Theory and Modelling of Light-Matter Interactions in Photonic Crystal Cavity Systems Coupled to Quantum Dot Ensembles

by

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Abstract

Photonic crystal microcavity quantum dot lasers show promise as high quality-factor, low threshold lasers, that can be integrated on-chip, with tunable room temperature operations. However, such semiconductor microcavity lasers are notoriously difficult to model in a self-consistent way and are primarily modelled by simplified rate equation approximations, typically fit to experimental data, which limits investigations of their optimization and fundamental light-matter interaction processes. Moreover, simple cavity mode optical theory and rate equations have recently been shown to fail in explaining lasing threshold trends in triangular lattice photonic crystal cavities as a function of cavity size, and the potential impact of fabrication disorder is not well understood. In this thesis, we develop a simple but powerful numerical scheme for modelling the quantum dot active layer used for lasing in these photonic crystal cavity structures, as an ensemble of randomly positioned artificial two-level atoms. Each two-level atom is defined by optical Bloch equations solved by a quantum master equation that includes phenomenological pure dephasing and an incoherent pump rate that effectively models a multi-level gain system. Light-matter interactions of both passive and lasing structures are analyzed using simulation defined tools and post-simulation Green function techniques. We implement an active layer ensemble of up to 24,000 statistically unique quantum dots in photonic crystal cavity simulations, using a self-consistent finite-difference time-domain method. This method has the distinct advantage of capturing effects such as dipole-dipole coupling and radiative decay, without the need for any phenomenological terms, since the time-domain solution self-consistently captures these effects. Our analysis demonstrates a powerful ability to connect with recent experimental trends, while remaining completely general in its set-up; for example, we do not invoke common approximations such as the rotating-wave or slowly-varying envelope approximations, and solve dynamics with zero a priori knowledge.
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Common Symbols and Acronyms

Acronyms
FDTD  finite-difference time domain
FP   Fabry-Pérot
FWHM full width at half maximum
LDOS local optical density of states
MPB  MIT Photonic Bands
PC   photonic crystal
PML perfectly matched layers
QD   quantum dot
TLA  two-level atom
OBE  Optical Bloch Equation
MB   Maxwell Bloch

Common Meanings of Symbols used
r  - position vector
ω  - angular frequency
t  - time
V  - system volume
k  - wavevector
$a$ - lattice pitch

$c$ - the speed of light in vacuum

$\mathbf{E}$ - the electric field

$\mathbf{P}$ - polarization

$\mathbf{G}$ - photonic Green tensor

$f$ - normalized system eigenmode

$\tilde{f}$ - quasi-normal system eigenmode

$\epsilon_0$ - vacuum permittivity

$\epsilon$ - relative permittivity of a material

$\mu_0$ - vacuum permeability

$\mu$ - relative permeability of a material

$\epsilon_B$ - constant background relative permittivity

$\Gamma$ - decay rate; $\gamma'$ typically denotes a non-radiative decay rate. Alternatively, imaginary part of complex eigenfrequency $\tilde{\omega}$.

$d$ - dipole moment

$Q$ - the quality factor of a resonance $Q = \omega/\Gamma$

$L[\hat{O}]$ - Lindblad superoperator: $L[\hat{O}] = (\hat{O}\rho\hat{O}^\dagger - \frac{1}{2}\{\hat{O}^\dagger\hat{O},\rho\})$
Chapter 1

Introduction

1.1 Introduction

Engineers and scientists across many industries are constantly pushing the boundaries on how small usable devices can be made. As devices are shrunk, their power consumption is usually reduced, increasing the systems' efficiency, functionality, and ultimately their ability to beat out competitors. This is especially prevalent in the electronics industry, and is also the case in photonics. Small-scale photonic devices are able to interact with light in unique ways, which can allow for improved efficiencies over larger macroscopic devices. A particular area of optical physics, “nanophotonics”, studies light at sub-micron lengths and examines its interactions with nanometer size structures. In recent years, this field of research has flourished as industrial techniques become more advanced in manufacturing ultra-precise microstructures. Most notably, continued improvements in nano-scale fabrication have benefited telecommunications devices [Toulouse [2005]], high-precision measuring instruments such as a near-field scanning optical microscope [Drezet et al. [2015]], micro-cavity lasers [Ulrich et al. [2007]; Stockman [2008]], and various quantum system applications including quantