure 5.1(b)). A topographical representation of this model of photonic crystal waveguide is depicted in Figure 6.1, which was also studied

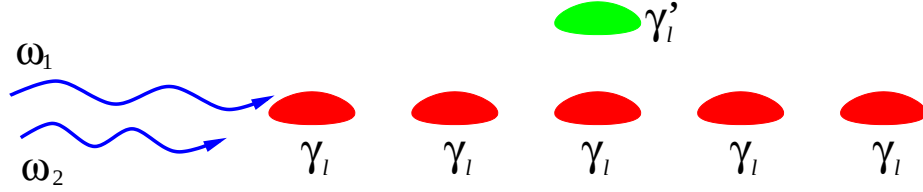


Figure 6.1: Schematic illustration of the two different frequencies, ω_1 and ω_2 , interacting through an off-channel Kerr nonlinear dielectrics in a 2D photonic crystal lattice. The γ_l represents the dielectric property of the waveguide channel, and the γ'_l denotes γ_l for the Kerr site with $l \in (1, 2)$. Here, only the waveguide channel lattice sites (solid red oval shapes) and out-of-channel Kerr impurity lattice site (solid green oval shape) are shown.

in the case of the single frequency mode in the previous chapter. We consider weak couplings for the interaction between the waveguide channel and the Kerr defect at the $(0, m)$ site in order to model the transmission characteristics of the guided modes. The coupling strength $\{c_l\}$ can be varied by changing the separation of the waveguide channel and the off-channel Kerr site or by changing the nonlinearity of the Kerr site. The Kerr nonlinearity may be changed by using dielectrics of different optical properties or by

changing the size, shape, or geometry of the defect. Indeed, the weak coupling, $\{c_l\}$, including on-site and nearest-neighbor couplings, a_l and b_l , respectively, may depend on the chemistry and geometry of the dielectric materials of the photonic crystal lattice and the defect itself. Additionally, here, we extend the generalization of two-frequency model explained on page 75 in the previous Chapter V with the following remark: The form of the two-frequency interaction we use in the later discussions is based on Eq. (5.3-3) of Reference [164] and gives a very general expression for the Kerr coefficients of the interaction. As discussed in that reference the interaction is often simplified and made less general for certain engineering applications. This is accomplished by reducing the number of independent Kerr coefficients needed to specify the interaction.

Interest in off-channel characteristics of the Kerr nonlinear media is that the field dependence of their dielectric properties allows two different frequency waveguide modes to interact with one another by a modulation of the off-channel site dielectric properties [42, 45, 47, 48, 163]. This modulation can be maximized in frequency regions at which localized modes on the off-channel features are resonantly excited by one or both of the waveguide modes [48, 71]. The resonantly localized modes cause the waveguide modes to affect one another's propagation down the waveguide channel. For example, one mode can be used to model numerically the transmission characteristics of the other mode. Also, the one mode can be used to switch on or off the other mode's propagation down the same waveguide channel, including the amplitude modification and other possibilities arising from a localized mode bound to the off-channel feature as marked by McGurn in [71].

6.1 The Equations

For the numerical computation of the transmission of the waveguide modes with an off-channel feature, we use the notation $\{c_l\}$, $l \in [1, 2]$, which corresponds to guided modes ω_1 and ω_2 for the weak couplings and the other usual notations in Section 5.3 for all other parameters. Thus the difference equations for $|n| \geq 1$, $(0, 0)$, and $(0, m)$ sites in the order can be written as

$$E_{n,0}^l = \gamma_l \left[a_l E_{n,0}^l + b_l (E_{n+1,0}^l + E_{n-1,0}^l) \right], \quad (6.1a)$$

$$E_{0,0}^l = \gamma_l \left[a_l E_{0,0}^l + b_l (E_{1,0}^l + E_{-1,0}^l) \right] + \gamma'_l c_l [1 + \lambda \delta] E_{0,m}^l, \quad (6.1b)$$

$$\text{and } E_{0,m}^l = \gamma'_l a_l \left[1 + \lambda \left(d_l |E_{0,m}^l|^2 + e_l |E_{0,m}^{l'}|^2 \right) \right] E_{0,m}^l + \gamma_l c_l E_{0,0}^l \quad (6.1c)$$

where $\delta = \left(d_l |E_{0,m}^l|^2 + e_l |E_{0,m}^{l'}|^2 \right)$. The γ'_l denotes γ_l of the off-channel Kerr site at $(0, m)$.

The solutions or boundary conditions for these equations describing the propagation of the waveguide modes can have a planewave solution form

$$E_{n,0}^l = \begin{cases} u_l e^{ik_l n} + v_l e^{-ik_l n}, & n \leq 0, \\ (xt_l) e^{ik_l n}, & n \geq 0, \end{cases} \quad (6.2a)$$

as explained in Section 5.3, and the solution at the off-channel Kerr site

$$E_{0,m}^l = s_l e^{i\theta_l} = s_l, \quad \because \theta_l = 0, \quad (6.2b)$$

for $l = 1$ or 2 . The $E_{0,m}^l$ is complex in general, so it has a magnitude s_l and phase $e^{i\theta_l}$, as shown in Eq. (6.2b); but, we assume $\theta_l = 0$. As usual, u_l , v_l , and (xt_l) denote amplitudes of the incident, reflected, and transmitted field of the frequency ω_l ($l = 1$ or 2), respectively. Substituting these boundary conditions (Eqs. (6.2a) and (6.2b)) into the Eqs. (6.1a)-(6.1c) result in a set of six difference equations (not shown here, but

their derivation is straight forward) describing the propagation of two guided modes at frequencies within a stop band of the photonic crystal forming the waveguide. After some algebra, the transmission and reflection coefficients for scattering of the waveguide modes in the off-channel Kerr features can be expressed as

$$T_l = \left| \frac{(xt_l)}{u_l} \right|^2 = \frac{4 \sin^2 k_l}{4 \sin^2 k_l + \left[\frac{c_l}{b_l}(r_l - \gamma_l c_l)(1 + 2 \frac{b_l}{a_l} \cos k_l) \right]^2} \quad (6.3a)$$

$$\text{and } R_l = \left| \frac{v_l}{u_l} \right|^2 = \frac{\left[\frac{c_l}{b_l}(r_l - \gamma_l c_l)(1 + 2 \frac{b_l}{a_l} \cos k_l) \right]^2}{4 \sin^2 k_l + \left[\frac{c_l}{b_l}(r_l - \gamma_l c_l)(1 + 2 \frac{b_l}{a_l} \cos k_l) \right]^2} \quad (6.3b)$$

where $r_l = \frac{s_l}{t_l}$, $l = 1$ or 2 . Here, the Kerr field solutions, r_l , are expressed in terms of the transmitted field amplitudes. The nonlinear equations for these solutions are obtained as

$$d_1(\lambda x^2)|t_1|^2|r_1|^2r_1 + \left[1 + e_1(\lambda x^2)|t_2|^2|r_2|^2 - \frac{1}{\gamma'_1 a_1} \right] r_1 + \frac{\gamma_1 c_1}{\gamma'_1 a_1} = 0 \quad (6.4a)$$

$$\text{and } d_2(\lambda x^2)|t_2|^2|r_2|^2r_2 + \left[1 + e_2(\lambda x^2)|t_1|^2|r_1|^2 - \frac{1}{\gamma'_2 a_2} \right] r_2 + \frac{\gamma_2 c_2}{\gamma'_2 a_2} = 0. \quad (6.4b)$$

Note that we take the off-channel Kerr site at $(0,1)$ for numerical convenience.

6.1.1 Results and Discussions

The difference equation formalism reviewed for two frequencies of the present problem can be used to study both the linear and nonlinear transmissions of the waveguide modes. In particular, we analyze the effect of the Kerr nonlinearity in the resonant scattering of the waveguide modes. Note that we first apply the linear limit, i.e., $e_2 = d_2 = 0$, in Eq. (6.4b) that results in a linear solution of the r_2 : $r_2 = \gamma_2 c_2 / (1 - \gamma'_2 a_2)$, which renders the resonant transmission of the ω_2 mode into the linear profile. This not only simplifies the problem, but also allows one to consider the ω_1 mode as the primary interest for the numerical analysis without the loss of its qualitative nature of transmission or reflection

coefficient or its interaction with the ω_2 mode through off-channel nonlinearity. Basically, the discussion here focuses on the self-interactions of the two guided modes controlled by the off-channel dielectric modulations.

We adopt descriptions of the coupling ratios of Section 5.3 on page 78 to the current problem in order to generate the data for the simulation of the transmission, or reflection coefficient, or field excitation about the off-channel site, etc. Here, we simply list the values of those ratios, including the other constant parameters necessary for this problem: $a_2/a_1 = 0.8952$, $b_1/a_1 = 0.0852$, $b_2/a_1 = 0.0701$, $k_1 \approx 3.0$, $k_2 \approx 1.8$, $\lambda_1 x^2 = \lambda_2 x^2 = 0.0025$, and $e_1 = d_1 = 1$. Besides these, the weak coupling ratios, which are relevant to off-channel features only, are taken such that $c_1/a_1 = c_2/a_1 = 0.02$ [71]. Note that the values of these constant parameters will be the same for each simulation/result in this section, below.

Figure 6.2 shows the results for a special condition (single mode condition) on our formalism in Eqs. (6.3a) - (6.4b). This means the field amplitudes u_2 , v_2 , t_2 , and r_2 ,

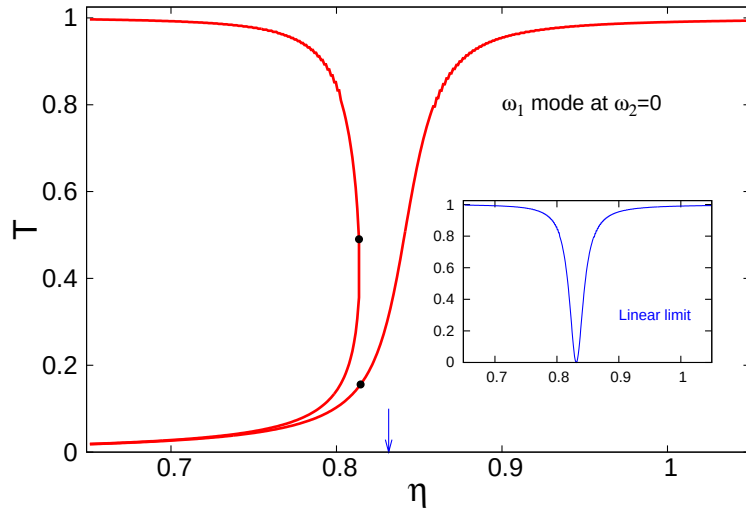


Figure 6.2: Plot of the transmission coefficient versus $\eta = \gamma'/\gamma$ for the condition of single mode $\omega (\equiv \omega_1)$ at stop band frequency interacting with an off-channel Kerr feature. The system exhibits bistability below the jump points indicated by the two black dots. The linear limit (see an arrow head down) of the single mode occurs at $\eta \approx 0.8315$. The insert shows the result for the linear limit with a resonance.

describing the ω_2 mode in these equations, are set to zero, which results in single mode equations containing only the field amplitudes u_1 , v_1 , t_1 , and r_1 , describing the ω_1 mode transmission of interaction. We expect, upon this special condition, the method here could describe a type of behavior the single off-channel Kerr waveguide could display. Essentially, the result in Figure 6.2 is the specific case study of the variety of results that will be presented in Figures 6.3 and 6.4. The result in Figure 6.2 shows a plot of transmissivity as a function of $\eta = \gamma'/\gamma$ when only the ω_1 mode exists in the system. Notice here that we removed numerical subscripts on γ' and γ ; the reason is we use only one frequency mode in order to produce this result.

As can be seen in the plot, the resonant scattering of the waveguide mode with the localized off-channel Kerr field occurs at $\eta = 0.8315$, which is the linear limit in this case. The limit is also indicated by an arrow headed down in the figure or alternatively this limit is shown by the linear transmission resonance of the mode as seen in the insert. As we expected in a discussion of the single mode condition in the previous paragraph, Figure 6.2 describes, essentially, a type of bistable resonance. Here, below the linear limit (more accurately, below the limit of the input η corresponding to the jump points indicated by two black dots) the system exhibits bistability that describes the possibility of two resonant transmission states and both are the stable states that depend on the initial values (inputs). The bistability in this case may arise from the Kerr nonlinearity introduced into an off-channel site that inherently generates a localized mode. Such an off-channel localized mode affects transmission of the waveguide mode incident into the waveguide channel. The bistable states arising from the waveguide structure in this discussion may have the application in the bistable devices.

Now, we proceed to general discussions of both the ω_1 and ω_2 modes present (nonzero) in the model equations of the problem in the limit $d_2 = e_2 = 0$. The most interesting consequence of the off-channel Kerr-induced transmission in this problem is the bistable resonance at the lower region of η_1 , which is the region below the linear limit of the problem. Compared to the results in Figure 6.2, where a single mode interacting with the off-channel feature shows limited types of behaviors, the interactions of the two frequencies here can present the variety of behaviors the system could display. For example, it may exhibit bistability including the peak, dip, kink, valley, and island features of transmissions when two guided modes, ω_1 and ω_2 , are incoming into the waveguide channel and interacting each other via the off-channel Kerr site. Note that we restricted the resonant excitation of the ω_2 mode to the linear model by using the numerical constraints as described on page 100 and elsewhere in this discussion. Nevertheless, such a linearly excited ω_2 mode significantly affects the ω_1 mode transmission of interaction that will be discussed below.

Figure 6.3 shows the transmission into the waveguide channel and the linear resonant scattering of the ω_2 mode from the localized modes of the off-channel Kerr site. Notice that the linear scattering resonances of the ω_2 mode occurs at $\eta_1 \approx 1.0307, 0.8770, 0.8341, 0.7753, 0.6935$, and 0.6446 , respectively, corresponding to six different ratios of $\eta' = \gamma'_2/\gamma'_1 = 0.9012, 1.0591, 1.1125, 1.1977, 1.3385$, and 1.4325 . This result, the linear transmission of the ω_2 mode as a function of the parameter space η_1 of the ω_1 mode, does not display bistability because we simplified the problem with the condition of the $e_2 = d_2 = 0$ in the numerical treatment. It is very important to note here that the transmission resonances in the ω_2 as seen on the η_1 -axis are correlated to the kinks and peaks

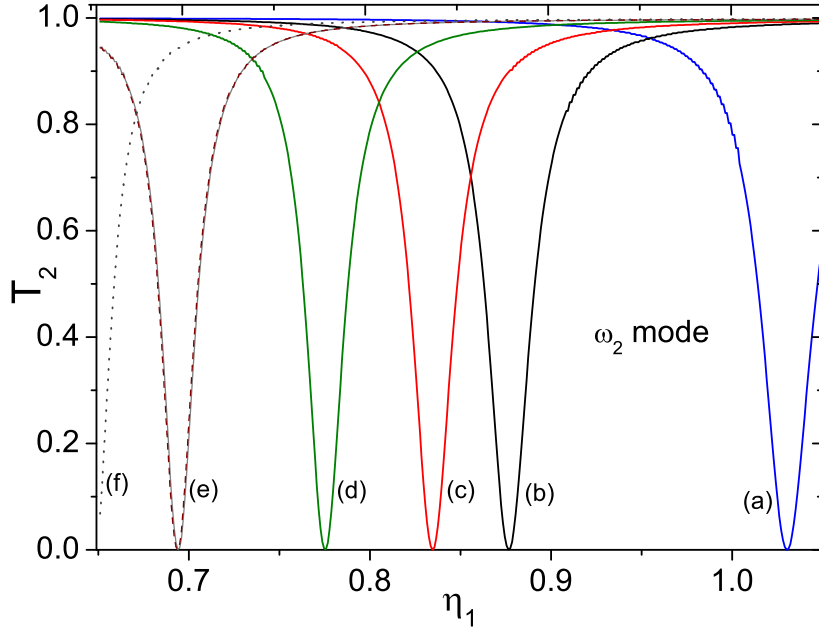


Figure 6.3: Plot of the resonant transmission coefficient versus η_1 of the ω_2 mode for the system with an off-channel Kerr site. Curves labelled (a), (b), (c), (d), (e), and (f) respectively are for six different ratios of $\eta' = \gamma'_2/\gamma'_1 = 0.9012, 1.0591, 1.1125, 1.1977, 1.3385,$ and 1.4325 . The results show the linear transmission resonances in the ω_2 mode at $\eta_1 = \gamma'_1/\gamma_1 \approx 1.0307, 0.8770, 0.8341, 0.7753, 0.6935,$ and 0.6446 corresponding to the six ratios of η' .

in the ω_1 transmission profiles. This will be explained in detail in a case study of the ω_1 mode in the next result. Actually, the data for Figure 6.3 and 6.4 were generated from the same computer run by using the same set of the ratios of η' , but they are stored in two different figures for the presentation purpose only.

Figure 6.4 simulates transmissivity of the induced ω_1 mode as a function of the $\eta_1 = \gamma'_1/\gamma_1$ for six different ratios of $\eta' = \gamma'_2/\gamma'_1 =$ (a) 0.9012, (b) 1.0591, (c) 1.1125, (d) 1.1977, (e) 1.3385, and (f) 1.4325. In this result, the ω_2 mode affects the transmissions of the ω_1 mode through the localized mode excited in the off-channel Kerr site.

Notice that the data on each plot here corresponds to the data for the curves labelled (a), (b), (c), (d), (e), and (f) in Figure 6.3, meaning the data for plot (a) in Figure 6.4 and the curve (a) in Figure 6.3 were generated simultaneously under the same

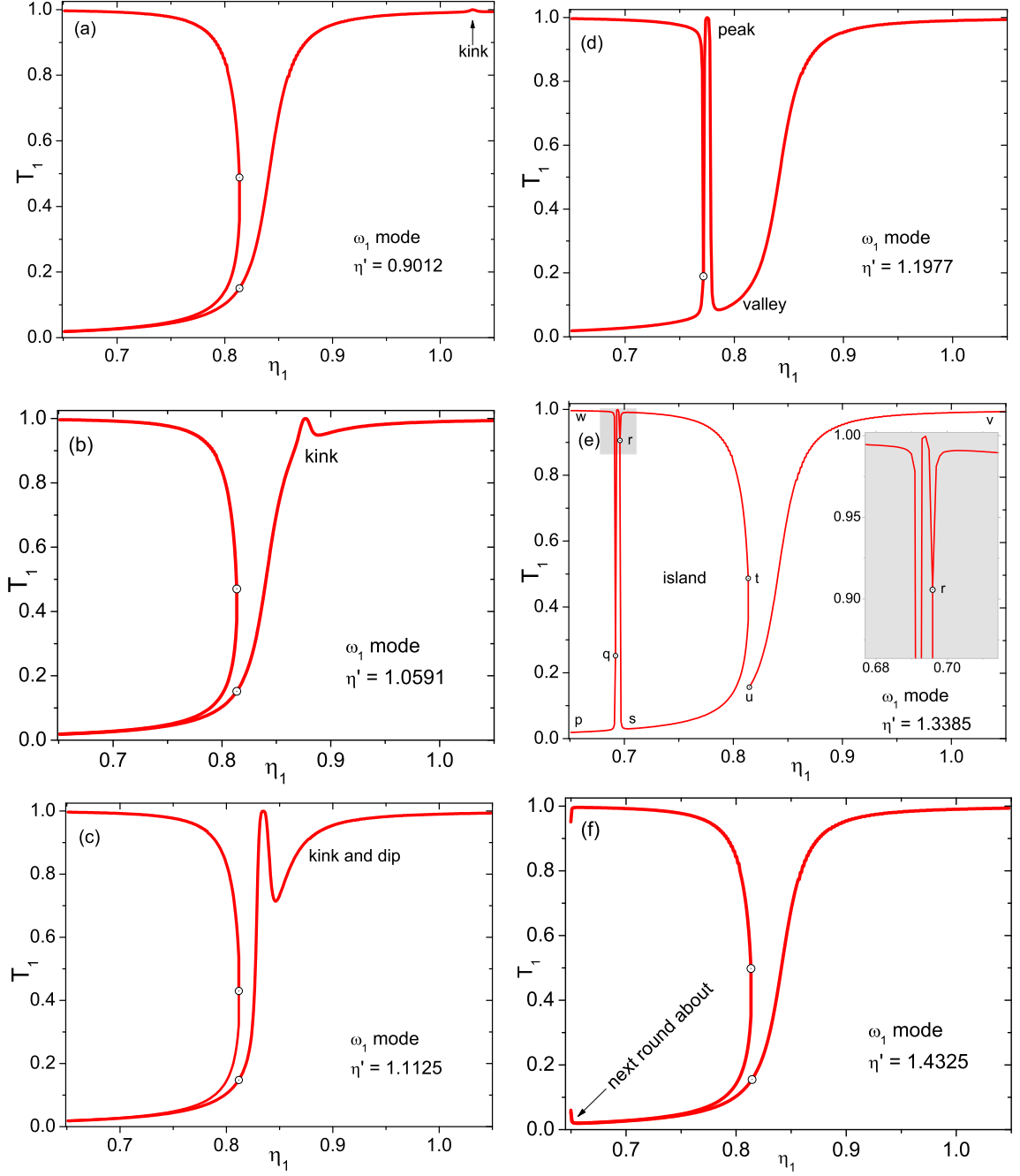


Figure 6.4: Plots of the simulated transmission coefficient versus $\eta_1 = \gamma'_1/\gamma_1$ of the waveguide mode interacting through a Kerr off-channel site for the ratios of $\eta' =$ (a) 0.9012, (b) 1.0591, (c) 1.1125, (d) 1.1977, (e) 1.3375 to 1.3385, and (f) 1.4325. Particularly, the nonlinear behaviors of the transmissions of the ω_1 mode induced by the linear ω_2 mode are shown on the plots. The kink, dip, valley, and island as seen in the plots are resulted from the effect of the resonant excitations of the ω_2 mode. The insert in the plot (e) is an enlarged version of the kink formed on the same plot. The open circles on the solution curves show the switching points of the bistable scatterings.

numerical conditions, and so on for (b) through (f) in both figures. Essentially, the plots (a) through (f), for the six ratios of η' in the order from smaller to larger, display the transmission behaviors of the ω_1 mode incoming down the waveguide channel and past the off-channel site, with the incoming ω_2 mode perturbing the transmission of the ω_1 mode by virtue of the contribution to the Kerr effect.

Now we analyze the plots (results) presented in Figure 6.4 case by case in the following paragraphs in order to explain the features of each individual plot. The bistable solutions on these plots may be explained as follows. Plot (a) shows transmission of the ω_1 mode for the ratio of $\eta' = \gamma'_2/\gamma'_1 = 0.9012$. Corresponding to this ratio, the resonant scattering of the ω_2 mode occurs at $\eta_1 \approx 1.0307$, as seen in Figure 6.3. Since $\eta_1 \approx 1.0307$ is far above the linear limit ($\eta_1 \approx 0.8315$) of the system, the effect of the ω_2 on the ω_1 mode transmission of interaction is very small, which can be realized only with a little kink (bump) at $\eta_1 \approx 1.0307$ in this plot.

Plot (b) shows the transmission coefficient of the ω_1 mode for the ratio of $\eta' = 1.0591$, a higher ratio than in the case of plot (a). In this plot, the resonant scattering of the ω_2 mode, as seen in Figure 6.3, occurs at $\eta_1 \approx 0.8770$. This value is still above the linear limit, but not as far above as in the previous case in plot (a). Because of this reason, the resonance of the ω_2 mode affects transmission of the ω_1 mode in the near vicinity of the $\eta_1 \approx 0.8770$, resulting in an easily noticeable kink on the linear part of the ω_1 mode transmission. Plot (c) is similar to plot (b), however, the effect of the ω_2 mode on the transmission of the ω_1 mode is larger in this case.

Plot (d) shows transmission of the ω_1 mode for the ratio of $\eta' = 1.1977$. In this case, the resonant scattering of the ω_2 mode occurs at $\eta_1 \approx 0.7753$. As seen in the plot,

the effect causes the bistable region to downshift below the limit $\eta_1 \approx 0.7753$. This limit was maintained at $\eta_1 \approx 0.8315$ in previous plots where the ω_2 affects weakly or negligibly on the resonant transmission of the ω_1 mode. In addition, the effect is seen as a peak (like a giant kink) around $\eta_1 \approx 0.7753$ and a deep valley just beside the peak.

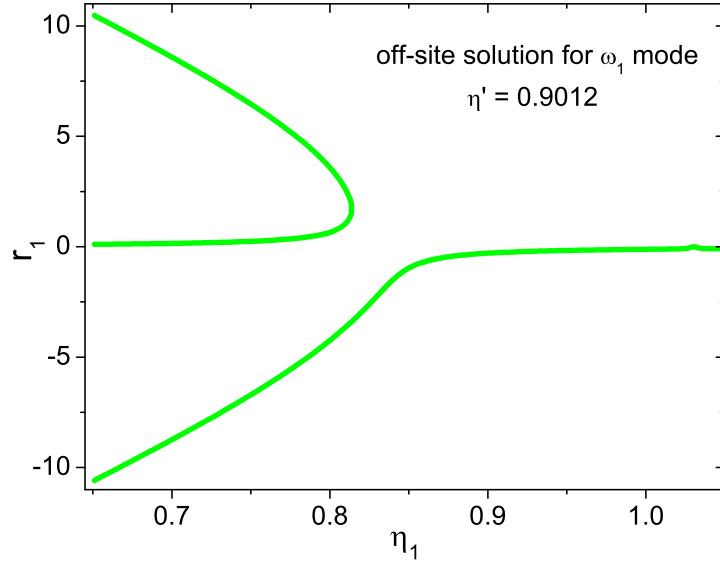
The result in plot (e) is presented for the ratio of $\eta' = 1.3385$ for the transmission of the ω_1 mode. Corresponding to this ratio, the resonant scattering of the ω_2 mode falls at $\eta_1 \approx 0.6935$, which is further below than the linear limit ($\eta_1 \approx 0.8315$) of the system. As a result, the effect of the ω_2 mode is the strongest, particularly, in the case of the present plot. The system gives the upper (the curve $r - t$) and lower (the curve $r - s - t$) slices of the solutions that allow us to form an island-like topographical feature between the new (lowest or critical) limit at $\eta_1 \approx 0.6939$ and the original linear limit at $\eta_1 \approx 0.8315$. In this result, the transmission coefficient is traced out through the lower slices of the solutions. Here, the curve $p - q - r - s - t - u - v$ is in the forward bias of the input, when the transission is traced out through the upper slices, the curve $v - u - t - r - q - w$ is in the reversed bias of the input. The four open circles at points q , r , t , and u indicate the switching points of the solutions as usual.

The solutions of the island-like feature in plot (e) may be called a meta-bistability, because it is difficult to force always consistently the system to exhibit stable solutions over the region of the island. This part of the result is still under our investigation and any sort of new characteristics of island-like features found out of the investigation will be reported in future research. In addition, the plot shows a tendency to downshift the island's area below the new limit; however, the plot also indicates a tendency of shifting the bistable region upward by forming a mini-kink over the features that the plot displays.

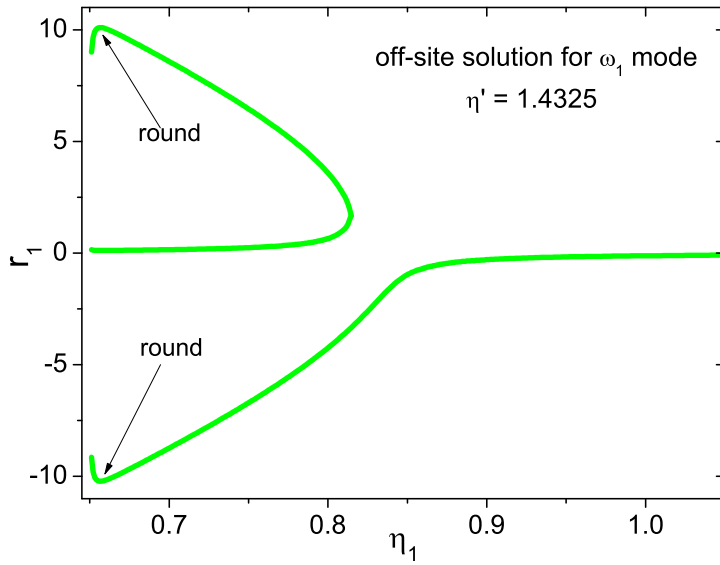
The mini-kink profile is shown in an enlarged form (see the shaded area) inside plot (e) itself. For a higher ratio of η' than $\eta' = 1.3385$, the bistable range tends to recover its initial state. This is why the transmission profiles as displayed in plot (a) is seen almost identical as in plot (f), the recovered plot.

Plot (f) clearly presents the result showing a complete recovery of the original bistable profile of the system, and the result is also showing the beginning of the next new limit of the island by forming the rounded ends in the solution curves at $\eta_1 \approx 0.6509$, as seen in the plot. Indeed, this result, as usual, plots the resonant transmission of the ω_1 mode for the ratio of $\eta' = 1.4325$ showing the bistability below the original linear limit at $\eta_1 \approx 0.8315$. The corresponding transmission resonances of the ω_2 mode occurs at $\eta_1 \approx 0.6446$ (not seen in the plot as this value is out of the plotting range), which is below the new limit at $\eta_1 \approx 0.6939$ (as discussed in plot (e)). This shows that the scattering resonances for the ω_2 mode are gradually moved downwards as the ratios of η' are gradually increased.

Also, the area of the island-like feature is increased as each of the ratios of η' are increased, which is obvious from the round corner ends of the solution curves, as indicated in the plot at $\eta_1 \approx 0.6509$ (just like the round corner at point s in plot (e)). This concept can be understood better using the result in Fig 6.5, where the field solutions r_1 versus η_1 of the ω_1 mode using numerical conditions in Figure 6.4(a) and (f) are plotted. As can be seen in Figure 6.5, the field solution curves on both plots are found almost identical, except around the $\eta_1 \approx 0.6509$. In fact, the field solution at $\eta_1 \approx 0.6509$ in Figure 6.5(b) is seen to be perturbed due to a different (but higher) ratio of the η' than its value in Figure 6.5(a). Such a perturbation in the field solution causes an increase the area of



(a) Field solution for the plot in Figure 6.4(a)



(b) Field solution for the plot in Figure 6.4(f)

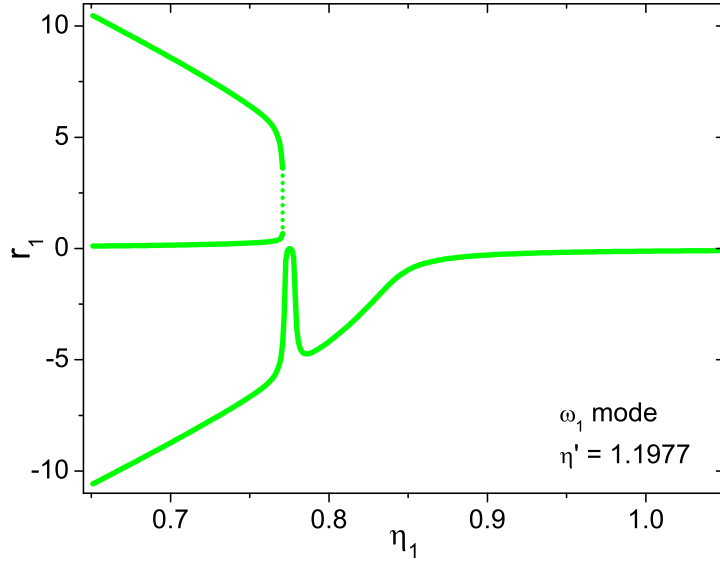
Figure 6.5: Plots of the field solution, r_1 , versus η_1 of the ω_1 mode for (a) $\eta' = 0.9012$ and (b) $\eta' = 1.4325$ corresponding to the transmission results shown in Figure 6.4(a) and (f) on page 105.

the island-like feature in the ω_1 mode transmission of the interaction. In the present problem of the ω_1 mode interaction, the perturbation arises from the ratio of η' as well as the coherently scattering resonances of the ω_2 . A very small kink as seen at $\eta_1 \approx 1.0307$

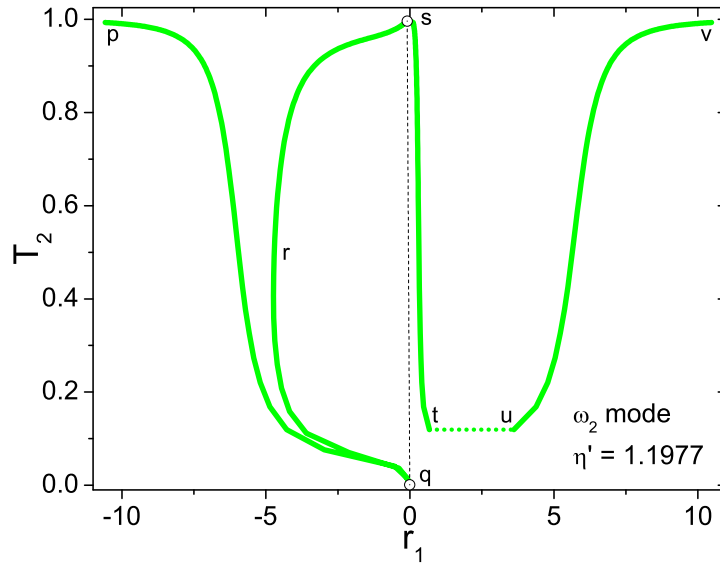
in Figure 6.5(a) is due to the ω_2 resonance, which is not the point of discussion in this instance.

In brief, the smaller or fairly larger ratio of η' as simulated in the present problem does not affect the transmission resonances significantly from the result presented in Figure 6.2 for the single mode; yet, they are interesting owing to the presence of the optical bistability. More importantly, a moderately chosen ratios of η' may exhibit very interesting results as seen in plots (b) through (e) in Figure 6.4, which may be useful to explore the functions of the novel optical bistable devices in the regime around or below the switching points.

As a closing remark of the discussions in this subsection, we want to address a method to determine the possible bistable states for the ω_2 mode under the condition of $e_2 = d_2 = 0$. The method of the field solution as given in Figure 6.5 may be used for this purpose. As we noticed previously in this subsection, the linear transmission of the ω_2 mode as a function of the parameter space η_1 of the ω_1 mode does not display bistable states. However, the transmission of the ω_2 mode as a function of the field solution r_1 of the ω_1 mode can exhibit bistable characteristics for certain sets of solution profiles. The height of the kink/peak of the field solution in the (η_1, r_1) space describes the range of the bistable states in the ω_2 transmission in the r_1 -space. In this method, for example, Figure 6.6 plots the field solutions of the transmission in Figure 6.4(d) and the corresponding transmission of the ω_2 mode as a function of the field solution r_1 . As seen in plot (a) in Figure 6.6, the kink spans over the range $\approx -5 < r_1 < 0$, so that the corresponding bistability for ω_2 transmission is found within the same limit (i.e., $\approx -5 < r_1 < 0$) of the field solution axis, as seen in the plot in Figure 6.6(b)). The dotted



(a) Field solution for the plot in Figure 6.4(d)



(b) Transmissivity for the ω_2 mode

Figure 6.6: (a) Plot of the field solution, r_1 , versus η_1 of the ω_1 mode for $\eta' = 1.1977$, which is the field solution profile for the plot in Figure 6.4(d), and (b) corresponding transmission result for the ω_2 mode in the r_1 -space of the ω_1 mode. Open circles at points q and s are the switching points of the bistability as usual.

line in plot (a) gives the transmission solution in the dotted line $t - u$ in plot (b). As can be seen in plot (b), the curves $p - q - s - t - u - v$ may be taken as the transmission

solution in the forward direction and the curves $v - u - t - s - r - q - p$ as the solution in the reverse direction, as usual .

6.2 Case Study of the Two Guided Modes in Off-Channel Features

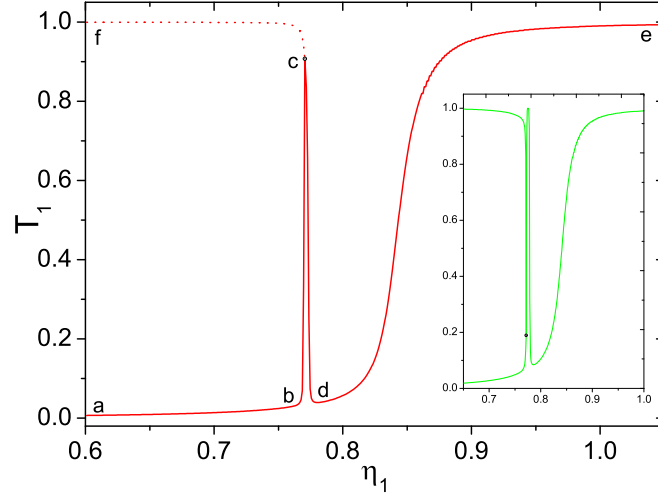
Here, we continue the problem of two frequencies into the single off-channel Kerr impurity introduced on page 97. But, in this case, both guided modes, ω_1 and ω_2 , are allowed to interact nonlinearly at the off-channel site, meaning all the nonlinearity constraints of the modes are given to nonzero weight, i.e., $e_l = d_l \neq 0$ for $l = \{1, 2\}$, in model Eqs. (6.4a)-(6.4b). Such a condition is favorable to creating a complicated, but interesting, problem in the treatment of the two frequency modes in which the fields interact with themselves and each other. However, our main concern is to achieve stable solutions of the fields corresponding to the guided modes in the system.

In order to simplify this discussion, the guided modes are studied under the numerical controls of only the e_l and d_l for $l = \{1, 2\}$ and the other parameters of the system are carried over from the previous subsection. The variation of other parameters of the system as well, of course, allows the fields to display interesting forms of transmission features; but, the motivation of considering the parameters e_l and d_l in the current problem is that they appear as the major factors for introducing nonlinear interaction between modes and on the modes themselves. In the following, we proceed to the discussion of the transmission features of the modes depending mainly on the initial conditions for the three different specific cases of e_l and d_l .

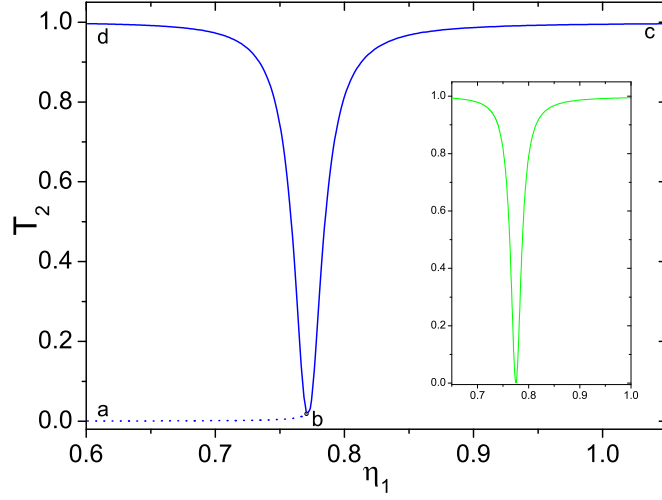
6.2.1 Case (i): Very Weak Effect of ω_2

In Figure 6.7, the plots for a typical interaction of ω_1 and ω_2 modes interacting with each other nonlinearly at the single off-channel site are presented by setting the nonlinear constraints of $e_1 = d_1 = 1$, $e_2 = d_2 = 0.06$ and adopting all other material parameters. This includes the fields' initial values being the same as in the case of the ω_1 nonlinearly and ω_2 linearly excited interaction given in Figure 6.4(d) on page 105. In fact, we have attempted here to perturb the previous system by using small changes of only e_2 and d_2 characterizing the nonlinearity of the ω_2 mode. The plots reveal the transmission properties of the guided modes and their interaction through the excitations of both the fields about the common off-channel site. Plot (a) shows the transmission of the ω_1 mode, while plot (b) shows the transmission of the ω_2 mode. It is seen in the curves, as predicted earlier in this discussion, that both modes exhibit bistable states below the limit of $\eta_1 \approx 0.76$, corresponding to the switching points (labelled open circle). The bistability, particularly the solutions found as dotted curves, shows both modes are seen to be similar to the usual case of the off-channel problem of nonlinear interaction. However, for $e_2 = d_2 = 0$, the ω_2 transmission reduces to a linear resonant profile, as shown in the insert in plot (b) or as given in the curve (d) in Figure 6.3 on page 104, where the ω_1 exhibits bistable transmission as usual. The inset in plot (a) shows usual bistable profile of ω_1 given in Figure 6.4(d) on page 105 for the unperturbed case of ω_2 . Notice that in Figure 6.7(b), this was the first time the ω_2 mode exhibited bistability in the present discussion of two frequency modes with perturbed ω_2 mode.

As the nonlinear interaction of ω_2 increases, the effect is seen in the resonant transmission of ω_1 mode. Specifically, the segment of dotted solutions of ω_2 tend to shift



(a) Transmissivity for the ω_1 mode



(b) Transmissivity for the ω_2 mode

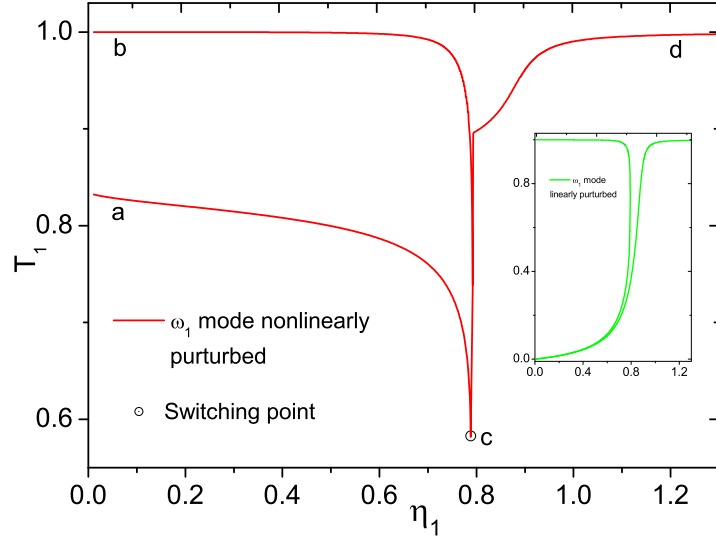
Figure 6.7: (a) Plot of the transmission coefficient, T_1 , versus η_1 of the ω_1 mode and (b) the corresponding nonlinear transmission result, T_2 , of the ω_2 mode in the η_1 -space of the ω_1 mode for the ratio of $\eta' = 1.1977$ while both guided modes are interacting with the nonlinear site. Open circles are the bistable switching points of the modes. Notice that this plot is the both modes nonlinearly interacting version of only ω_1 nonlinearly and ω_2 linearly interacting case shown in Figure 6.4(d) on page 105. The inserts in plot (a) and (b), respectively, are the resonant transmission results for ω_1 and ω_2 modes in the case of $e_2 = d_2 = 0$.

the branches of ω_1 transmission so that the dotted curved is raised and the peak at point c is lowered. We can trace the path of the system by changing η_1 . In this, as the η_1 is changed, the system begins at point a and continues to evolve the transmission through

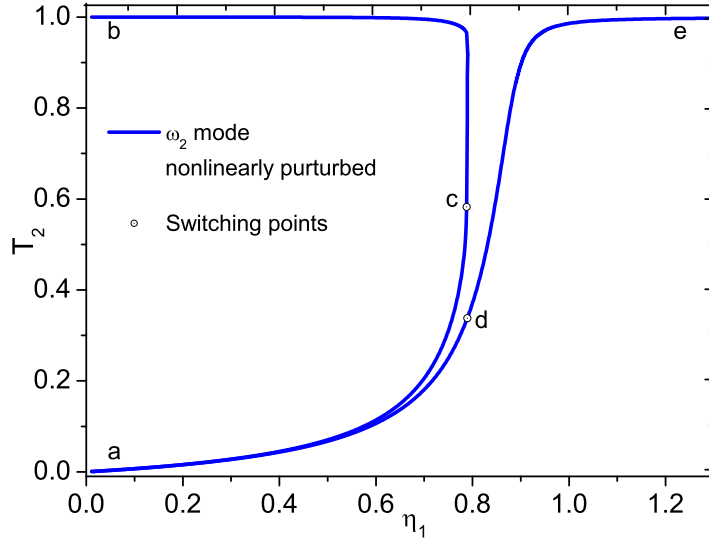
the solution labelled $b - c - d - e$. If the transverse occurs in the reversed direction, the transmission follows the upper branch of the solution curve $e - d - c - f$. The bistability of ω_2 at $\eta_1 < 0.76$ in plot (b) can be described by tracing the curves $a - b - c$ (in forward) and $c - b - d$ (in reversed) direction of the η_1 -space.

6.2.2 Case (ii): Weak Interactions of Both ω_1 and ω_2

It is interesting when all of the nonlinear interactions are of the same order. Such a situation is achieved in present model by using the constants, specifically, $e_1 = d_1 = 1$, $e_2 = d_2 = 1$, $\lambda x^2 = 0.02535$ and $\eta' = 1.0751$. Other parameters of the system in this case remain the same as in the above cases. The result of the computation for the bistable transmission of the modes, using the set of parameterization of this case is presented in Figure 6.8. The ω_1 mode solutions in plot (a) trace out bistable curves $a - c$ and $b - c$, followed by the linear solution curve $c - d$. As seen in plot (a), the transmission in curve $a - c$ has been raised up to $T_1 \approx 0.8$ due to the nonlinear effect of the ω_2 . In general, the solutions in plots (a) and (b) can be coupled through the switching point c at (η_1, T_1) or $(\eta_1, T_2) = (0.79, 0.58)$. The presence of the branch, $b - c$, of ω_2 in (b) tends to lift the $T_1 \approx 0$ solutions of the ω_1 mode to the $T_1 > 0$. In this model, the solution of one mode is followed by another, which is evident from the switching point c on both plots. These plots occur at the same point in that the forward bias in the system is as seen in the previous cases, while the reverse bias is an unusual transmission because it may follow either $c - a$ or $c - b$ states, depending on the initial conditions of the modes about the off-channel site. Such states may be useful for storing binary information in complex optical devices.



(a) Transmissivity for the ω_1 mode

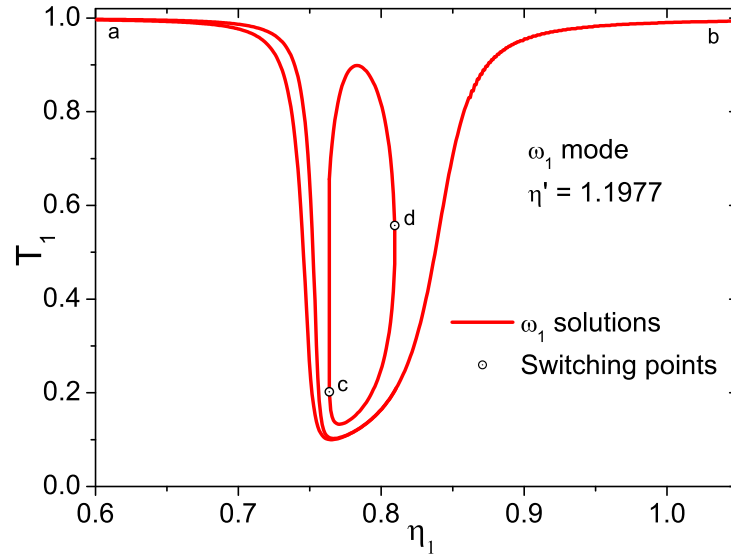


(b) Transmissivity for the ω_2 mode

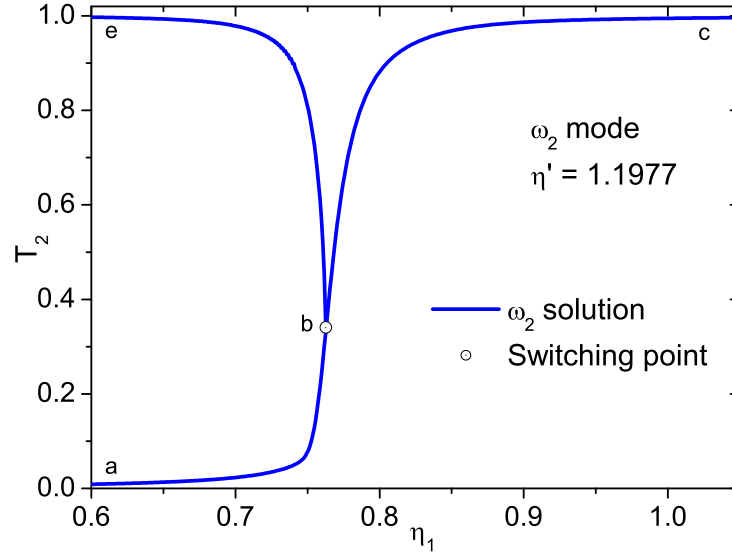
Figure 6.8: Plot of the transmission coefficients, (a) T_1 of the ω_1 mode and (b) T_2 of the ω_2 mode, in the η_1 -space of the ω_1 mode. Both modes are interacting with the nonlinear site for constant parameters same as in Case (i) but for $e_1 = d_1 = 1$, $e_2 = d_2 = 1$, $\lambda_1 x^2 = \lambda_2 x^2 = 0.02535$, and $\eta' = 1.0751$. Open circles are the bistable switching points of the modes. Inset in (a) shows the bistable transmission of the ω_1 for off-channel feature when ω_2 perturbing linearly as in previous section.

6.2.3 Case (iii): Stronger Effect of ω_1

In Figure 6.9, the transimssion coefficients for the ω_1 and ω_2 modes using stronger perturbations are studied in parameter space of the ω_1 mode. The numerical process is run



(a) Transmissivity for the ω_1 mode



(b) Transmissivity for the ω_2 mode

Figure 6.9: (a) Plot of the transmission coefficient solution, T_1 , versus η_1 of the ω_1 mode and (b) the corresponding nonlinear transmission result, T_2 , for the ω_2 mode in the η_1 -space of the ω_1 mode for the ratio of $\eta' = 1.1977$ while both guided modes are interacting with the nonlinear site. Open circles are the bistable switching points.

by initializing the nonlinear constraint $e_1 = 3$ while using fixed values of $d_1 = 3.5$ and $e_2 = d_2 = 1$. All other material parameters, including the fields' initial values adopted in Case (i) have been used on this case as well. The e_1 , as predicted, allows the solutions

r_1 and r_2 to behave more smoothly in the η_1 -space of the ω_1 mode. Note that only the stable solutions of the modes are shown in Figure 6.9. The case study of the plots in this figure will proceed as follows.

Figure 6.9(a) plots the transmission coefficient, T_1 , versus η_1 for the ω_1 mode interacting nonlinearly with the ω_2 mode transmission. The ω_1 mode transmission about the points $0.60 < \eta_1 < 0.76$ in the plot displays two branches, a lower and upper branch of solutions looking like a hysteresis loop. Between $0.76 < \eta_1 < 0.81$, an additional loop of solutions exists with the lowest branch for $0.76 < \eta_1$ being single valued. Notice that the modes display an interesting transmission topography of an oval shape with multiple solutions for input range of η_1 between the switching points c and d , as seen in the plot. In the oval region, the system may follow the upper or lower branch in the forward or reverse bias depending on the initial values of the system.

Figure 6.9(b) plots the transmission coefficient, T_2 , of ω_2 mode in the η_1 -space of the ω_1 mode. In this, the ω_2 mode interacts nonlinearly with the resonant excitation of the off-channel site. As a result, as we assumed earlier in this discussion, the ω_2 reveals the bistable transmission for a range of η_1 below the limit ($\eta_1 = 0.76$), corresponding to the switching point again.

CHAPTER VII

Summary and Conclusion

In this dissertation, we have investigated nonlinear electromagnetic modes of photonic crystal waveguides mediated by in- and/or off-channel Kerr nonlinear dielectric properties. Basically, this research has intensified the study of optical phenomenon in both linear and nonlinear waveguides (optical bistability) in the hope that these systems can be used for all-optical switching, including other applications. The research methods were based on the numerical simulation/modeling of the light modes existing in the 1D and 2D photonic crystal systems of interest.

Chapter III introduced fundamentals of computation of photonic crystal characteristics. In this chapter, the FDTD and PWE methods, including several analytical treatments, were implemented in order to study the propagating and localizing field modes arising from single site impurities in the photonic crystal lattice. The impurities caused light localization about a point or line-like region. We have shown a controlling mechanism (cavity-like excitation) over the propagation of light modes in a microcavity structure within the stop band of the photonic crystal. By creating a line of single site impurities, we have propagated the modes exhibiting the property of a linear waveguide. In addition, we developed 1D nonlinear FDTD algorithms which were used to investigate the localization properties of the field modes. In this case, we found the nonlinear bound modes and impurity modes that contained high quality factors, which indicated a strong confinement of the light modes in the photonic crystals. By considering a 2D photonic crystal in the computer simulation, we analyzed waveguide and resonator modes

using their field distribution patterns and symmetries. The results of the simulation were considered for investigating the general properties of the modes, which allowed us to suggest the coupling method of the resonantly excited mode of one symmetry within the waveguide, or an excitation of a different symmetry in the photonic crystal designs.

The guided modes in the linear waveguide were further incorporated with the nonlinear modes of a photonic crystal, and this embedded effect into the system posed an intricate problem to our research. Therefore, the dissertation work involves addressing the solution of nonlinear partial differential equations. In this respect, the focus of the dissertation was on a better understanding and application of the Kerr nonlinear modes (intensity dependent) existing within the photonic crystal waveguides. For this purpose, particularly, analytical descriptions and/or numerical simulations for predicting the behavior of light modes in nonlinear photonic crystal waveguides were presented. In order to understand the physical phenomena appearing in such waveguides, the fields were analyzed using computer simulations. To this end, Chapter IV proposed a novel approach, the difference equation waveguide, for investigating the full generality of increasing complexity of the Kerr-type modes. This chapter also reports the relevance and importance of the nonlinear modes of the difference equation that was taken as an alternative to computer simulations based on FDTD methods or finite-element approaches, as cited in the introduction of this dissertation.

Chapter V explained many of the waveguide and in- or off-channel feature geometries, particularly the 2D photonic crystal waveguide systems, which were shown to exhibit new transmission anomalies of the waveguide modes. The difference equation approach allowed for the expression of the modal properties of the waveguide system in

terms of closed-form algebraic expressions. The guided light modes were described using the algorithms for difference equation waveguides. In general, for our purposes, the waveguide modes were characterized by the parameters: α (on-site coupling), β (nearest-neighbor interaction), γ (dielectric property), λ (Kerr nonlinearity constant), etc.; α and β are defined as functions of the mid-gap frequency $\omega a_c/2\pi c = 0.441$ in the stop band of the 2D photonic crystal that was originally studied experimentally. The solutions of the light modes in the system formed recursively defined sequences similar to the form of difference equations in linear algebra, and these were solved to demonstrate the wide and interesting behavior present in the system. The most interesting property was the bistable transmissions of the waveguide modes, which was exhibited by the off-channel nonlinear interaction in the photonic crystal lattice. In addition, the introduction of two nonlinear off-sites in the lattice led to the observation of new features, including the shifting, lifting, and self-steepening effects in the transmission profiles of the waveguide modes. Therefore, the off-channel transmission characteristics of the modes indicated potential nonlinear functions of the modulated dielectrics, which can be used to design optical switching and multiplexing. Additionally, the results of the scattering of the modes were compared with the linear limit of the Kerr media, i.e., in the absence of the $|E|^2$ term in the Kerr dielectrics.

As an extension of the difference equation approach for modeling nonlinear systems, the transmission in a Kerr nonlinear barrier was studied as a function of the parameters characterizing the nonlinearity. This problem presented the general features of transmission maxima, giving a summary of mode types that can be excited within the barrier. For a particular parameter space of the transmission coefficient, we observed

Fano-type transmission shapes [74], in which the transmission resonances were shifted using the perturbations in the Kerr nonlinearity parameter.

Chapter VI presented the theory for waveguide modes of two different frequencies, ω_1 and ω_2 , that travel down a single waveguide channel and interact with one another due to the Kerr nonlinear media off-channel features. These frequencies also resonantly excite localized modes on the Kerr off-channel media, and the resonant excitations can be used to enhance the interaction of the two waveguide modes with one another or to modulate the fields on the off-channel features. The interactions between the frequencies require Kerr-type nonlinear optical systems in which, through a modulation of the dielectric properties of materials by applied electric fields, one wave can interact with and control the modulation of another wave. Such features were illustrated in the results obtained from our model using the two frequencies. In that study, we found the transmission properties of the ω_1 mode exhibiting the kink-, dip-, peak-, valley-, and island-like features in the parameter space of the ω_2 mode resonances. More interestingly, in computing these transmission profiles, we found the various switching points (jump points) at which the systems changed their transmission states rapidly.

In addition, by studying the coefficients of the new dielectric model of the perturbative functions and how they modulate with the intensities of the field modes, we have shown that the ω_2 mode strongly interacts with the ω_1 mode and destroys the peaks. However, the system reproduced the new features in the transmission profiles by lifting the lower branch of the transmissions to higher values and displaying oval islands and hysteresis loops in the parameter space of the ω_1 mode. The Kerr nonlinear system proposed in this case has a feature that not only exhibits resonant phenomena retaining

enhanced nonlinear properties, but also suggests a mechanism for possible technological applications, such as switches in amplitude modulation and in signal amplification. The nonlinear effects here depend only on the use of the Kerr interaction to allow a waveguide mode of particular frequency to modulate the dielectric properties seen by the second mode of another frequency.

In conclusion, in addition to developing general purpose methodologies, we have suggested a novel approach for investigating the transmission properties of photonic crystal waveguide modes. Our approach is based on the analysis of the difference equations derived using Green's function theory. The difference equations of a system emphasize the importance of the impurity modes localized in the photonic crystal lattice. By implementing this technique, we have studied properties of several important in- and off-channel geometries that may be used as the components in optical integrated circuits. We will continue working on our research endeavor by considering more realistic models in Kerr dielectrics, particularly for the case of two frequency modes. The results will be included in a forthcoming publication of this dissertation research. Since the terms in the difference equation can be used conveniently to represent the dielectric modulation of the electric field in the lattice cylinder, our method can be useful for solving more complicated geometries. However, even this approach is quite complicated when one is designing large-scale photonic crystal circuits. Thus it requires substantial computational resources. The method can also be extended to manipulating useful optical phenomena (solitons, intrinsic localized modes, supercontinuum generation, signal conversions, etc.) where the Kerr effect is significant in nonlinear photonic crystal structures. It is hoped that this dissertation research will stimulate increased interest in materials exhibiting nonlinear

optical properties, which have potential applications to all-optical switching, optical data storage, optical information processing, electro-optic switching, and, in general, optical computing and telecommunications systems technologies.

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APPENDIX A

Poynting Vector for a Two-Frequency Kerr Interaction: Analytical Proof

The wave equation for electric field vector parallel to the x -axis and propagating to the z -direction on a Kerr nonlinear medium can be written as

$$\frac{d^2 E}{dz^2} + \frac{\omega^2}{c^2} n^2 \left(1 + \lambda |E|^2\right) E = 0, \quad (\text{A.1})$$

where the Kerr dielectric constant depends on the electric field intensity, a term containing the Kerr parameter, λ , in the equation. We introduce the two-frequency problem by using a generalization of the Kerr dielectric constant: the dielectric constant of the first frequency mode must be dependent on the amplitude squared of the first frequency electric field and the amplitude squared of the second frequency electric field co-propagating with the first [165, 166]. Likewise, the dielectric constant of the second frequency mode must be dependent on the amplitude squared of the first frequency electric field and the amplitude squared of the second frequency electric field. Thus, invoking the nonlinear part of the dielectric constant, the coupled equations for the two electric field modes in Kerr dielectrics can be written as

$$\frac{d^2 E_1}{dz^2} + A_1 \left(1 + \lambda_1 |E_1|^2 + \lambda_2 |E_2|^2\right) E_1 = 0, \quad (\text{A.2})$$

$$\frac{d^2 E_2}{dz^2} + A_2 \left(1 + \lambda_3 |E_1|^2 + \lambda_4 |E_2|^2\right) E_2 = 0, \quad (\text{A.3})$$

where the factors λ_1 , λ_2 , λ_3 , and λ_4 describe the nonlinearity effects.

Assuming the two different plane waves, with the field amplitudes E_1^0 and E_2^0 , incident on the Kerr dielectric media, the field solutions are of the forms

$$E_1 = E_1^0 \epsilon_1(z) e^{i\phi_1(z)} \text{ and } E_2 = E_2^0 \epsilon_2(z) e^{i\phi_2(z)}, \quad (\text{A.4})$$

where ϵ_1 , ϵ_2 , ϕ_1 , and ϕ_2 are real. Then, $|E_1|^2 = |E_1^*|^2 = E_1^{02} \epsilon_1^2$, $|E_2|^2 = |E_2^*|^2 = E_2^{02} \epsilon_2^2$, $E_1^* E_1 = E_1 E_1^* = E_1^{02} \epsilon_1^2$, etc. Using the solution forms of Eq. (A.4), the important differentials used in the present treatment can be defined as

$$\begin{aligned} \frac{dE_l}{dz} &= E_l^0 \left[\frac{d\epsilon_l}{dz} + i\epsilon_l \frac{d\phi_l}{dz} \right] e^{i\phi_l} \\ \text{and } \frac{d^2 E_l}{dz^2} &= E_l^0 \left[\frac{d^2 \epsilon_l}{dz^2} + 2i \frac{d\phi_l}{dz} \frac{d\epsilon_l}{dz} + i\epsilon_l \frac{d^2 \phi_l}{dz^2} - \epsilon_l \left(\frac{d\phi_l}{dz} \right)^2 \right] e^{i\phi_l}, \end{aligned} \quad (\text{A.5})$$

where $l \in 1$ or 2 . Substituting Eqs. (A.4) and (A.5) into Eq. (A.2) or (A.3), we get

$$\frac{d^2 \epsilon_l}{dz^2} + 2i \frac{d\phi_l}{dz} \frac{d\epsilon_l}{dz} + i\epsilon_l \frac{d^2 \phi_l}{dz^2} - \epsilon_l \left(\frac{d\phi_l}{dz} \right)^2 + A_l [1 + \alpha_{l,l} \epsilon_l^2 + \alpha_{l,l'} \epsilon_{l'}^2] \epsilon_l = 0, \quad (\text{A.6})$$

where the indexes $(l, l') \in (1, 2)$ or $(2, 1)$. The $\alpha_{l,l}$ and $\alpha_{l,l'}$ describe the factors containing the λ_s (introduced through Eq. (A.2) or (A.3)) and E_l^0 or $E_{l'}^0$ in the derivation. The real and imaginary parts in Eq. (A.6) can be separated as

$$\frac{d^2 \epsilon_l}{dz^2} - \epsilon_l \left(\frac{d\phi_l}{dz} \right)^2 + A_l [1 + \alpha_{l,l} \epsilon_l^2 + \alpha_{l,l'} \epsilon_{l'}^2] \epsilon_l = 0 \quad \text{and} \quad 2 \frac{d\phi_l}{dz} \frac{d\epsilon_l}{dz} + \epsilon_l \frac{d^2 \phi_l}{dz^2} = 0, \quad (\text{A.7})$$

respectively. The imaginary part gives

$$\frac{d}{dz} \left[\epsilon_l^2 \frac{d\phi_l}{dz} \right] = 0 \implies \epsilon_l^2 \frac{d\phi_l}{dz} = W_l = \text{a constant}. \quad (\text{A.8})$$

The Poynting vector [155] of the problem is defined as

$$S_l \propto \text{Re} \left[\frac{1}{i} E_l^* \frac{dE_l}{dz} \right] \quad (\text{A.9})$$

where $l \in 1$ or 2 , again. After a few algebraic steps, we obtain,

$$\text{Re} \left[\frac{1}{i} E_l^* \frac{dE_l}{dz} \right] = |E_l^0|^2 \epsilon_l^2 \frac{d\phi_l}{dz}, \text{ but } \epsilon_l^2 \frac{d\phi_l}{dz} = W_l = \text{a constant.} \quad (\text{A.10})$$

Therefore, $S_l \propto W_l = \text{a constant}$.

Another version of this suggested by Professor Gorczyca is: subtracting complex conjugate of Eq. (A.2) times E_1 from E_1^* times Eq. (A.2) results in

$$E_1^* \frac{d^2 E_1}{dz^2} - \frac{d^2 E_1^*}{dz^2} E_1 = 0, \text{ or } \frac{d}{dz} \left[E_1^* \frac{dE_1}{dz} - \frac{dE_1^*}{dz} E_1 \right] = 0. \quad (\text{A.11})$$

Then, $E_1^* \frac{dE_1}{dz} - \frac{dE_1^*}{dz} E_1 = \text{a constant}$, and after using the algebraic property, $Z - Z^* = 2i\Im(Z)$, for a complex number Z , we obtain $2i E_1^* \frac{dE_1}{dz} = \text{a constant}$, which can be used to support the statement of Eq. (A.10), i.e., the real part of the complex Poynting vector is a constant [82]. Notice that the differentials obtained from Maxwell's equations for the z -directed electric field, i.e., $\frac{dH}{dz} \propto iE$ or $\frac{dE}{dz} \propto iH$, can be used in order to define the Poynting vector $S \propto EH^*$.

APPENDIX B

FDTD Process Recipes

B.1 Nonlinear FDTD for Kerr Polarization Current

Using the intensity dependent dielectric model,

$$\varepsilon_r^*(\omega) = \varepsilon_r + \sigma/(j\omega\varepsilon_0) + \alpha\chi^{(3)}(\omega)|E(\omega)|^2, \quad (\text{B.1})$$

the nonlinear polarization, $\vec{P}_K^{NL}(\omega)$, in frequency domain can be introduced into electric flux density: $\vec{D}(\omega) = \varepsilon(\omega)\vec{E}(\omega) = \varepsilon_0\varepsilon_r^*(\omega)\vec{E}(\omega) = \varepsilon_0\varepsilon_r\vec{E}(\omega) + \frac{\sigma}{j\omega}\vec{E}(\omega) + \vec{P}_K^{NL}(\omega)$ with $\vec{P}_K^{NL}(\omega) = \varepsilon_0\alpha\chi^{(3)}(\omega)|\vec{E}(\omega)|^2$. This can be used to explain the Kerr nonlinear polarization. Applying the inverse Fourier transform on the method yields the polarization in time domain as

$$\begin{aligned} P_K^{NL}(t) &= \varepsilon_0 \int_{-\infty}^{\infty} \alpha\chi^{(3)}(t-t')|E(t')|^2 E(t) dt' \\ &= \varepsilon_0\alpha\chi_0^{(3)} E(t) \int_{-\infty}^{\infty} \delta(t-t')|E(t')|^2 dt' = \varepsilon_0\alpha\chi_0^{(3)} E^3(t), \end{aligned} \quad (\text{B.2})$$

where we have used the instantaneous response-model, i.e., $\chi^{(3)}(t) \cong \chi_0^{(3)}\delta(t)$ as explained in [59, 120, 121]. In this, $\delta(t)$ is the delta function and it represents the instantaneous response of Kerr interaction, α is a weight constant that dictates the relative strengths of different nonlinear interactions, and $\chi_0^{(3)}$ is the nonlinear coefficient (third order susceptibility).

Taylor series expansion of $E^3(t)$ around $t = t_{n-1}$ and evaluating it at $t = t_n$ will give the new values of $E^3(t)$ and then $P_K^{NL}(t)$ that can be used to define the Kerr polarization current as $J_K^{NL}(t) = \partial P_K^{NL}(t)/\partial t$. As deduced in Sullivan's paper [120],

$$\begin{aligned}
E^3(t_n) &\cong E^3(t_{n-1}) + \frac{\partial}{\partial t} (E^3(t_{n-1})) \Delta t = E^3(t_{n-1}) + \dots \\
3E^2(t_{n-1}) \left(\frac{E(t_n) - E(t_{n-1})}{\Delta t} \right) \Delta t &= 3E^2(t_{n-1})E(t_n) - 2E^3(t_{n-1}). \quad (\text{B.3})
\end{aligned}$$

Combining Eqs. (B.2) and (B.3) results in polarization term as $P_K(t_n) = \varepsilon_0 \alpha \chi_0^{(3)} E^3(t_n) \cong \varepsilon_0 \alpha \chi_0^{(3)} (3E^2(t_{n-1})E(t_n) - 2E^3(t_{n-1}))$. Then,

$$\begin{aligned}
J_K(t_n) &= \frac{\partial P_K(t_n)}{\partial t} \cong \varepsilon_0 \alpha \chi_0^{(3)} \frac{\partial}{\partial t} (3E^2(t_{n-1})E(t_n) - 2E^3(t_{n-1})) \\
&= \frac{3r}{\Delta t} \{ E^2(t_p)E(t_q) - 5E^2(t_p)E(t_n) + 2E(t_p)E^2(t_n) + 2E^3(t_p) \} \quad (\text{B.4})
\end{aligned}$$

where $p = n - 1$, $q = n + 1$, and $r = \varepsilon_0 \alpha \chi_0^{(3)}$. The finite-difference of current can be written as $J_K(t_n) = \frac{1}{2} (J_K(t_{n+1}) + J_K(t_n))$. Thus, solving for $J_K(t_{n+1})$ results in

$$J_K^{n+1} = \frac{6r}{\Delta t} \{ (E^p)^2 E^{n+1} - 5(E^p)^2 E^n + 2E^p (E^n)^2 + 2(E^p)^3 \} - J_K^n. \quad (\text{B.5})$$

This equation updates the Kerr polarization current density.

B.2 Boundary Conditions

The 1D FDTD boundary fields, $E_z(1)$ and $E_z(M)$, at the far-left and far-right respectively, are updated by approximating advection of wave equation. Knowing all other interior nodes such as $E_z^{n+1}(2)$, $E_z^n(1)$, $E_z^n(2)$, etc., the space-time at $(\frac{\Delta x}{2}, (n + \frac{1}{2})\Delta t)$ for $E_z^{n+1}(1)$ or $E_z^{n+1}(M)$ in case of the first order ABC:

$$\underbrace{E_z^{n+1}(1 \text{ or } M)}_{\text{future}} = \underbrace{E_z^n(2 \text{ or } M - 1)}_{\text{present}} + S_{ff} \times \left(\underbrace{E_z^{n+1}(2 \text{ or } M - 1)}_{\text{future}} - \underbrace{E_z^n(1 \text{ or } M)}_{\text{present}} \right), \quad (\text{B.6})$$

where the terms are: $S_{ff} = (S_f - 1)/(S_f + 1)$, $S_f = s_c/\sqrt{\mu_r \varepsilon_r}$, with the Courant factor, $S_c = c\Delta t/\Delta x$, detailed in [94–96, 167], that determines numerical stability in the FDTD simulation. For second order ABC the $E_z^{n+1}(1)$ and $E_z^{n+1}(M)$ are:

$$E_z^{n+1}(1) = \frac{-1}{(S' + 2)} \{ (S' - 2) (E_z^{n+1}(3) + E_z^{n-1}(1)) + 2T'P - 4S'E_z^n(2) \} - E_z^{n-1}(3), \quad (\text{B.7})$$

$$E_z^{n+1}(M) = -\frac{1}{(S' + 2)} \left\{ \begin{array}{l} (S' - 2) (E_z^{n+1}(M - 2) + E_z^{n-1}(M)) \\ + 2T'Q - 4S'E_z^n(M - 1) \end{array} \right\} - E_z^{n-1}(M - 2), \quad (\text{B.8})$$

where $S' = S'_c + 1/S'_c$, $T' = S'_c - 1/S'_c$, $S'_c = S_c/\sqrt{\mu_r \varepsilon_r}$, $P = E_z^n(1) + E_z^n(3) - E_z^{n+1}(2) - E_z^{n-1}(2)$, and $Q = E_z^n(M) + E_z^n(M - 2) - E_z^{n+1}(M - 1) - E_z^{n-1}(M - 1)$.

Total-field scattered-field boundary: The computational domain is divided into scattered-field (SF) and total-field (TF) regions as $E_{tot} = E_{inc} + E_{sca}$, $H_{tot} = H_{inc} + H_{sca}$. If $i - 1/2$, i , and $i + 1/2$ are each in TF or SF side, then the correct forms of the fields at $\lambda = \Delta t/(\varepsilon \Delta x)$ and $\Lambda = \Delta t/(\mu \Delta x)$ are:

$$E_{tot}^{n+1}[i] = E_{tot}^n[i] + \lambda(H_{tot}^{n+1/2}[i + 1/2] - H_{tot}^{n+1/2}[i - 1/2]), \quad (\text{B.9a})$$

$$H_{tot}^{n+1/2}[i - 1/2] = H_{tot}^{n-1/2}[i - 1/2] + \Lambda(E_{tot}^n[i] - E_{tot}^n[i - 1]). \quad (\text{B.9b})$$

$$E_{sca}^{n+1}[i] = E_{sca}^n[i] + \lambda(H_{sca}^{n+1/2}[i + 1/2] - H_{sca}^{n+1/2}[i - 1/2]), \quad (\text{B.9c})$$

$$H_{sca}^{n+1/2}[i - 1/2] = H_{sca}^{n-1/2}[i - 1/2] + \Lambda(E_{sca}^n[i] - E_{sca}^n[i - 1]). \quad (\text{B.9d})$$

However, if i_L is in TF region, and the interface between TF and SF lies between i_L and $i_{L-1/2}$, then the correct version of total field results in the form, such that

$$E_{tot}^{n+1}[i_L] = \underbrace{E_{tot}^n[i_L] + \lambda(H_{tot}^{n+1/2}[j] - H_{sca}^{n+1/2}[k])}_{\text{assumed stored in computer memory}} - \underbrace{\lambda H_{inc}^{n+1/2}[k]}_{\text{assumed known}}, \quad (\text{B.10})$$

$$H_{sca}^{n+1/2}[k] = \underbrace{H_{sca}^{n-1/2}[k] + \Lambda(E_{tot}^n[i_L] - E_{sca}^n[i_L - 1])}_{\text{assumed stored in computer memory}} - \underbrace{\Lambda E_{inc}^n[i_L]}_{\text{assumed known}}, \quad (\text{B.11})$$

where $j = i_L + 1/2$ and $k = i_L - 1/2$. Note that the H -field corresponding to $E_{tot}^{n+1}[i_L]$ is located at $i_L - 1/2$.

B.3 TM_z FDTD Algorithm Employing PML Boundary

The E_z component splits up: $E_z = E_{zx} + E_{zy}$ while the H_x and H_y components remain in the usual forms. If the computational region is characterized by the medium $(\mu_1, \varepsilon_1, \sigma)$ and the PML region is by $(\mu_2, \varepsilon_2, \sigma^*)$ then Maxwell's equations give

$$H_x^{n+\frac{1}{2}}[i, j_+] = C_{hxx}[i, j_+] H_x^{n-\frac{1}{2}}[i, j_+] + C_{hxez}[i, j_+] (E_z^n[i, j+1] - E_z^n[i, j]), \quad (\text{B.12})$$

$$H_y^{n+\frac{1}{2}}[i_+, j] = C_{hyh}[i_+, j] H_y^{n-\frac{1}{2}}[i_+, j] + C_{hyez}[i_+, j] (E_z^n[i+1, j] - E_z^n[i, j]), \quad (\text{B.13})$$

$$E_{zx}^{n+1}[i, j] = C_{ezxe}[i, j] E_{zx}^n[i, j] + C_{ezxhy}[i, j] \left(H_y^{n+\frac{1}{2}}[i_+, j] - H_y^{n+\frac{1}{2}}[i_-, j] \right), \quad (\text{B.14})$$

$$E_{zy}^{n+1}[i, j] = C_{ezye}[i, j] E_{zy}^n[i, j] + C_{ezyhx}[i, j] \left(H_x^{n+\frac{1}{2}}[i, j_+] - H_x^{n+\frac{1}{2}}[i, j_-] \right), \quad (\text{B.15})$$

where $j_{\pm} = j \pm \frac{1}{2}$, $i_{\pm} = i \pm \frac{1}{2}$, and the field coefficients C, s are described as

$$\begin{aligned} C_{hxx}[i, j + \frac{1}{2}] &= \frac{2\mu_2 - \Delta t \sigma_y^*[i, j + \frac{1}{2}]}{2\mu_2 + \Delta t \sigma_y^*[i, j + \frac{1}{2}]}, \quad C_{hxez}[i, j + \frac{1}{2}] = \frac{-1}{2\mu_2 + \Delta t \sigma_y^*[i, j + \frac{1}{2}]} \frac{2\Delta t}{\Delta y}, \\ C_{hyh}[i + \frac{1}{2}, j] &= \frac{2\mu_2 - \Delta t \sigma_x^*[i + \frac{1}{2}, j]}{2\mu_2 + \Delta t \sigma_x^*[i + \frac{1}{2}, j]}, \quad C_{hyez}[i + \frac{1}{2}, j] = \frac{1}{2\mu_2 + \Delta t \sigma_x^*[i + \frac{1}{2}, j]} \frac{2\Delta t}{\Delta x}, \\ C_{ezxe}[i, j] &= \frac{2\varepsilon_2 - \Delta t \sigma_x[i, j]}{2\varepsilon_2 + \Delta t \sigma_x^*[i, j]}, \quad C_{ezxhy}[i, j] = \frac{1}{2\varepsilon_2 + \Delta t \sigma_x[i, j]} \frac{2\Delta t}{\Delta x}, \\ C_{ezye}[i, j] &= \frac{2\varepsilon_2 - \Delta t \sigma_y[i, j]}{2\varepsilon_2 + \Delta t \sigma_y[i, j]}, \quad \text{and } C_{ezyhx}[i, j] = \frac{-1}{2\varepsilon_2 + \Delta t \sigma_y[i, j]} \frac{2\Delta t}{\Delta y}. \end{aligned}$$

Using expansion rules: $\frac{2\varepsilon - \Delta t \sigma}{2\varepsilon + \Delta t \sigma} = \exp\left(-\frac{\Delta t \sigma}{\varepsilon}\right)$ and $\frac{1}{2\varepsilon + \Delta t \sigma} \frac{2\Delta t}{\Delta} = \frac{1}{\sigma \Delta} \left(1 - \exp\left(-\frac{\Delta t \sigma}{\varepsilon}\right)\right)$.

The TM_z fields in the main grid inside PML can be written, in general, as

$$H_x^{n+\frac{1}{2}}[i, j_+] = C_{ahx} H_x^{n-\frac{1}{2}}[i, j_+] - C_{bhx} \frac{\Delta t}{\Delta y} (E_z^n[i, j+1] - E_z^n[i, j]), \quad (\text{B.16})$$

$$H_y^{n+\frac{1}{2}}[i_+, j] = C_{ahy} H_y^{n-\frac{1}{2}}[i_+, j] + C_{bhy} \frac{\Delta t}{\Delta x} (E_z^n[i+1, j] - E_z^n[i, j]), \quad (\text{B.17})$$

$$E_z^{n+1}[i, j] = C_{aez} E_z^n[i, j] + C_{bez} \left[\frac{\Delta t}{\Delta x} (P_y) - \frac{\Delta t}{\Delta y} (P_x) \right], \quad (\text{B.18})$$

$C_{ahx} = \frac{2\mu - \sigma^* \Delta t}{2\mu + \sigma^* \Delta t} = C_{ahy}$, $C_{bhx} = \frac{2}{2\mu + \sigma^* \Delta t} = C_{bhy}$, $C_{aez} = \frac{2\varepsilon - \sigma \Delta t}{2\varepsilon + \sigma \Delta t}$, $C_{bez} = \frac{2}{2\varepsilon + \sigma \Delta t}$, $P_y = H_y^{n+\frac{1}{2}}[i_+, j] - H_y^{n+\frac{1}{2}}[i_-, j]$, and $P_x = H_x^{n+\frac{1}{2}}[i, j_+] - H_x^{n+\frac{1}{2}}[i, j_-]$.

APPENDIX C

Programming Source Codes for Waveguide and Impurity Modes

C.1 Fortran 77 for Waveguide and Resonator

c Simulation of localized modes of 2D photonic crystal (1) waveguide and (2) resonator,
c using FDTD technique on a square lattice with dielectric cylinders at the lattice
c points. The photonic crystal is taken from McCall *et al.* experimental results in PRL,
c Vol 67, 2017 (1991). Poynting vector in the waveguide is along the +x-axis in the
c sense of TMz polarization. Unimodular design of source code is developed for clear
c explanation of the simulation process. The PML region is divided according to
c Taflove's book (Computational Electrodynamics: The Finite-Difference
c Time-Domain Method, Third Edition) supplementary material.
c The program also generates a grid.eps file for visualizing the FDTD grids.
integer ax,ay,ng,nmax,nx,ny,npml,device,nrow,ncol,i,j,k,l,n,nth,isrc,jsrc,ip1,jp1
real pi,c0,dx,dy,dt,m,r,delta,sigmamax,factor,pulse,t0,tw
parameter(ax=9,ay=9,ng=27,npml=12,nmax=16384)
! ax & ay: number of periods @x & @y axis, ng: number of grids/period
parameter(nx=ax*ng+1,ny=ay*ng+1,pi=3.14159274e0)
! nx & ny: no. of nodes @x & @y axis in the main grid
real sigmae,sigmam,mur,eps0,mu0,ea,eb,a0,r0,w0
data sigmae/0.0/,sigmam/0.0/,mur/1.0/,ea/9.0/,eb/1.0/,a0/0.0127/,r0/0.0048/,
w0/0.440/
c input parameters for constructing the proposed photonic crystal are described as follows: ea & eb: dielectric constants
of the cylinders and air, r0: radius of the cylinders, a0: lattice constant, w0: normalized frequency at the center of the
second stop gap, all these five parameters are taken from McCall *et al.* experimental results, sigmae: electrical conductivity,
sigmam: magnetic conductivity, and mur: permeability all remain same in both cylinders and air.
! declare all arrays used in the program:
real sige(nx-1,ny-1),sigm(nx-1,ny),miur(nx-1,ny-1),eaxy(nx-1,ny-1),ebxy(nx-1,ny-1)
real ez(nx-1,ny-1),hx(nx-1,ny),hy(nx,ny-1),epsr(nx-1,ny-1),x(ng,ng),y(ng,ng)
real ezca(nx-1,ny-1),ezcb(nx-1,ny-1),hxca(nx-1,ny),hxcb(nx-1,ny),hyca(nx,ny-1),
hycb(nx,ny-1)
real ezall(nx-1+2*npml,ny-1+2*npml),hxall(nx-1+2*npml,ny+2*npml),
hyall(nx+2*npml,ny-1+2*npml)
real t(nmax),ezpower(nmax)
real sigmax(2*npml),sigmay(2*npml),sig,bcfactor,expfactor
real dummy1(npml,npml),dummy2(npml,npml),dummy3(npml,npml),
dummy4(npml,npml)
real dummy5(npml,npml),dummy6(npml,npml),dummy7(npml,npml)
real dummy8(npml,npml),dummy9(npml,npml),dummy10(npml,npml)
real ezxpml1(npml,npml),ezypml1(npml,npml),hxpml1(npml,npml),
hypml1(npml,npml)
real sigmaxz1(npml,npml),sigmaxx1(npml,npml),sigmaxy1(npml,npml)
real sigmayz1(npml,npml),sigmayx1(npml,npml),sigmayy1(npml,npml)
real ezxpml2(npml,npml),ezypml2(npml,npml),hxpml2(npml,npml),
hypml2(npml,npml)
real sigmaxz2(npml,npml),sigmaxx2(npml,npml),sigmaxy2(npml,npml)
real sigmayz2(npml,npml),sigmayx2(npml,npml),sigmayy2(npml,npml)
real ezxpml3(npml,npml),ezypml3(npml,npml),hxpml3(npml,npml),
hypml3(npml,npml)
real sigmaxz3(npml,npml),sigmaxx3(npml,npml),sigmaxy3(npml,npml)
real sigmayz3(npml,npml),sigmayx3(npml,npml),sigmayy3(npml,npml)
real ezxpml4(npml,npml),ezypml4(npml,npml),hxpml4(npml,npml),
hypml4(npml,npml)
real sigmaxz4(npml,npml),sigmaxx4(npml,npml),sigmaxy4(npml,npml)
real sigmayz4(npml,npml),sigmayx4(npml,npml),sigmayy4(npml,npml)
real ezxpmlA(nx-1,npml),ezypmlA(nx-1,npml),hxpmlA(nx-1,npml),
hypmlA(nx,npml)
real sigmayzA(nx-1,npml),sigmayxA(nx-1,npml),sigmayyA(nx,npml)
real ezxpmlB(nx-1,npml),ezypmlB(nx-1,npml),hxpmlB(nx-1,npml),
hypmlB(nx,npml)
real sigmayzB(nx-1,npml),sigmayxB(nx-1,npml),sigmayyB(nx,npml)
real dummy11(nx-1,npml),dummy12(nx-1,npml),dummy13(nx,npml)
real ezxpmlC(npml,ny-1),ezypmlC(npml,ny-1),hxpmlC(npml,ny),
hypmlC(npml,ny-1)
real sigmaxzC(npml,ny-1),sigmaxxC(npml,ny),sigmaxyC(npml,ny-1)
real ezxpmlD(npml,ny-1),ezypmlD(npml,ny-1),hxpmlD(npml,ny),
hypmlD(npml,ny-1)
real sigmaxzD(npml,ny-1),sigmaxxD(npml,ny),sigmaxyD(npml,ny-1)

```

real ezpml1(npml,npml),ezpml2(npml,npml),ezpml3(npml,npml),ezpml4(npml,npml)
real ezpmlA(nx-1,npml),ezpmlB(nx-1,npml),ezpmlC(npml,ny-1),ezpmlD(npml,ny-1)
! input the choice of simulation device
write(*,*)'Which photonic crystal device? 1 = waveguide, 0 = microcavity'
read(*,*)device
if (device .eq. 1) then
  r0=r0      ! for waveguide
elseif (device .eq. 0) then
  r0=r0/2.    ! reducing size of dielectric cylinders to model the resonator
endif
nrow=(ay-1)/2    ! nrow=3: the w.g. or res. located at (3+1)th row from the bottom
ncol=(ax-1)/2
c input material and free-space properties:
data c0/2.99792458e8/tw/30.0e-12/ ! c0: speed of light in free space, tw: pulse width
mu0=4.0*pi*1.0e-7 ! permeability of free space
eps0=1.0/(c0*c0*mu0) ! permittivity of free space
factor=mu0/eps0
w0=w0*(2*pi*c0/a0) ! actual frequency of the guided mode
t0=4.*tw
c input space and time discretizations:
dx=a0/float(ng)
dy=dx
dt=1.0/sqrt(1.0/(dx*dx)+1.0/(dy*dy))/c0
c source and probe locations:
isrc=(nx-1-1)/2+1
jsrc=(ny-1-1)/2+1
ip1=(nx-1-1)/2+1
jp1=(ny-1-1)/2+1
c input nth time step for the grid observation:
write(*,*)'Input time step (<',nmax,') to observe the Ez, Hx, and Hy field grids:'
read(*,*)nth
c create a grid.eps file and draw cross & circle for visualizing the FDTD field grids
open(1, file='grid.eps', status='unknown')
write(1,*)"!PS"
write(1,*)" /scalefactor 2.28 def" ! for regular picture
! write(1,*)" /scalefactor 18.5 def" ! for enlarged picture
write(1,*)"scalefactor scalefactor scale"
write(1,*)"1 scalefactor div setlinewidth"
write(1,*)" /cross {moveto"
write(1,*)" -.2 0 rmoveto .4 0 rlineto"
write(1,*)" -.2 -.2 rmoveto 0 .4 rlineto stroke} def"
write(1,*)" /circle { .4 0 360 arc fill} def" ! for a circle
write(1,*)" /scircle { .3 0 360 arc fill} def" ! for smaller circle
! draw a star to indicate source location in the grid
write(1,*)" /starside"
write(1,*)" { 5 0 lineto" ! add line to path, 10 0 for bigger star
write(1,*)" currentpoint translate" ! move origin
write(1,*)" -144 rotate } def" ! rotate coord. sys.
write(1,*)" /star " ! stack: x y
write(1,*)" { moveto currentpoint translate 4 {starside} repeat"
write(1,*)" closepath gsave .5 setgray fill grestore"
write(1,*)" 200 200 fill} def" ! opposite of 'fill' is 'stroke'
! include the text 'PML-ABC'
write(1,*)" /pml {/Times-Roman findfont 10 scalefont"
write(1,*)" setfont 80 -97 moveto (PML-ABC) 217 rotate show} def" ! for waveguide
! write(1,*)" setfont 80 -97 moveto (PML-ABC) 217 rotate show} def" ! for resonator
! initialize ez,hx,hy fields including ez-all
do 200 j=1,ny-1
do 200 i=1,nx-1
do 200 k=1,nx
ez(i,j)=0.
hy(k,j)=0.
200 continue
do 201 j=1,ny
do 201 i=1,nx-1
hx(i,j)=0.
201 continue
do 204 j=1,ny-1+2*npml
do 204 i=1,nx-1+2*npml
do 204 k=1,nx+2*npml
ezall(i,j)=0.
hyall(k,j)=0.
204 continue
do 205 j=1,ny+2*npml
do 205 i=1,nx-1+2*npml
hxall(i,j)=0.
205 continue
! initialize materials

```

```

do 207 j=1,ny-1
do 207 i=1,nx-1
    eaxy(i,j)=ea
    ebxy(i,j)=eb
    sige(i,j)=sigmae
    sigm(i,j)=sigmam
    miur(i,j)=mur
207 continue
! describe main grids for Ez field in the computational domain (nx-1) x (ny-1)
do 1 j=1,ny-1
do 1 i=1,nx-1
    epsr(i,j)=eps0
!   write(1,*)i,j," cross" ! actual position
1 continue
! visualize the regions of main grid including pml boundary outside:
do 2 j=1,ny-1+2*npml
do 2 i=1,nx-1+2*npml
    write(1,*)i,j," cross"
2 continue
! describe photonic crystal by inserting cylinders at the lattice points
do 3 j=1,ng
do 3 i=1,ng
    x(i,j)=(float(i-1)-float((ng)/2))*dx
    y(i,j)=(float(j-1)-float((ng)/2))*dx
3 continue
do 5 j=1,ay
do 5 i=1,ax
do 5 l=1,ng
do 5 k=1,ng
    if (sqrt(x(k,l)*x(k,l)+y(k,l)*y(k,l)) .lt. r0) then
        epsr((i-1)*ng+k,(j-1)*ng+l)=eaxy(k,l)*eps0
!       write(1,*)(i-1)*ng+k,(j-1)*ng+l," circle" ! actual position
        write(1,*)(i-1)*ng+k+npml,(j-1)*ng+l+npml," circle" ! for picture due to pml
    endif
5 continue
c design photonic crystal device of interest:
if (device .eq. 1) then ! waveguide
! straight waveguide with the width: nrow*ng+1 to (nrow+1)*ng
do 6 j=nrow*ng+1,(nrow+1)*ng
do 6 i=1,ax*ng
    epsr(i,j)=ebxy(i,j)*eps0
    write(1,*)"0 1 0 setrgbcolor"
!   write(1,*)i,j," cross" ! actual positions
    write(1,*)i+npml,j+npml," scircle" ! for the picture after adding pml layer
6 continue
elseif (device .eq. 0) then ! resonator
do 250 j=nrow*ng+1,(nrow+1)*ng
do 250 i=ncol*ng+1,(ncol+1)*ng
    if (sqrt(float(i-((nx-2)/2+1))*2.+float(j-((ny-2)/2+1))*2.)*dx .lt. r0+r0/10.) then
        epsr(i,j)=ebxy(i,j)*eps0
        write(1,*)"0 1 0 setrgbcolor"
!       write(1,*)i,j," cross" ! actual position
        write(1,*)i+npml,j+npml," scircle" ! for the picture after adding pml layer
    endif
250 continue
endif
! update the coefficients for Ez, Hx, and Hy fields inside the main grid
do 208 j=1,ny-1
do 208 i=1,nx-1
do 208 k=1,nx
    ezca(i,j)=(1.-(sige(i,j)*dt)/(2.*epsr(i,j)))/(1.+(sige(i,j)*dt)/(2.*epsr(i,j)))
    ezcb(i,j)=1./(1.+(sige(i,j)*dt)/(2.*epsr(i,j)))
    hyca(k,j)=(1.-(sigm(k,j)*dt)/(2.*miur(k,j)))/(1.+(sigm(k,j)*dt)/(2.*miur(k,j)))
    hycb(k,j)=1./(1.+(sigm(k,j)*dt)/(2.*miur(k,j)))
208 continue
do 209 j=1,ny
do 209 i=1,nx-1
    hxca(i,j)=(1.-(sigm(i,j)*dt)/(2.*miur(i,j)))/(1.+(sigm(i,j)*dt)/(2.*miur(i,j)))
    hxcb(i,j)=1./(1.+(sigm(i,j)*dt)/(2.*miur(i,j)))
209 continue
! visualize pml region outside of the main grids: (nx-1)+2*npml x (ny-1)+2*npml
do 251 j=1,ny-1+2*npml
do 251 i=1,nx-1+2*npml
    if ((i .ge. 2 .and. i .lt. npml+1 .and. j .ge. 2 .and. j .lt. ny-1+2*npml) .or.
        & (i .ge. nx-1+npml .and. i .lt. nx-1+2*npml .and.
        & j .ge. 2 .and. j .lt. ny-1+2*npml) .or.
        & (i .ge. 2 .and. i .lt. nx-1+2*npml .and.
        & j .ge. 2 .and. j .lt. npml+1) .or.
        & (i .ge. 2 .and. i .lt. nx-1+2*npml .and.
        & j .ge. ny-1+npml .and. j .lt. ny-1+2*npml)) then

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write(1,*)"1 0 0 setrgbcolor"
write(1,*)i,j," circle"
endif
251 continue
! describe pml-abc
m=4, ! order
r=1.0e-10
delta=npml*dx
sigmamax=-(m+1.)*eps0*c0*log(r)/(delta*2.)
bcfactor = sigmamax*(dx/2.)*(m+1.)/(delta**m*dx*(m+1.))
do 7 i=2*npml,1,-1
    sigmax(i)=sigmamax*((float(i)*dx/2.+dx/2.)*(m+1.)-
    (float(i)*dx/2.-dx/2.)*(m+1.))/(delta**m*dx*(m+1.))
7 continue
do 8 i=2*npml,1,-1 ! reversing the sigmax(i)
    sig=sigmax(i)
    sigmay(2*npml+1-i)=sig
8 continue
do 9 i=1,2*npml
    sigmax(i)=sigmay(i)
9 continue
! initialize the pml-losses and pml-fields in the left-top square: Area 1
! for losses: sigmax-z1, sigmax-x1, sigmax-y1
do 10 j=2,2*npml,2
    sig=sigmax(j)
do 10 i=1,npml
    dummy1(i,j/2)=sig
10 continue
do 11 j=1,2*npml,2
    sig=sigmax(j)
do 11 i=1,npml
    dummy2(i,(j+1)/2)=sig
11 continue
do 12 j=1,npml ! for sigmax,s
do 12 i=1,npml
    sigmaxz1(i,j)=dummy1(j,i)
    sigmaxx1(i,j)=dummy1(j,i)
    sigmaxy1(i,j)=dummy2(j,i)
12 continue
do 13 j=npml,1,-1 ! for sigmay,s
do 13 i=npml,1,-1
    dummy3(npml+1-i,npml+1-j)=dummy1(j,i)
13 continue
do 14 j=1,npml
do 14 i=1,npml
    sigmayz1(i,j)=dummy3(j,i)
    sigmayy1(i,j)=sigmayz1(i,j)
14 continue
do 15 j=npml,1,-1
do 15 i=npml,1,-1
    dummy4(npml+1-i,npml+1-j)=dummy2(j,i)
15 continue
do 16 j=1,npml
do 16 i=1,npml
    sigmayx1(i,j)=dummy4(j,i)
16 continue
! for fields:
do 17 j=1,npml
do 17 i=1,npml
    ezxpml1(i,j)=0.
    ezypl1(i,j)=0.
    hxpml1(i,j)=0.
    hypml1(i,j)=0.
17 continue
! initialize pml-losses and pml-fields in the right-top square: Area 2
! for losses:
do 18 j=1,npml ! for sigmax,s
do 18 i=1,npml
    sigmaxz2(npml+1-j,npml+1-i)=sigmaxz1(j,i)
    sigmaxx2(npml+1-j,npml+1-i)=sigmaxx1(j,i)
    sigmaxy2(npml+1-j,npml+1-i)=sigmaxy1(j,i)
18 continue
do 19 j=1,npml ! for sigmay,s
do 19 i=1,npml
    sigmayz2(i,j)=sigmayz1(j,i)
    sigmayx2(i,j)=sigmayx1(j,i)
    sigmayy2(i,j)=sigmayy1(j,i)
19 continue
! for fields:
do 20 j=1,npml
do 20 i=1,npml
    ezxpml2(i,j)=0.
    ezypl2(i,j)=0.

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    hxpml2(i,j)=0.
    hypml2(i,j)=0.
20  continue
! initialize pml-losses and pml-fields in the left-bottom square: Area 3
do 21 j=1,npml ! for sigmax,s
do 21 i=1,npml
    sigmaxz3(i,j)=sigmaxz1(i,j)
    sigmaxx3(i,j)=sigmaxx1(i,j)
    sigmay3(i,j)=sigmay1(i,j)
21  continue
do 22 j=npml,1,-1 ! for sigmay,s
do 22 i=npml,1,-1
    dummy5(npml+1-i,npml+1-j)=sigmayz1(j,i)
    dummy6(npml+1-i,npml+1-j)=sigmayx1(j,i)
    dummy7(npml+1-i,npml+1-j)=sigmayy1(j,i)
22  continue
do 23 j=1,npml
do 23 i=1,npml
    sigmayz3(i,j)=dummy5(j,i)
    sigmayx3(i,j)=dummy5(j,i)
    sigmayy3(i,j)=dummy5(j,i)
23  continue
! for fields
do 24 j=1,npml
do 24 i=1,npml
    ezxpml3(i,j)=0.
    ezipml3(i,j)=0.
    hxpml3(i,j)=0.
    hypml3(i,j)=0.
24  continue
! initialize the pml-losses and pml-fields in the right-bottom square: Area 4
! for losses:
do 25 j=1,npml ! for sigmax,s
do 25 i=1,npml
    sigmaxz4(npml+1-j,npml+1-i)=sigmaxz1(j,i)
    sigmaxx4(npml+1-j,npml+1-i)=sigmaxx1(j,i)
    sigmay4(npml+1-j,npml+1-i)=sigmay1(j,i)
25  continue
do 26 j=npml,1,-1 ! for sigmay,s
do 26 i=npml,1,-1
    dummy8(npml+1-i,npml+1-j)=sigmayz1(j,i)
    dummy9(npml+1-i,npml+1-j)=sigmayx1(j,i)
    dummy10(npml+1-i,npml+1-j)=sigmayy1(j,i)
26  continue
do 27 j=1,npml
do 27 i=1,npml
    sigmayz4(i,j)=dummy8(j,i)
    sigmayx4(i,j)=dummy9(j,i)
    sigmayy4(i,j)=dummy10(j,i)
27  continue
! for fields:
do 28 j=1,npml
do 28 i=1,npml
    ezxpml4(i,j)=0.
    ezipml4(i,j)=0.
    hxpml4(i,j)=0.
    hypml4(i,j)=0.
28  continue
! initialize the pml-losses and pml-fields in the top-middle rectangle: Area 5->A
! for losses:
do 29 i=1,nx-1 ! sigma changes only for sigmax,s
do 29 j=1,npml
    sigmayzA(i,j)=sigmayz1(1,j)
    sigmayxA(i,j)=sigmayx1(1,j)
29  continue
do 30 i=1,nx
do 30 j=1,npml
    sigmayyA(i,j)=sigmayy1(1,j)
30  continue
! for fields:
do 31 j=1,npml
do 31 i=1,nx-1
    ezxpmlA(i,j)=0.
    ezipmlA(i,j)=0.
    hxpmlA(i,j)=0.
31  continue
do 32 j=1,npml
do 32 i=1,nx
    hypmlA(i,j)=0.
32  continue
! initialize the pml-losses and pml-fields in the bottom-middle rectangle: Area 6->B
! for losses:
do 33 j=npml,1,-1 ! for sigmay,s

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do 33 i=nx-1,1,-1
  dummy11(nx-1+1-i,npml+1-j)=sigmayzA(i,j)
  dummy12(nx-1+1-i,npml+1-j)=sigmayxA(i,j)
33 continue
do 34 j=1,npml
  do 34 i=1,nx-1
    sigmayzB(i,j)=dummy11(i,j)
    sigmayxB(i,j)=dummy12(i,j)
34 continue
do 35 j=npml,1,-1
  do 35 i=nx,1,-1
    dummy13(nx+1-i,npml+1-j)=sigmayyA(i,j)
35 continue
do 36 j=1,npml
  do 36 i=1,nx
    sigmayyB(i,j)=dummy13(i,j)
36 continue
! for fields:
do 37 j=1,npml
  do 37 i=1,nx-1
    ezxpmlB(i,j)=0.
    ezyplB(i,j)=0.
    hxpmlB(i,j)=0.
37 continue
do 38 j=1,npml
  do 38 i=1,nx
    hypmlB(i,j)=0.
38 continue
! initialize the pml-losses and pml-fields in the left-middle rectangle: Area 7->C
! for losses:
do 39 j=1,ny-1      ! sigma changes only for sigmax,s
  do 39 i=1,npml
    sigmaxzC(i,j)=sigmaxz1(i,1) ! i generated this using a different ...
    sigmaxyC(i,j)=sigmaxz1(i,1)
39 continue
! note sigmay_z1() is equivalent to sigmay_y1() that's why sigmaxzC(i,j)=sigmaxyC(i,j)
do 40 j=1,ny
  do 40 i=1,npml
    sigmaxxC(i,j)=sigmaxy1(i,1)
40 continue
! for fields:
do 41 j=1,ny-1
  do 41 i=1,npml
    ezxpmlC(i,j)=0.
    ezyplC(i,j)=0.
    hypmlC(i,j)=0.
41 continue
do 42 j=1,ny
  do 42 i=1,npml
    hxpmlC(i,j)=0.
42 continue
! initialize the pml-losses and pml-fields in the right-middle rectangle: Area 8->D
! for losses:
do 43 j=1,ny-1      ! for sigmax,s
  do 43 i=1,npml
    sigmaxzD(npml+1-i,ny-j)=sigmaxzC(i,j)
    sigmaxyD(npml+1-i,ny-j)=sigmaxyC(i,j)
43 continue
do 44 j=1,ny      ! for sigmax,s
  do 44 i=1,npml
    sigmaxxD(npml+1-i,ny+1-j)=sigmaxxC(i,j)
44 continue
! for fields:
do 45 j=1,ny-1
  do 45 i=1,npml
    ezxpmlD(i,j)=0.
    ezyplD(i,j)=0.
    hypmlD(i,j)=0.
45 continue
do 46 j=1,ny
  do 46 i=1,npml
    hxpmlD(i,j)=0.
46 continue
expfactor=exp(-bcfactor*dt/eps0)
c open files to store output data for further analysis:
open(2,file='grid_ezall.dat',status='unknown')
open(3,file='grid_hxall.dat',status='unknown')
open(4,file='grid_hyall.dat',status='unknown')
open(7,file='time_ezall.dat',status='unknown')
open(8,file='time_hxall.dat',status='unknown')
open(9,file='time_hyall.dat',status='unknown')
open(10,file='power.dat',status='unknown')
open(11,file='dxdt.dat',status='unknown')

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! start big do loop for the time steps -----
do 900 n=1,nmax
! H fields inside the main grid
do 47 j=2,ny-1
do 47 i=1,nx-1
hx(i,j)=hxca(i,j)*hx(i,j)-hxcb(i,j)*dt*(ez(i,j)-ez(i,j-1))/(dy*mu0)
47 continue
do 48 j=1,ny-1
do 48 i=2,nx-1
hy(i,j)=hyca(i,j)*hy(i,j)+hycb(i,j)*dt*(ez(i,j)-ez(i-1,j))/(dx*mu0)
48 continue
do 49 i=1,nx-1 ! boundary A
hx(i,ny)=expfactor*hx(i,ny)-(1.-expfactor)*(ezxpmlA(i,1)+ezypmlA(i,1)-
ez(i,ny-1))/(bcfactor*factor*dy)
49 continue
do 50 i=1,nx-1 ! boundary B
hx(i,1)=expfactor*hx(i,1)-(1.-expfactor)*(ez(i,1)-ezxpmlB(i,npml)-
ezypmlB(i,npml))/(bcfactor*factor*dy)
50 continue
do 51 j=1,ny-1 ! boundary C
hy(1,j)=expfactor*hy(1,j)+(1.-expfactor)*(ez(1,j)-ezxpmlC(npml,j)-
ezypmlC(npml,j))/(bcfactor*factor*dx)
51 continue
do 52 j=1,ny-1 ! boundary D
hy(nx,j)=expfactor*hy(nx,j)+(1.-expfactor)*(ezxpmlD(1,j)+ezypmlD(1,j)-
ez(nx-1,j))/(bcfactor*factor*dx)
52 continue
! H fields inside the Back PML: Area A
do 53 j=1,npml-1
do 53 i=1,nx-1
hxpmlA(i,j)=exp(-sigmayxA(i,j)*dt/eps0)*hxpmlA(i,j)-(1.-
exp(-sigmayxA(i,j)*dt/eps0))/(sigmayxA(i,j)*factor*dy)*(ezxpmlA(i,j+1)+
ezypmlA(i,j+1)-ezxpmlA(i,j)-ezypmlA(i,j))
53 continue
do 54 j=1,npml
do 54 i=2,nx-1
hypmlA(i,j)=hypmlA(i,j)+dt*(ezxpmlA(i,j)+ezypmlA(i,j)-ezxpmlA(i-1,j)-
ezypmlA(i-1,j))/(mu0*dx)
54 continue
do 55 j=1,npml ! boundary left
hypmlA(1,j)=expfactor*hypmlA(1,j)+(1.-expfactor)*(ezxpmlA(1,j)+ezypmlA(1,j)-
ezxpml1(npml,j)-ezypml1(npml,j))/(bcfactor*factor*dx)
55 continue
do 56 j=1,npml ! boundary right
hypmlA(nx,j)=expfactor*hypmlA(nx,j)+(1.-expfactor)*(ezxpml2(1,j)+ezypml2(1,j)-
ezxpmlA(nx-1,j)-ezypmlA(nx-1,j))/(bcfactor*factor*dx)
56 continue
do 57 i=1,nx-1 ! boundary upper
hxpmlA(i,npml)=hxpmlA(i,npml-1)
57 continue
! H fields inside the Front PML: Area B
do 58 j=2,npml
do 58 i=1,nx-1
hxpmlB(i,j)=exp(-sigmayxB(i,j)*dt/eps0)*hxpmlB(i,j)-(1.-exp(-sigmayxB(i,j)*
dt/eps0))/(sigmayxB(i,j)*factor*dy)*(ezxpmlB(i,j)+ezypmlB(i,j)-ezxpmlB(i,j-1)-
ezypmlB(i,j-1))
58 continue
do 59 j=1,npml
do 59 i=2,nx-1
hypmlB(i,j)=hypmlB(i,j)+dt*(ezxpmlB(i,j)+ezypmlB(i,j)-ezxpmlB(i-1,j)-
ezypmlB(i-1,j))/(mu0*dx)
59 continue
do 60 j=1,npml ! boundary left
hypmlB(1,j)=expfactor*hypmlB(1,j)+(1.-expfactor)*(ezxpmlB(1,j)+ezypmlB(1,j)-
ezxpml3(npml,j)-ezypml3(npml,j))/(bcfactor*factor*dx)
60 continue
do 61 j=1,npml ! boundary right
hypmlB(nx,j)=expfactor*hypmlB(nx,j)+(1.-expfactor)*(ezxpml4(1,j)+ezypml4(1,j)-
ezxpmlB(nx-1,j)-ezypmlB(nx-1,j))/(bcfactor*factor*dx)
61 continue
do 62 i=1,nx-1 ! boundary bottom
hxpmlB(i,1)=hxpmlB(i,2)
62 continue
! H fields inside the Left PML: Area C
do 63 j=2,ny-1
do 63 i=1,npml
hxpmlC(i,j)=hxpmlC(i,j)-dt*(ezxpmlC(i,j)+ezypmlC(i,j)-ezxpmlC(i,j-1)-
ezypmlC(i,j-1))/(mu0*dy)
63 continue
do 64 j=1,ny-1
do 64 i=2,npml
hypmlC(i,j)=exp(-sigmaxyC(i,j)*dt/eps0)*hypmlC(i,j)+(1.-exp(-sigmaxyC(i,j)*
dt/eps0))/(sigmaxyC(i,j)*factor*dx)*(ezxpmlC(i,j)+ezypmlC(i,j)-ezxpmlC(i-1,j)-

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    ezyplC(i-1,j))
64 continue
do 65 i=1,npml ! boundary down
    hxpmlC(i,1)=expfactor*hxpmlC(i,1)-(1.-expfactor)*(ezxpmlC(i,1)+ezyplC(i,1)-
    ezxpml3(i,npml)-ezypl3(i,npml))/(bcfactor*factor*dy)
65 continue
do 66 i=1,npml ! boundary upper
    hxpmlC(i,ny)=expfactor*hxpmlC(i,ny)-(1.-expfactor)*(ezxpml1(i,1)+ezypl1(i,1)-
    ezxpmlC(i,ny-1)-ezyplC(i,ny-1))/(bcfactor*factor*dy)
66 continue
do 67 j=1,ny-1 ! boundary left
    hypmlC(1,j)=hypmlC(2,j)
67 continue
! H fields inside the Right PML: Area D
do 68 j=2,ny-1
    do 68 i=1,npml
        hxpmlD(i,j)=hxpmlD(i,j)-dt*(ezxpmlD(i,j)+ezyplD(i,j)-ezxpmlD(i,j-1)-
        ezyplD(i,j-1))/(mu0*dy)
68 continue
do 69 j=1,ny-1
    do 69 i=1,npml-1
        hypmlD(i,j)=exp(-sigmaxyD(i,j)*dt/eps0)*hypmlD(i,j)+(1.-exp(-sigmaxyD(i,j)*
        dt/eps0))/(sigmaxyD(i,j)*factor*dx)*(ezxpmlD(i+1,j)+ezyplD(i+1,j)-
        ezxpmlD(i,j)-ezyplD(i,j))
69 continue
do 70 i=1,npml ! boundary down
    hxpmlD(i,1)=expfactor*hxpmlD(i,1)-(1.-expfactor)*(ezxpmlD(i,1)+ezyplD(i,1)-
    ezxpml4(i,npml)-ezypl4(i,npml))/(bcfactor*factor*dy)
70 continue
do 71 i=1,npml ! boundary upper
    hxpmlD(i,ny)=expfactor*hxpmlD(i,ny)-(1.-expfactor)*(ezxpml2(i,1)+ezypl2(i,1)-
    ezxpmlD(i,ny-1)-ezyplD(i,ny-1))/(bcfactor*factor*dy)
71 continue
do 72 j=1,ny-1 ! boundary right
    hypmlD(npml,j)=hypmlD(npml-1,j)
72 continue
! H fields inside the PML Area 1
do 73 j=1,npml-1
    do 73 i=1,npml
        hxpml1(i,j)=exp(-sigmayx1(i,j)*dt/eps0)*hxpml1(i,j)-(1.-exp(-sigmayx1(i,j)*
        dt/eps0))/(sigmayx1(i,j)*factor*dy)*(ezxpml1(i,j+1)+ezypl1(i,j+1)-
        ezxpml1(i,j)-ezypl1(i,j))
73 continue
do 74 i=1,npml
    hxpml1(i,npml)=hxpml1(i,npml-1)
74 continue
do 75 j=1,npml
    do 75 i=2,npml
        hypml1(i,j)=exp(-sigmayx1(i,j)*dt/eps0)*hypml1(i,j)+(1.-exp(-sigmayx1(i,j)*
        dt/eps0))/(sigmayx1(i,j)*factor*dx)*(ezxpml1(i,j)+ezypl1(i,j)-ezxpml1(i-1,j)-
        ezypl1(i-1,j))
75 continue
do 76 j=1,npml
    hypml1(1,j)=hypml1(2,j)
76 continue
! H fields inside the PML Area 2
do 77 j=1,npml-1
    do 77 i=1,npml
        hxpml2(i,j)=exp(-sigmayx2(i,j)*dt/eps0)*hxpml2(i,j)-(1.-exp(-sigmayx2(i,j)*
        dt/eps0))/(sigmayx2(i,j)*factor*dy)*(ezxpml2(i,j+1)+ezypl2(i,j+1)-
        ezxpml2(i,j)-ezypl2(i,j))
77 continue
do 78 i=1,npml
    hxpml2(i,npml)=hxpml2(i,npml-1)
78 continue
do 79 j=1,npml
    do 79 i=1,npml-1
        hypml2(i,j)=exp(-sigmayx2(i,j)*dt/eps0)*hypml2(i,j)+(1.-exp(-sigmayx2(i,j)*
        dt/eps0))/(sigmayx2(i,j)*factor*dx)*(ezxpml2(i+1,j)+ezypl2(i+1,j)-
        ezxpml2(i,j)-ezypl2(i,j))
79 continue
do 80 j=1,npml ! boundary right
    hypml2(npml,j)=hypml2(npml-1,j)
80 continue
! H fields inside the PML Area 3
do 81 j=1,npml
    do 81 i=2,npml
        hypml3(i,j)=exp(-sigmayx3(i,j)*dt/eps0)*hypml3(i,j)+(1.-exp(-sigmayx3(i,j)*
        dt/eps0))/(sigmayx3(i,j)*factor*dx)*(ezxpml3(i,j)+ezypl3(i,j)-ezxpml3(i-1,j)-
        ezypl3(i-1,j))
81 continue
do 82 j=1,npml
    hypml3(1,j)=hypml3(2,j)

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82 continue
do 83 j=2,npml
do 83 i=1,npml
  hxpm3(i,j)=exp(-sigmayx3(i,j)*dt/eps0)*hxpm3(i,j)-(1.-exp(-sigmayx3(i,j)*
  dt/eps0))/(sigmayx3(i,j)*factor*dy)*(ezxpm3(i,j)+ezypm3(i,j)-ezxpm3(i,j-1)-
  ezypm3(i,j-1))
83 continue
do 84 i=1,npml ! boundary bottom
  hxpm3(i,1)=hxpm3(i,2)
84 continue
! H fields inside the PML Area 4
do 85 j=2,npml
do 85 i=1,npml
  hxpm4(i,j)=exp(-sigmayx4(i,j)*dt/eps0)*hxpm4(i,j)-(1.-exp(-sigmayx4(i,j)*
  dt/eps0))/(sigmayx4(i,j)*factor*dy)*(ezxpm4(i,j)+ezypm4(i,j)-ezxpm4(i,j-1)-
  ezypm4(i,j-1))
85 continue
do 86 i=1,npml
  hxpm4(i,1)=hxpm4(i,2)
86 continue
do 87 j=1,npml
do 87 i=1,npml-1
  hypm4(i,j)=exp(-sigmayx4(i,j)*dt/eps0)*hypm4(i,j)+(1.-exp(-sigmayx4(i,j)*
  dt/eps0))/(sigmayx4(i,j)*factor*dx)*(ezxpm4(i+1,j)+ezypm4(i+1,j)-
  ezxpm4(i,j)-ezypm4(i,j))
87 continue
do 88 j=1,npml ! boundary right
  hypm4(npml,j)=hypm4(npml-1,j)
88 continue
! E field inside the main grid
do 89 j=1,ny-1
do 89 i=1,nx-1
  ez(i,j)=ezca(i,j)*ez(i,j)+ezcb(i,j)*dt*((hy(i+1,j)-hy(i,j))/dx-
  (hx(i,j+1)-hx(i,j))/dy)/epsr(i,j)
89 continue
! include source through E field
if (device .eq. 1) then
do 90 j=nrow*ng+1,(nrow+1)*ng ! check loop number 6 above
! pulse=exp(-(n*w0*dt-3.)*2.)*sin(w0*n*dt) ! modulated Gaussian pulse
pulse=sin(w0*n*dt) ! plane wave source
ez(1,j)=ez(1,j)+pulse
90 continue
elseif (device .eq. 0) then
  pulse=exp(-(n*dt-t0)**2./tw**2.)
  ez(isrc,jsrc)=ez(isrc,jsrc)+pulse
endif
! Ez fields inside the Back PML: Area A
do 91 j=1,npml
do 91 i=1,nx-1
  ezxpmA(i,j)=ezxpmA(i,j)+dt*(hypm4(i+1,j)-hypm4(i,j))/(eps0*dx)
91 continue
do 92 j=2,npml
do 92 i=1,nx-1
  ezypmA(i,j)=exp(-sigmayzA(i,j)*dt/eps0)*ezypmA(i,j)-(1.-exp(-sigmayzA(i,j)*
  dt/eps0))/(sigmayzA(i,j)*dy)*(hxpm4(i,j)-hxpm4(i,j-1))
92 continue
do 93 i=1,nx-1
  ezypmA(i,1)=exp(-sigmayzA(i,1)*dt/eps0)*ezypmA(i,1)-(1.-exp(-sigmayzA(i,1)*
  dt/eps0))/(sigmayzA(i,1)*dy)*(hxpm4(i,1)-hx(i,ny))
93 continue
! Ez fields inside the Front PML: Area B
do 94 j=1,npml
do 94 i=1,nx-1
  ezxpmB(i,j)=ezxpmB(i,j)+dt*(hypmB(i+1,j)-hypmB(i,j))/(eps0*dx)
94 continue
do 95 j=1,npml-1
do 95 i=1,nx-1
  ezypmB(i,j)=exp(-sigmayzB(i,j)*dt/eps0)*ezypmB(i,j)-(1.-exp(-sigmayzB(i,j)*
  dt/eps0))/(sigmayzB(i,j)*dy)*(hxpmB(i,j+1)-hxpmB(i,j))
95 continue
do 96 i=1,nx-1
  ezypmB(i,npml)=exp(-sigmayzB(i,npml)*dt/eps0)*ezypmB(i,npml)-(1.-
  exp(-sigmayzB(i,npml)*dt/eps0))/(sigmayzB(i,npml)*dy)*(hx(i,1)-hxpmB(i,npml))
96 continue
! Ez fields inside the Left PML: Area C
do 97 j=1,ny-1
do 97 i=1,npml-1
  ezxpmC(i,j)=exp(-sigmaxzC(i,j)*dt/eps0)*ezxpmC(i,j)+(1.-exp(-sigmaxzC(i,j)*
  dt/eps0))/(sigmaxzC(i,j)*dx)*(hypmC(i+1,j)-hypmC(i,j))
97 continue
do 98 j=1,ny-1
  ezxpmC(npml,j)=exp(-sigmaxzC(npml,j)*dt/eps0)*ezxpmC(npml,j)+(1.-
  exp(-sigmaxzC(npml,j)*dt/eps0))/(sigmaxzC(npml,j)*dx)*(hy(1,j)-hypmC(npml,j))

```

```

98 continue
do 99 j=1,ny-1
do 99 i=1,npml
ezypmlC(i,j)=ezypmlC(i,j)-dt*(hxpmlC(i,j+1)-hxpmlC(i,j))/(eps0*dy)
99 continue
! Ez fields inside the Right PML: Area D
do 100 j=1,ny-1
do 100 i=2,npml
ezxpmlD(i,j)=exp(-sigmaxzD(i,j)*dt/eps0)*ezxpmlD(i,j)+(1.-exp(-sigmaxzD(i,j)*
dt/eps0))/(sigmaxzD(i,j)*dx)*(hypmlD(i,j)-hypmlD(i-1,j))
100 continue
do 101 j=1,ny-1
ezxpmlD(1,j)=exp(-sigmaxzD(1,j)*dt/eps0)*ezxpmlD(1,j)+(1.-exp(-sigmaxzD(1,j)*
dt/eps0))/(sigmaxzD(1,j)*dx)*(hypmlD(1,j)-hypmlD(1,j))
101 continue
do 102 j=1,ny-1
do 102 i=1,npml
ezypmlD(i,j)=ezypmlD(i,j)-dt*(hxpmlD(i,j+1)-hxpmlD(i,j))/(eps0*dy)
102 continue
! Ez fields inside the PML Area 1
do 103 j=1,npml
do 103 i=1,npml-1
ezxpml1(i,j)=exp(-sigmaxz1(i,j)*dt/eps0)*ezxpml1(i,j)+(1.-exp(-sigmaxz1(i,j)*
dt/eps0))/(sigmaxz1(i,j)*dx)*(hypml1(i+1,j)-hypml1(i,j))
103 continue
do 104 j=1,npml
ezxpml1(npml,j)=exp(-sigmaxz1(npml,j)*dt/eps0)*ezxpml1(npml,j)+(1.-
exp(-sigmaxz1(npml,j)*dt/eps0))/(sigmaxz1(npml,j)*dx)*(hypml1(1,j)-
hypml1(npml,j))
104 continue
do 105 j=2,npml
do 105 i=1,npml
ezypml1(i,j)=exp(-sigmayz1(i,j)*dt/eps0)*ezypml1(i,j)-(1.-exp(-sigmayz1(i,j)*
dt/eps0))/(sigmayz1(i,j)*dy)*(hxpml1(i,j)-hxpml1(i,j-1))
105 continue
do 106 i=1,npml
ezypml1(i,1)=exp(-sigmayz1(i,1)*dt/eps0)*ezypml1(i,1)-(1.-exp(-sigmayz1(i,1)*
dt/eps0))/(sigmayz1(i,1)*dy)*(hxpml1(i,1)-hxpmlC(i,ny))
106 continue
! Ez fields inside the PML Area 2
do 107 j=1,npml
do 107 i=2,npml
ezxpml2(i,j)=exp(-sigmaxz2(i,j)*dt/eps0)*ezxpml2(i,j)+(1.-exp(-sigmaxz2(i,j)*
dt/eps0))/(sigmaxz2(i,j)*dx)*(hypml2(i,j)-hypml2(i-1,j))
107 continue
do 108 j=1,npml
ezxpml2(1,j)=exp(-sigmaxz2(1,j)*dt/eps0)*ezxpml2(1,j)+(1.-exp(-sigmaxz2(1,j)*
dt/eps0))/(sigmaxz2(1,j)*dx)*(hypml2(1,j)-hypmlA(nx,j))
108 continue
do 109 j=2,npml
do 109 i=1,npml
ezypml2(i,j)=exp(-sigmayz2(i,j)*dt/eps0)*ezypml2(i,j)-(1.-exp(-sigmayz2(i,j)*
dt/eps0))/(sigmayz2(i,j)*dy)*(hxpml2(i,j)-hxpml2(i,j-1))
109 continue
do 110 i=1,npml
ezypml2(i,1)=exp(-sigmayz2(i,1)*dt/eps0)*ezypml2(i,1)-(1.-exp(-sigmayz2(i,1)*
dt/eps0))/(sigmayz2(i,1)*dy)*(hxpml2(i,1)-hxpmlD(i,ny))
110 continue
! Ez fields inside the PML Area 3
do 111 j=1,npml
do 111 i=1,npml-1
ezxpml3(i,j)=exp(-sigmaxz3(i,j)*dt/eps0)*ezxpml3(i,j)+(1.-exp(-sigmaxz3(i,j)*
dt/eps0))/(sigmaxz3(i,j)*dx)*(hypml3(i+1,j)-hypml3(i,j))
111 continue
do 112 j=1,npml
ezxpml3(npml,j)=exp(-sigmaxz3(npml,j)*dt/eps0)*ezxpml3(npml,j)+(1.-
exp(-sigmaxz3(npml,j)*dt/eps0))/(sigmaxz3(npml,j)*dx)*(hypmlB(1,j)-
hypml3(npml,j))
112 continue
do 113 j=1,npml-1
do 113 i=1,npml
ezypml3(i,j)=exp(-sigmayz3(i,j)*dt/eps0)*ezypml3(i,j)-(1.-exp(-sigmayz3(i,j)*
dt/eps0))/(sigmayz3(i,j)*dy)*(hxpml3(i,j+1)-hxpml3(i,j))
113 continue
do 114 i=1,npml
ezypml3(i,npml)=exp(-sigmayz3(i,npml)*dt/eps0)*ezypml3(i,npml)-(1.-
exp(-sigmayz3(i,npml)*dt/eps0))/(sigmayz3(i,npml)*dy)*(hxpmlC(i,1)-hxpml3(i,npml))
114 continue
! Ez fields inside the PML Area 4
do 115 j=1,npml
do 115 i=2,npml
ezxpml4(i,j)=exp(-sigmaxz4(i,j)*dt/eps0)*ezxpml4(i,j)+(1.-exp(-sigmaxz4(i,j)*
dt/eps0))/(sigmaxz4(i,j)*dx)*(hypml4(i,j)-hypml4(i-1,j))
115 continue
do 116 j=1,npml
ezxpml4(1,j)=exp(-sigmaxz4(1,j)*dt/eps0)*ezxpml4(1,j)+(1.-exp(-sigmaxz4(1,j)*

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    dt/eps0))/(sigmaxz4(1,j)*dx)*(hypml4(1,j)-hypmlB(nx,j))
116 continue
do 117 j=1,npml-1
do 117 i=1,npml
    ezypl4(i,j)=exp(-sigmayz4(i,j)*dt/eps0)*ezypl4(i,j)-(1.-exp(-sigmayz4(i,j)*
    dt/eps0))/(sigmayz4(i,j)*dy)*(hxpml4(i,j+1)-hxpml4(i,j))
117 continue
do 118 i=1,npml
    ezypl4(i,npml)=exp(-sigmayz4(i,npml)*dt/eps0)*ezypl4(i,npml)-(1.
    -exp(-sigmayz4(i,npml)*dt/eps0))/(sigmayz4(i,npml)*dy)*(hxpmlD(i,1)-hxpml4(i,npml))
118 continue
! calculate ez=ezx+ezy in the PML areas
do 300 j=1,npml
do 300 i=1,npml
    ezpml1(i,j)=ezxpml1(i,j)+ezypl1(i,j)
    ezpml2(i,j)=ezxpml2(i,j)+ezypl2(i,j)
    ezpml3(i,j)=ezxpml3(i,j)+ezypl3(i,j)
    ezpml4(i,j)=ezxpml4(i,j)+ezypl4(i,j)
300 continue
do 301 j=1,npml
do 301 i=1,nx-1
    ezpmlA(i,j)=ezxpmlA(i,j)+ezyplA(i,j)
    ezpmlB(i,j)=ezxpmlB(i,j)+ezyplB(i,j)
301 continue
do 302 j=1,ny-1
do 302 i=1,npml
    ezpmlC(i,j)=ezxpmlC(i,j)+ezyplC(i,j)
    ezpmlD(i,j)=ezxpmlD(i,j)+ezyplD(i,j)
302 continue
! mapping all Ez field grids into a single matrix
do 303 j=1,npml ! Area 3
do 303 i=1,npml
    ezall(i,j)=ezpml3(i,j)
303 continue
do 304 j=1,ny-1 ! Area C
do 304 i=1,npml
    ezall(i,j+npml)=ezpmlC(i,j)
304 continue
do 305 j=1,npml ! Area 1
do 305 i=1,npml
    ezall(i,j+npml+ny-1)=ezpml1(i,j)
305 continue
do 306 j=1,npml ! Area B
do 306 i=1,nx-1
    ezall(i+npml,j)=ezpmlB(i,j)
306 continue
do 307 j=1,ny-1 ! main grid
do 307 i=1,nx-1
    ezall(i+npml,j+npml)=ez(i,j)
307 continue
do 308 j=1,npml ! Area A
do 308 i=1,nx-1
    ezall(i+npml,j+npml+ny-1)=ezpmlA(i,j)
308 continue
do 309 j=1,npml ! Area 4
do 309 i=1,npml
    ezall(i+npml+nx-1,j)=ezpml4(i,j)
309 continue
do 310 j=1,ny-1 ! Area D
do 310 i=1,npml
    ezall(i+npml+nx-1,j+npml)=ezpmlD(i,j)
310 continue
do 311 j=1,npml ! Area 2
do 311 i=1,npml
    ezall(i+npml+nx-1,j+npml+ny-1)=ezpml2(i,j)
311 continue
! mapping all Hx field grids into a single matrix
do 313 j=1,npml
do 313 i=1,npml
    hxall(i,j)=hxpml3(i,j) ! Area 3
    hxall(i,j+npml+ny-1)=hxpml1(i,j) ! Area 1
    hxall(i+npml+nx-1,j)=hxpml4(i,j) ! Area 4
    hxall(i+npml+nx-1,j+npml+ny-1)=hxpml2(i,j) ! Area 2
313 continue
do 314 j=1,ny
do 314 i=1,npml
    hxall(i,j+npml)=hxpmlC(i,j) ! Area C
    hxall(i+npml+nx-1,j+npml)=hxpmlD(i,j) ! Area D
314 continue
do 315 j=1,npml
do 315 i=1,nx-1
    hxall(i+npml,j)=hxpmlB(i,j) ! Area B
    hxall(i+npml,j+npml+ny-1)=hxpmlA(i,j) ! Area A

```

```

315 continue
do 316 j=1,ny
do 316 i=1,nx-1
  hxall(i+npml,j+npml)=hx(i,j) ! main grid
316 continue
! mapping all Hy field grids into a single matrix
do 317 j=1,npml
do 317 i=1,npml
  hyall(i,j)=hypml3(i,j) ! Area 3
  hyall(i,j+npml+ny-1)=hypml1(i,j) ! Area 1
  hyall(i+npml+nx-1,j)=hypml4(i,j) ! Area 4
  hyall(i+npml+nx-1,j+npml+ny-1)=hypml2(i,j) ! Area 2
317 continue
do 318 j=1,ny-1
do 318 i=1,npml
  hyall(i,j+npml)=hypmlC(i,j) ! Area C
  hyall(i+npml+nx-1,j+npml)=hypmlD(i,j) ! Area D
318 continue
do 319 j=1,npml
do 319 i=1,nx
  hyall(i+npml,j)=hypmlB(i,j) ! Area B
  hyall(i+npml,j+npml+ny-1)=hypmlA(i,j) ! Area A
319 continue
do 320 j=1,ny-1
do 320 i=1,nx
  hyall(i+npml,j+npml)=hy(i,j) ! main grid
320 continue
! record the fields at each grid at nth time step
if (n .eq. nth) then
do 170 j=1,ny-1+2*npml
do 170 i=1,nx-1+2*npml
  write(2,999)float(i),float(j),ezall(i,j) ! save data in grid_ezall.dat
  write(20,999)float(i),float(j),ezall(i,j)
170 continue
do 171 j=1,ny+2*npml
do 171 i=1,nx-1+2*npml
  write(3,999)float(i),float(j),hxall(i,j) ! save data in grid_hxall.dat
  write(21,999)float(i),float(j),hxall(i,j)
171 continue
do 172 j=1,ny-1+2*npml
do 172 i=1,nx+2*npml
  write(4,999)float(i),float(j),hyall(i,j) ! save data in grid_hyall.dat
  write(22,999)float(i),float(j),hyall(i,j)
172 continue
endif
! calculate Poynting vector product
t(n)=float(n)+1.
ezpower(n)=0.
do 173 j=npml+1,ny-1 ! power inside the pml region for both devices
do 173 i=npml+1,nx-1
! do 173 j=npml+1+nrow*ng+1,npml+(nrow+1)*ng ! power inside the w.g. channel
! do 173 i=npml+1,nx-1
  ezpower(n)=ezpower(n)+abs(ezall(i,j)**2.)
173 continue
write(10,997)t(n),ezpower(n)
! record time/pulse response at ports:
  write(7,998)ezall(ip1,jp1) ! save data in time_ezall.dat
  write(8,998)hxall(ip1,jp1) ! save data in time_hxall.dat
  write(9,998)hyall(ip1,jp1) ! save data in time_hyall.dat
900 continue ! ends big do loop for the time steps
  write(11,997)dx,dt
999 format(1x,e15.6,1x,e15.6,1x,e15.6)
998 format(1x,e15.6)
997 format(1x,e15.6,1x,e15.6)
  write(1,*)"1 0 0 setrgbcolor"
  write(1,*)ncol*ng+1+2*npml-2,nrow*ng+1+2*npml+2," star" ! for resonator
!   write(1,*)npml,nrow*ng+1+3*npml-10," star" ! for waveguide
  write(1,*)"0 0 0 setrgbcolor"
  write(1,*)ncol*ng+1+2*npml+3,ny-1+6," pml"
  write(1,*)"showpage"
close(1)
close(2)
close(3)
close(4)
close(7)
close(8)
close(9)
stop ''
end

```

C.2 Matlab for Impurity Modes

```
% This program computes defect modes in 1-d photonic crystal using FDTD method.
% eps1=1 and eps2=12.85 (GaAs), the lattice constant a=1 micron with thickness
% l1=0.7 and l2=a-l1 respectively
clear all; % clears the variable space
close all; % close all figures
c0=3e8; % speed of light in free-space
mu0=4.0*pi*1.0e-7; % permeability of free-space
eps0=1.0/(c0*c0*mu0); % permittivity of free-space
imp0=sqrt(mu0/eps0); % free-space impedance
epsr=[1. 12.85]; % air, GaAs at 300K
mur=[1. 1.]; epsdef=13;a=1e-6; c=3e8;imax=72;
% for impurity band: defect is put between l1 and l2 but on l1 side
l1=0.7;l11=0.3;l12=l1-l11; l2=1-l1;
ml1=round(imax*l1);ml2=round(imax*l2);ml11=round(imax*l11); ml12= round(imax*l12);
% force to satisfy ml11+ml12=ml1
if ml1 ~= ml11+ml12
    ml1=ml11+ml12; imax=ml1+ml2;
end
%
dy=a/imax;s=1;dt=1/c/sqrt(1/dy^2);% dt=s*dy/c;
% source location for ftdt algorithm
sloc=round(1*imax/5);
% Gaussian pulse properties
nw=3200;nc=3*nw;Nlambda=20;tw=0.167e-12;tc=3*tw;
% coefficients for E and H algorithms
se=[s*(imp0/epsr(1)) s*(imp0/epsr(2))];sh=[s/(imp0*mur(1)) s/(imp0*mur(2))];
%
def=1:2:30;
% maximum number of time steps
nmax=2^14;numk=0;
% open files for storing some important data
ft=fopen('6pi_over_10a.dat','w');smallField= fopen('field1.dat','w');
largeField=fopen('field2.dat','w');FrequencyData= fopen('freqFDTD.dat','w');
%
% for figure
ax=axes; hold on;
%
for l=1:length(def); % dielectric constant loop started
    sedef=s*imp0/def(l);%s*imp0/epsdef; % defect
    % k-vector in first Brillouin zone
    % for k=-pi/a:0.1*pi/a:pi/a; % main loop on k-vector
    k=0.5*pi/a;
    %
    numk=numk+1;
    ez=zeros(1,imax);hx=zeros(1,imax);rotate=exp(i*k*a); clear R;
    % for t=0:dt:nmax*dt-dt; % start time step loop
    for n=1:nmax; %
        t=n*dt;
        ez(sloc)=ez(sloc)+exp(-(t-0.5e-12).^2/1.0e-25)*exp(i*.20e15*t);
        % % FOR Ez-POLARIZED X-DIRECTED PROPAGATION (Ez,Hx)
        hx(1)=hx(1)+sh(1)*(ez(1)-ez(length(ez))*rotate);
        % % update Hx field
        hx(2:ml1-1)=hx(2:ml1-1)+sh(1)*(ez(2:ml1-1)-ez(1:ml1-2));
        hx(ml1:imax)=hx(ml1:imax)+sh(2)*(ez(ml1:imax)-ez(ml1-1:imax-1));
        % % update Ez field
        ez(1:ml1-1)=ez(1:ml1-1)+se(1)*(hx(2:ml1)-hx(1:ml1-1));
        ez(ml11:ml11+ml12-1)=ez(ml11:ml11+ml12-1)+sedef*(hx(ml11+1:ml1)- hx(ml11:ml1-1));
        ez(ml1:imax-1)=ez(ml1:imax-1)+se(2)*(hx(ml1+1:imax)-hx(ml1:imax-1));
        % % periodic boundary condition on Ez field
        ez(imax)=ez(imax)+se(2)*(hx(1)/rotate-hx(length(ez)));
        % % record the Response, the function of time, at an observation port
        pot=round(2*imax/5); R(round(n+1))=(ez(pot));
    %
end; % time step loop ended
%
% % Field distribution computation -----
% figure(1);
% % plot(real(R));
% if abs(R)<=1
%     plot(real(R),'r');
%     fprintf(smallField,'%6.2f %14.9f \n',[1:nmax+1;real(R)]);
% else
%     plot(real(R),'b');
%     fprintf(largeField,'%6.2f %14.9f \n',[1:nmax+1;real(R)]);
% end
% figure(2);
```

```

% fourier=real(fft(R)); % fourier=abs(fftshift(fft(R)));
% % plot(fourier);
% freq=1/dt*(1:length(fourier))./length(R);
% index1=1;index2=1000;%length(fourier);
% freq_index=index1:index2;
% freq_interest=freq(freq_index)./1.0e15; % PHz, petahertz
% % plot(freq_interest,fourier(freq_index));
% % fprintf(ft, ' %14.9f %14.9f \n ',[freq_interest;fourier(freq_index)]);
% if abs(R)<=1
%     plot(freq_interest,fourier(freq_index),'r');
% else
%     plot(freq_interest,fourier(freq_index),'b');
% end
% figure(3);
% plot(real(fft(fft(R))/nmax));
%
% Band computation-----
fourier=abs(fft(R));
f=1/dt*(1:length(fourier))./length(R);
f=f*a/c; % f*a/c=normalized frequency, k*a/2pi=normalized wave vector
wCount=1;
if (fourier(1)/fourier(2))>1.0001
    wEigen(numk,wCount)=f(1);
    wCount=wCount+1;
end
for u=2:length(fourier)-1
    if (fourier(u)/fourier(u-1))>1.0001&&(fourier(u)/fourier(u+1))>1.0001
        wEigen(numk,wCount)=f(u);
        wCount=wCount+1;
    end
end
% record first few bands for the plots
nb=10; % number of bands
if (wCount-1)>=nb
    plot(ones(1,nb)*def(1),abs(wEigen(numk,1:nb)),'o', 'LineWidth',3);
    fprintf(FrequencyData, ' %14.9f %14.9f \n ',[ones(1,nb)*def(1);abs(wEigen(numk,1:nb))]);
else
    plot(ones(1,wCount-1)*def(1),abs(wEigen(numk,1:wCount-1)), 'o', 'LineWidth',3);
end
ylim([0 2]);xlim([0 30]);set(ax,'XGrid','on'); set(ax,'YGrid','on');
drawnow;
end; % main loop on dielectric constant ended
%
fclose(ft);fclose(smallField);fclose(largeField);fclose(FrequencyData);

```

APPENDIX D

Programming Source Codes for Difference Equation Waveguides

D.1 Single Mode onto In-Channel Nonlinear Features: mode.f

! This program computes the transmissivity vs gp/g for a single frequency
! guided mode of photonic crystal waveguide. The Kerr nonlinear impurity is
! located at a lattice site on the waveguide channel.

```
integer ntrial,it,nn
parameter (n=1)
real x(n),y(n),z(n)
real x1,y1,z1,tolx,tolf
real b,kv,gp,g,dn,cn,tc,rc,rt,l1,l2,l3,ytc,ztz,yrc,zrc,yrt,zrt
c constants: x...initial guess, n...dimension
ntrial=100 ! ntrial...number of tries
tolx=0.001 ! tol x ...error in the horizontal (x) direction
tolf=0.001 ! tolf ...error in the vertical (f) direction
b=0.0869
c b=0.1738 ! two times the original 'b=0.0869', kv=1.5
kv=2.5
cn=cos(kv)
dn=1.+2.*b*cn
g=1./dn
c same calculation but for three different Kerr parameters t,t2,t3
l1=0.000
l2=0.175
l3=0.421
c guessing initial values corresponding to l1,l2,l3:
x(1)=1.
y(1)=50.
z(1)=-100.
c big do loop starts
do 200 it=1,1200
gp=0.40*g+0.0012*it
c gp=g
c call Newton-Raphson
call mnewt(ntrial, x, n, tolx,tolf,gp,g,l1)
call mnewt(ntrial, y, n, tolx,tolf,gp,g,l2)
call mnewt(ntrial, z, n, tolx,tolf,gp,g,l3)
c store the solutions in the computer memory
x1 = x(1)
y1 = y(1)
z1 = z(1)
c compute transmission coefficients
call tcoeff(x1,tc,rc,rt,b,kv,g)
call tcoeff(y1,yc,ycr,yrt,b,kv,g)
call tcoeff(z1,ztc,zrc,zrt,b,kv,g)
c print transmission coefficients in output files
write(6,998) gp/g,x1,tc,rc,rt
write(21,99) gp/g,tc
write(22,99) gp/g,ycr
write(23,99) gp/g,ztc
200 continue
998 format(5f16.8)
99 format(2x,e15.8,2x,e15.8)
c call gnuplot to display the result of the file: mplot.gnu
! call system ('gnuplot mplot.gnu')
! call system ('convert mplot.eps mplot.pdf')
end
c main program ends

c include subroutine files
include 'mnewt.f'
include 'usrfun.f'
include 'tcoeff.f'
include 'ludcmp.f'
include 'lubksb.f'
! mnewt.f
subroutine mnewt(ntrial,x,n,tolx,tolf,gp,g,l)
integer n,ntrial,np
real tolf,tolx,x(n)
parameter (np=15)
real gp,g,l
c uses lubksb,ludcmp,usrfun
```

```

integer i,k,indx(np)
real d,errf,errx,fjac(np,np),fvec(np),p(np)
do 14 k=1,ntrial
  call usrfun(x,n,np,fvec,fjac,gp,g,l)
  errf=0.
  do 11 i=1,n
    errf=errf+abs(fvec(i))
  11 continue
  if(errf.le.tolf)return
  do 12 i=1,n
    p(i)=-fvec(i)
  12 continue
  call ludcmp(fjac,n,np,indx,d)
  call lubksb(fjac,n,np,indx,p)
  errx=0.
  do 13 i=1,n
    errx=errx+abs(p(i))
    x(i)=x(i)+p(i)
  13 continue
  if(errx.le.tolx)return
  14 continue
  return
end
! ludcmp.f
subroutine ludcmp(fjac,n,np,indx,d)
parameter (nmax=100,tiny=1.0e-20)
dimension fjac(np,np),indx(n),vv(nmax)
d=1.
do 12 i=1,n
  aamax=0.
  do 11 j=1,n
    if (abs(fjac(i,j)).gt.aamax) aamax=abs(fjac(i,j))
  11 continue
  if (aamax.eq.0.) pause 'singular matrix.'
  vv(i)=1./aamax
  12 continue
do 19 j=1,n
  if (j.gt.1) then
    do 14 i=1,j-1
      sum=fjac(i,j)
      if (i.gt.1)then
        do 13 k=1,i-1
          sum=sum-fjac(i,k)*fjac(k,j)
        13 continue
      fjac(i,j)=sum
    endif
    continue
  14 endif
  aamax=0.
  do 16 i=j,n
    sum=fjac(i,j)
    if (j.gt.1)then
      do 15 k=1,j-1
        sum=sum-fjac(i,k)*fjac(k,j)
      15 continue
      fjac(i,j)=sum
    endif
    dum=vv(i)*abs(sum)
    if (dum.ge.aamax) then
      imax=i
      aamax=dum
    endif
  16 continue
  if (j.ne.imax)then
    do 17 k=1,n
      dum=fjac(imax,k)
      fjac(imax,k)=fjac(j,k)
      fjac(j,k)=dum
    17 continue
    d=-d
    vv(imax)=vv(j)
  endif
  indx(j)=imax
  if(j.ne.n)then
    if(fjac(j,j).eq.0.)fjac(j,j)=tiny
    dum=1./fjac(j,j)
    do 18 i=j+1,n
      fjac(i,j)=fjac(i,j)*dum
    18 continue
  endif
  19 continue
  if(fjac(n,n).eq.0.)fjac(n,n)=tiny
  return
end
! lubksb.f

```

```

subroutine lubksb(fjac,n,np,indx,p)
dimension fjac(np,np),indx(n),p(n)
ii=0
do 12 i=1,n
  ll=indx(i)
  sum=p(ll)
  p(ll)=p(i)
  if (ii.ne.0)then
    do 11 j=ii,i-1
      sum=sum-fjac(i,j)*p(j)
11    continue
  else if (sum.ne.0.) then
    ii=i
  endif
  p(i)=sum
12 continue
do 14 i=n,1,-1
  sum=p(i)
  if(i.lt.n)then
    do 13 j=i+1,n
      sum=sum-fjac(i,j)*p(j)
13    continue
  endif
  p(i)=sum/fjac(i,i)
14 continue
return
end
! usrfun.f: this subroutine calculates the nonlinear function and its derivative
subroutine usrfun(x,n,np,f,dfdx,gp,g,l)
dimension x(n),f(n),dfdx(np,np)
real x1
real g,gp,l
x1 = x(1)
c specify the function: f(x)=0
f(1) =gp*(1.+1*x1*x1)*x1-g
c define derivatives: dfdx
dfdx(1,1)=gp*(1.+3.*1*x1*x1)
c
return
end
! tcoeff.f: this subroutine calculates the transmission coefficients
subroutine tcoeff(z,tc,rc,rt,b,kv,g)
real z
real b,kv,g,sn,cn s2,c2,gb,gr,g2,tn,td,rn,rd,tc,rc,rt
intrinsic sin,cos
sn=sin(kv)
cn=cos(kv)
s2=sn*sn
c2=cn*cn
gb=1./(g*b)
gr=gb*(z-g)
g2=gr*gr
tn=4.*s2
td=4.+g2-4.*gr*cn
rn=4.*c2+g2-4.*gr*cn
rd=4.+g2-4.*gr*cn
tc=tn/td
rc=rn/rd
rt=rc+tc
return
end

```

D.2 Transmission Maxima for the Single Mode: mode_gt.f

```

! The program computes transmission maxima in the (g,t) space of photonic
! crystal waveguide containing single in-channel Kerr nonlinearity.
! In this case, we chose exact or analytical solutions for cubic
! polynomials instead of using the Newton-Raphson solver. Formula used
! here are given in Jan J. Tuma and Ronald A. Walsh, 'Engineering
! Mathematics Handbook', McGraw-Hill, 1998. In addition, a part of codes
! in cubic subroutine was taken from Dr. Nam Sun Wang, Department of
! Chemical & Biomolecular Engineering, University of Maryland
c Declare variables -----
complex x(3)
real x(3)
!
real bb,kv,gp,g,dn,cn,tc,rc,rt,x1,x2,x3,a,b,c,d,yc,ztc,zrc,zrc,yrt,zrt,lx2,r,t
real gpp(5000),gppp(5000),tcp(5000),tcpp(5000),gpmax,tcmx
integer i,j,it,imax
! Format the cubic nonlinear equation -----
! write(*,*) 'Solve a cubic equation f(x)=0:'
! write(*,*) ' gp*(1.+lx2*t**2*x*x)*x-g= 0'
! write(*,*) 'where a, b, c, and d are real.'
! Input parameters -----
imax=1200

```

```

bb=0.0869 ! NN interaction, reference: PRB 77 p. 115105 McGurn
kv=3.0 ! wave vector, reference: PRB 77 p. 115105 McGurn
cn=cos(kv)
dn=1.+2.*bb*cn
g=1./dn ! dispersion relation
lx2=0.005! nonlinearity,  $|x|^2=0.005$ , reference: PRB 77 p. 115105 McGurn
! 0.002, 0.005, 0.009 were used in the results
r=1.00001! scanning parameter for the transmission maxima
! Begin the t loop -----
do 200 j=1,50
    t=0.2*float(j-1)
    do 100 it=1,imax
        gp=0.40*g+0.0012*float(it)
        gpp(it)=gp ! it was gp/g in previous case
c compute the coefficients for cubic nonlinear equation -----
a=gp*lx2*t**2 !
b=0.
c=gp
d=-g
c call the routine to solve the cubic equation -----
call cubic(a, b, c, d, x, nroot)
c output the results -----
! write(*,*)
! write(*,'(a,i2,a)') ' There are', nroot, ' root(s):'
do i=1, nroot
    write(*,*) x(i) ! prints as '(real, imag)'
    write(*,*) real(x(i)) ! prints as 'real'
    x(i)=real(x(i)) ! stores the solutions in computer memory
enddo
x1 = x(1) ! only the first solution is physically meaningful
! x2 = x(2)
! x3 = x(3)
call tcoeff(x1,tc,rc,rt,bb,kv,g) ! compute transmission coefficients
! call tcoeff(x2,x2tc,x2rc,x2rt,bb,kv,g)
! call tcoeff(x3,x3tc,x3rc,x3rt,bb,kv,g)
write(11,99) gp,tc ! print transmission coefficient vs g on screen
! write(12,99) gp/g,x2tc
! write(13,99) gp/g,x3tc
tcp(it)=tc ! store the coefficients in computer memory
c print transmission at a fixed t
if(t.eq.8) then
    write(15,99) gp,tc
endif
100 continue
! do i=1,imax
! write(*,*)gpp(i),tcp(i)
! write(12,99)gpp(i),tcp(i)
! enddo
! scan the maximum values of transmission coefficients -----
if (tcp(1)/tcp(2) .gt. r) then
    tcpp(1)=tcp(1)
endif
do 300 i=2,imax
    if (tcp(i)/tcp(i-1) .gt. r .and. tcp(i)/tcp(i+1) .gt. r) then
        tcpp(i)=tcp(i) ! store all the maxima and minima
        gppp(i)=gpp(i)
        if (tcpp(i) .gt. 0.) then ! excludes all minima
            write(*,*) gppp(i), tcpp(i)
            gpmax=gppp(i)
            tcmax=tcpp(i)
            write(*,*)gpmax,tcmax
            write(*,*) t,gpmax
            write(10,99) t,gpmax
        endif
    endif
300 continue
! write(*,*) t,gpmax
! write(10,99) t,gpmax
200 continue
99 format(2x,e15.8,2x,e15.8)
c plot the result directly by calling gnuplot, great!!
! call system ('gnuplot gt.gnu')
stop
end
! End of main proram -----
! comment out the followings in order to use Newton-Raphson method
!
! ! Reference for subroutines: Numerical Recipe for F77 Chapter 9
! integer ntrial,it,nn
! parameter (n=1)

```

```

! real x(n),y(n),z(n)
! real x1,y1,z1,tolx,tolf
! real b,kv,gp,g,dn,cn,tc,rc,rt,l1,l2,l3
! c
! c constants: x...initial guess, n...dimension
! ntrial=100 ! ntrial...number of tries
! tolx=0.001 ! tolx ...error in the horizontal (x) direction
! tolf=0.001 ! tolf ...error in the vertical (f) direction
! b=0.0869
! c b=0.1738 ! two times the original 'b=0.0869'
! c kv=1.5
! kv=2.5
! cn=cos(kv)
! dn=1.+2.*b*cn
! g=1./dn
! c same calculation but for three different Kerr parameters t,t2,t3
! l1=0.000
! l2=0.175
! l3=0.421
! c guessing initial values corresponding to l1,l2,l3:
! x(1)=1.
! y(1)=1.
! z(1)=1.
! ! y(1)=50.
! ! z(1)=-100.
! do 200 it=1,1200
! gp=0.40*g+0.0012*it
! c gp=g
! call mnewt(ntrial, x, n, tolx,tolf,gp,g,l1)
! ! call mnewt(ntrial, y, n, tolx,tolf,gp,g,l1)
! ! call mnewt(ntrial, z, n, tolx,tolf,gp,g,l1)
! call mnewt(ntrial, y, n, tolx,tolf,gp,g,l2)
! call mnewt(ntrial, z, n, tolx,tolf,gp,g,l3)
! x1 = x(1)
! y1 = y(1)
! z1 = z(1)
! call tcoeff(x1,tc,rc,rt,b,kv,g)
! call tcoeff(y1,yc,rc,yrt,b,kv,g)
! call tcoeff(z1,zc,zrc,zrt,b,kv,g)
!
! write(6,998) gp/g,x1,tc,rc,rt
! write(21,99) gp/g,tc
! write(22,99) gp/g,yc
! write(23,99) gp/g,zc
! 200 continue
! 998 format(5f16.8)
! 99 format(2x,e15.8,2x,e15.8)
! call system ('gnuplot w1.gnu')
! ! call system ('convert w1.eps w1.pdf')
! end
! include 'mnewt.f'
! include 'usrfun.f'
! include 'tcoeff.f'
! include 'ludcmp.f'
! include 'lubksb.f'
!
! include 'tcoeff.f'
! subroutine giving exact or analytical solutions for cubic polynomials
c -----
c subroutine cubic(a, b, c, d, x, nroot)
c -----
c Declare variables
complex x(3)
data pi/3.141592654/
c Step 0: If a is 0 use the quadratic formula. -----
if(a .eq. 0.)then
call quad(b, c, d, x, nroot)
return
endif
c Cubic equation with 3 roots
nroot = 3
c Step 1: Calculate p and q -----
p = c/a - b*b/a/a/3.
q = (2.*b*b*b/a/a/a - 9.*b*c/a/a + 27.*d/a) / 27.
c Step 2: Calculate DD (discriminant) -----
DD = p*p*p/27. + q*q/4.
c Step 3: Branch to different algorithms based on DD -----
if(DD .lt. 0.)then
c Step 3b:
c 3 real unequal roots -- use the trigonometric formulation
phi = acos(-q/2./sqrt(abs(p*p*p)/27.))
temp1=2.*sqrt(abs(p)/3.)
y1 = temp1*cos(phi/3.)

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        y2 = -temp1*cos((phi+pi)/3.)
        y3 = -temp1*cos((phi-pi)/3.)
    else
c Step 3a:
c 1 real root & 2 conjugate complex roots OR 3 real roots (some are equal)
        temp1 = -q/2. + sqrt(DD)
        temp2 = -q/2. - sqrt(DD)
        u = abs(temp1)**(1./3.)
        v = abs(temp2)**(1./3.)
        if(temp1 .lt. 0.) u=-u
        if(temp2 .lt. 0.) v=-v
        y1 = u + v
        y2r = -(u+v)/2.
        y2i = (u-v)*sqrt(3.)/2.
    endif
c Step 4: Final transformation
        temp1 = b/a/3.
        y1 = y1-temp1
        y2 = y2-temp1
        y3 = y3-temp1
        y2r=y2r-temp1
c Assign answers
        if(DD .lt. 0.)then
            x(1) = cmplx( y1, 0.)
            x(2) = cmplx( y2, 0.)
            x(3) = cmplx( y3, 0.)
        elseif(DD .eq. 0.)then
            x(1) = cmplx( y1, 0.)
            x(2) = cmplx(y2r, 0.)
            x(3) = cmplx(y2r, 0.)
        else
            x(1) = cmplx( y1, 0.)
            x(2) = cmplx(y2r, y2i)
            x(3) = cmplx(y2r,-y2i)
        endif
    end
end

```

D.3 Single Frequency Mode into Off-Channel Features: mode_2off.f

```

! This program calculates the transmissivity vs gp/g for the single frequency guided
! mode of 2D PC waveguide mediated with two off-channel Kerr nonlinear sites in
! the lattice. Using this program we study the behavior of the system by
! changing the strength of pp with respect of gp. The pp and gp are described
! in this preamble below.
! References: mnewt,lubksb,ludcmp,usrfun in Numerical Recipe for F77
c x..initial guess, n..dimension, ntrial..number of tries, tol x ..error in the horizontal (x) direction
c tolf ..error in the vertical (f) direction
c b..relative coupling coefficient of NN sites (in-channel) : b/a
c c..relative coupling coefficient of NN sites (off-channel) : c/a
c kv..wave vector, g..gamma, gp..gamma prime, pp..gamma double prime
c t..lambda or Kerr parameter (first off-site), tt..Kerr parameter (second off-site)
c tc..transmission coefficient, rc..reflection coefficient, rt..R+T=1
integer ntrial,it,imax
parameter (n=2)
real tol,x,tolf, x(n),y(n),z(n)
real x1,x2, y1,y2, z1,z2
real b,c,g,gp,pp,kv,t,tt,tc1,rc1,rt1,gps
real tc2,rc2,rt2, ytc1,yc1,yrt1,yc2,yc2,yrt2, ztc1,zrc1,zrt1,ztc2,zrc2,zrt2
c for 100 level do loop =====
! specifying the constants
ntrial=100
tolx=0.001
tolf=0.001
imax=650
gps=0.40
!
    b=0.0869
    b=0.1738
    c=0.04
c
    c=0.02
    kv=2.5
    den=1.+2.*b*cos(kv)
    g=1./den
    t=0.00125
    tt=0.00
c
    pp=g
    pp=0.
! the condition tt=0 with pp=0 makes the system a single off-channel case
! guessing initial values: three sets of initial values
x(1)=1.
x(2)=1.
y(1)=50.
y(2)=50.

```

```

z(1)=-100.
z(2)=-100.
! do loop starts
  do 100 it=1,imax
    gp=g*gps+0.0012*it
    call mnewt(ntrial,x,n,tolx,tolf,b,c,g,gp,pp,t,tt)
    call mnewt(ntrial,y,n,tolx,tolf,b,c,g,gp,pp,t,tt)
    call mnewt(ntrial,z,n,tolx,tolf,b,c,g,gp,pp,t,tt)
    x1=x(1)
    x2=x(2)
    y1=y(1)
    y2=y(2)
    z1=z(1)
    z2=z(2)
! The 'call mnewt' calculates 'r' and 'rp' fields for each set of the
! initial values as (1)s and (2)s respectively. However, only 'r'
! solutions are present in transmission or reflection coefficient
! expressions. Check the model in original draft.
    call tcoeff(x1,b,c,g,kv,t,gp,tc1,rc1,rt1)
    call tcoeff(y1,b,c,g,kv,t,gp,yc1,rc1,yrt1)
    call tcoeff(z1,b,c,g,kv,t,gp,ztc1,zrc1,zrt1)
c we do not use this for the calculation of transmissivity or reflectivity
c because only 'r' fields are present in T or R, not the 'rp'
c call tcoeff(x2,b,c,g,kv,t,gp,tc2,rc2,rt2)
c call tcoeff(y2,b,c,g,kv,t,gp,yc2,rc2,yrt2)
c call tcoeff(z2,b,c,g,kv,t,gp,ztc2,zrc2,zrt2)
    write(6,998) gp/g,x1,tc1,rc1,rt1
    write(61,999) gp/g,tc1
    write(62,999) gp/g,yc1
    write(63,999) gp/g,ztc1
100 continue ! do loop ends
998 format(5f16.8)
999 format(2x,e15.8,2x,e15.8)
c for 200 level do loop =====
! specifying the constants
  ntrial=100
  tolx=0.001
  tolf=0.001
!   b=0.0869
  b=0.1738
  c=0.04
c   c=0.02
  kv=2.5
  den=1.+2.*b*cos(kv)
  g=1./den
  t=0.00125
  tt=0.00125
  pp=g !pp=g/2. or 1.98 or 1.99 are very interesting
c   pp=0.
! the condition tt=0 with pp=0 makes the system a single off-channel case
! guessing initial values: three sets of initial values
  x(1)=1.
  x(2)=1.
  y(1)=50.
  y(2)=50.
  z(1)=-100.
  z(2)=-100.
! do loop starts
  do 200 it=1,imax
    gp=g*gps+0.0012*it
    call mnewt(ntrial,x,n,tolx,tolf,b,c,g,gp,pp,t,tt)
    call mnewt(ntrial,y,n,tolx,tolf,b,c,g,gp,pp,t,tt)
    call mnewt(ntrial,z,n,tolx,tolf,b,c,g,gp,pp,t,tt)
    x1=x(1)
    x2=x(2)
    y1=y(1)
    y2=y(2)
    z1=z(1)
    z2=z(2)
! The 'call mnewt' calculates 'r' and 'rp' fields for each set of the
! initial values as (1)s and (2)s respectively. However, only 'r'
! solutions are present in transmission or reflection coefficient
! expressions. Check the model in original draft.
    call tcoeff(x1,b,c,g,kv,t,gp,tc1,rc1,rt1)
    call tcoeff(y1,b,c,g,kv,t,gp,yc1,rc1,yrt1)
    call tcoeff(z1,b,c,g,kv,t,gp,ztc1,zrc1,zrt1)
c we do not use this for the calculation of transmissivity or reflectivity
c because only 'r' fields are present in T or R, not the 'rp'
c call tcoeff(x2,b,c,g,kv,t,gp,tc2,rc2,rt2)

```



```

      call usrfun(x,n,NP,fvec,fjac,b,c,g,gp,pp,t,tt)
      errf=0.
      do 11 i=1,n
        errf=errf+abs(fvec(i))
11      continue
      if(errf.le.tolf)return
      do 12 i=1,n
        p(i)=-fvec(i)
12      continue
      call ludcmp(fjac,n,NP,indx,d)
      call lubksb(fjac,n,NP,indx,p)
      errx=0.
      do 13 i=1,n
        errx=errx+abs(p(i))
        x(i)=x(i)+p(i)
13      continue
      if(errx.le.tolx)return
14      continue
      return
      end
      subroutine usrfun(x,n,NP,f,dfdx,b,c,g,gp,pp,t,tt)
      dimension x(n),f(n),dfdx(NP,NP)
      real x1,x2
      real b,c,g,gp,pp,t,tt
      x1=x(1)
      x2=x(2)
      c the nonlinear function f(x) has two variables 'r' and 'rp'
      c specify the function: f(x)=0
      f1=x1-gp*(1.0+t*x1*x1)*x1
      f1=f1-pp*b*(1.0+tt*x2*x2)*x2
      f(1)=f1-g*c
      f2=x2-pp*(1.0+tt*x2*x2)*x2
      f(2)=f2-gp*b*(1.0+t*x1*x1)*x1
      c Jacobian matrix elements
      c define derivatives: dfdx
      dfdx(1,1)=1.0-gp*(1.0+3.0*t*x1*x1)
      dfdx(1,2)=-pp*b*(1.0+3.0*tt*x2*x2)
      dfdx(2,1)=-gp*b*(1.0+3.0*t*x1*x1)
      dfdx(2,2)=1.0-pp*(1.0+3.0*tt*x2*x2)
      return
      end
      c transmission and reflection coefficients-----
      subroutine tcoeff(z,b,c,g,kv,t,gp,tc,rc,rt)
      real z,b,c,g,kv,t,gp,tc,rc,rt
      real gb,gc,gr,sq,sn,tn,td,rn,rd
      gb=g*b
      gc=gp*c
      gr=gc/gb
      sq=gr*(1.0+t*z*z)*z
      sq=sq*sq
      sn=2.0*sin(kv)
      tn=sn*sn
      td=tn+sq
      tc=tn/td
      rn=sq
      rd=td
      rc=rn/rd
      rt=tc+rc
      end
      subroutine ludcmp(fjac,n,np,indx,d)
      parameter (nmax=100,tiny=1.0e-20)
      dimension fjac(np,np),indx(n),vv(nmax)
      d=1.
      do 12 i=1,n
        aamax=0.
        do 11 j=1,n
          if (abs(fjac(i,j)).gt.aamax) aamax=abs(fjac(i,j))
11        continue
        if (aamax.eq.0.) pause 'singular matrix.'
        vv(i)=1./aamax
12      continue
      do 19 j=1,n
        if (j.gt.1) then
          do 14 i=1,j-1
            sum=fjac(i,j)
            if (i.gt.1)then
              do 13 k=1,i-1
                sum=sum-fjac(i,k)*fjac(k,j)
13              continue
            fjac(i,j)=sum
14            endif
          continue
        endif
      end

```

```

aamax=0.
do 16 i=j,n
  sum=fjac(i,j)
  if (j.gt.1)then
    do 15 k=1,j-1
      sum=sum-fjac(i,k)*fjac(k,j)
15    continue
    fjac(i,j)=sum
  endif
  dum=vv(i)*abs(sum)
  if (dum.ge.aamax) then
    imax=i
    aamax=dum
  endif
16  continue
  if (j.ne.imax)then
    do 17 k=1,n
      dum=fjac(imax,k)
      fjac(imax,k)=fjac(j,k)
      fjac(j,k)=dum
17    continue
    d=-d
    vv(imax)=vv(j)
  endif
  indx(j)=imax
  if(j.ne.n)then
    if(fjac(j,j).eq.0.)fjac(j,j)=tiny
    dum=1./fjac(j,j)
    do 18 i=j+1,n
      fjac(i,j)=fjac(i,j)*dum
18    continue
  endif
19  continue
  if(fjac(n,n).eq.0.)fjac(n,n)=tiny
  return
end
subroutine lubksb(fjac,n,np,indx,p)
dimension fjac(np,np),indx(n),p(n)
ij=0
do 12 i=1,n
  ll=indx(i)
  sum=p(ll)
  p(ll)=p(i)
  if (ii.ne.0)then
    do 11 j=ii,i-1
      sum=sum-fjac(i,j)*p(j)
11    continue
  else if (sum.ne.0.) then
    ii=i
  endif
  p(i)=sum
12  continue
do 14 i=n,1,-1
  sum=p(i)
  if(i.lt.n)then
    do 13 j=i+1,n
      sum=sum-fjac(i,j)*p(j)
13    continue
  endif
  p(i)=sum/fjac(i,i)
14  continue
return
end

```

D.4 Two Frequency Modes into Off-Channel Features: 2mode_off.f

! This program calculates transmission coefficients for two different guided modes,
! w1 and w2, of 2D photonic crystal waveguide with single off-channel Kerr nonlinear
! feature. The transmission is studied in the parameter space of w1 mode considering
! the w2 mode is linear. References: mnewt, ludcmp, and lubksb are taken from
! Numerical Recipe for F77 Chapter 9. The material constants on this calculation are
! normally taken from McGurn's article in Organic Electronics, the constants
! including other variables are described in the preamble of the file mode_2off.f

```

integer ntrial,it
parameter (n=2)
real x(n),y(n),z(n)
real x1,x2,y1,y2,z1,z2,tolx,tolf
real a2,b1,b2,c1,c2,k1,k2,d1,d2,e1,e2,g1,g2,gp1,gp2,t1,t2,tc1,rc1,rt1
real ytc1,ycr1,yrt1,ztc1,zrc1,zrt1
real ytc2,ycr2,yrt2,ztc2,zrc2,zrt2
real ck1,ck2,gd1,gd2
c constants of nonlinear difference equations
a2=0.8953
b1=0.0852
b2=0.0701

```

```

c1=0.02
c2=0.02
k1=3.0
k2=1.8
ck1=cos(k1)
ck2=cos(k2)
gd1=1.+2.*b1*ck1
gd2=a2+2.*b2*ck2
g1=1./gd1
g2=1./gd2
d1=1.
d2=0.
e1=1.
e2=0.
t1=0.0025
t2=0.0025
c guessing initial values: three different initial values
x(1)=1.
x(2)=1.
y(1)=10.
y(2)=10.
z(1)=-100.
z(2)=-100.
c constants
ntrial=100
tolx=0.001
tolf=0.001
do 100 it=1,400
gp1=0.65*g1+0.0012*it
do 100 it=1,550
! gp1=0.40*g1+0.0012*it
! gp2=0.9012*gp1 ! p
! gp2=1.0591*gp1 ! q
! gp2=1.1125*gp1 ! r
! gp2=1.1977*gp1 ! s
! gp2=1.3375*gp1 ! t , cup
! gp2=1.3385*gp1 ! u , cap
! gp2=1.4325*gp1 ! v
! p2=1.9005*gp1
! gp2=1.2125*gp1
! gp2=1.2015*gp1
! gp2=gp1
call mnewt(ntrial,x,n,tolx,tolf,a2,c1,c2,g1,g2,gp1,gp2,d1,d2,e1,e2,t1,t2)
call mnewt(ntrial,y,n,tolx,tolf,a2,c1,c2,g1,g2,gp1,gp2,d1,d2,e1,e2,t1,t2)
call mnewt(ntrial,z,n,tolx,tolf,a2,c1,c2,g1,g2,gp1,gp2,d1,d2,e1,e2,t1,t2)
x1=x(1)
x2=x(2)
y1=y(1)
y2=y(2)
z1=z(1)
z2=z(2)
call tcoeff(x1,b1,c1,k1,g1,tc1,rc1,rt1)
call tcoeff(y1,b1,c1,k1,g1,yc1,rc1,yrt1)
call tcoeff(z1,b1,c1,k1,g1,ztc1,zrc1,zrt1)
call tcoeff(x2,b1,c1,k1,g1,tc2,rc2,rt2)
call tcoeff(y2,b1,c1,k1,g1,yc2,rc2,yrt2)
call tcoeff(z2,b1,c1,k1,g1,ztc2,zrc2,zrt2)
c call tcoeff(x2,b2,c2,k2,g2,tc2,rc2,rt2)
c call tcoeff(y2,b2,c2,k2,g2,yc2,rc2,yrt2)
c call tcoeff(z2,b2,c2,k2,g2,ztc2,zrc2,zrt2)
write(6,998) gp1/g1,x1,tc1,rc1,rt1
c write(6,998) gp1/g1,z1,ztc1,zrc1,zrt1
write(81,999) gp1/g1,tc1
write(82,999) gp1/g1,yc1
write(83,999) gp1/g1,ztc1
write(91,999) gp1/g1,tc2
write(92,999) gp1/g1,yc2
write(93,999) gp1/g1,ztc2
100 continue
998 format(5f16.8)
999 format(2x,e15.8,2x,e15.8)
! call system('gnuplot off.gnu')
end
subroutine mnewt(ntrial,x,n,tolx,tolf,a2,c1,c2,g1,g2,gp1,gp2,d1,d2,e1,e2,t1,t2)
INTEGER n,ntrial,NP
REAL tolf,tolx,x(n)
PARAMETER (NP=15)
real x1,x2
real a2,c1,c2,g1,g2,gp1,gp2,d1,d2,e1,e2,t1,t2
c USES lubksb,ludcmp,usrfun

```

```

INTEGER i,k,indx(NP)
REAL d,errf,errx,fjac(NP,NP),fvec(NP),p(NP)
do 14 k=1,ntrial
  call usrfun(x,n,NP,fvec,fjac,a2,c1,c2,g1,g2,gp1,gp2,d1,d2,e1,e2,t1,t2)
  errf=0.
  do 11 i=1,n
    errf=errf+abs(fvec(i))
11  continue
  if(errf.le.tolf)return
  do 12 i=1,n
    p(i)=-fvec(i)
12  continue
  call ludcmp(fjac,n,NP,indx,d)
  call lubksb(fjac,n,NP,indx,p)
  errx=0.
  do 13 i=1,n
    errx=errx+abs(p(i))
    x(i)=x(i)+p(i)
13  continue
  if(errx.le.tolx)return
14  continue
return
end
subroutine usrfun(x,n,NP,f,dfdx,a2,c1,c2,g1,g2,gp1,gp2,d1,d2,e1,e2,t1,t2)
  dimension x(n),f(n),dfdx(NP,NP)
  real x1,x2
  real a2,c1,c2,g1,g2,gp1,gp2,d1,d2,e1,e2,t1,t2
  real gi,ga,gai,gc1,gc2
  x1=x(1)
  x2=x(2)
c specify the function: f(x)=0
  gi=1./gp1
  ga=gp2*a2
  gai=1./ga
  gc1=g1*c1
  gc2=g2*c2
  f(1)=d1*t1*x1*x1*x1+(1.+ e1*t2*x2*x2-gi)*x1+gc1*gi
  f(2)=d2*t2*x2*x2*x2+(1.+ e2*t1*x1*x1-gai)*x2+gc2*gai
c define derivatives: dfdx
  dfdx(1,1)=3.*d1*t1*x1*x1+1.+ e1*t2*x2*x2-gi
  dfdx(1,2)=2.*t2*e1*x1*x2
  dfdx(2,1)=2.*t1*e2*x1*x2
  dfdx(2,2)=3.*d2*t2*x2*x2+1.+ e2*t1*x1*x1-gai
  return
end
c transmission and reflection coefficients-----
subroutine tcoeff(z,b,c,k,g,tc,rc,rt)
  real z,b,c,k,g
  real ck,cn,sn,l,ft,tn,td,tc,rn,rd,rc,rt
  intrinsic cos
  ck=cos(k)
  cn=ck*ck
  sn=1.-cn ! sin^2(k)=1-cos^2(k)
  l=c/b
  ft=l*(z-g*c)*(1.+2.*b*ck)
  ft=ft*ft
  tn=4.*sn
  td=tn+ft
  tc=tn/td
  rn=ft
  rd=td
  rc=rn/rd
  rt=rc+tc
  return
end
subroutine ludcmp(fjac,n,np,indx,d)
  parameter (nmax=100,tiny=1.0e-20)
  dimension fjac(np,np),indx(n),vv(nmax)
  d=1.
  do 12 i=1,n
    aamax=0.
    do 11 j=1,n
      if (abs(fjac(i,j)).gt.aamax) aamax=abs(fjac(i,j))
11  continue
    if (aamax.eq.0.) pause 'singular matrix.'
    vv(i)=1./aamax
12  continue
  do 19 j=1,n
    if (j.gt.1) then
      do 14 i=1,j-1
        sum=fjac(i,j)
        if (i.gt.1)then
          do 13 k=1,i-1

```

```

13         sum=sum-fjac(i,k)*fjac(k,j)
        continue
        fjac(i,j)=sum
    endif
14  continue
endif
aamax=0.
do 16 i=j,n
    sum=fjac(i,j)
    if (j.gt.1)then
        do 15 k=1,j-1
            sum=sum-fjac(i,k)*fjac(k,j)
15        continue
        fjac(i,j)=sum
    endif
    dum=vv(i)*abs(sum)
    if (dum.ge.aamax) then
        imax=i
        aamax=dum
    endif
16  continue
    if (j.ne.imax)then
        do 17 k=1,n
            dum=fjac(imax,k)
            fjac(imax,k)=fjac(j,k)
            fjac(j,k)=dum
17        continue
        d=-d
        vv(imax)=vv(j)
    endif
    indx(j)=imax
    if(j.ne.n)then
        if(fjac(j,j).eq.0.)fjac(j,j)=tiny
        dum=1./fjac(j,j)
        do 18 i=j+1,n
            fjac(i,j)=fjac(i,j)*dum
18        continue
    endif
19  continue
    if(fjac(n,n).eq.0.)fjac(n,n)=tiny
    return
end
c -----
subroutine lubksb(fjac,n,np,indx,p)
dimension fjac(np,np),indx(n),p(n)
ij=0
do 12 i=1,n
    ll=indx(i)
    sum=p(ll)
    p(ll)=p(i)
    if (ii.ne.0)then
        do 11 j=ii,i-1
            sum=sum-fjac(i,j)*p(j)
11        continue
    else if (sum.ne.0.) then
        ii=i
    endif
    p(i)=sum
12  continue
do 14 i=n,1,-1
    sum=p(i)
    if(i.lt.n)then
        do 13 j=i+1,n
            sum=sum-fjac(i,j)*p(j)
13        continue
    endif
    p(i)=sum/fjac(i,i)
14  continue
return
end

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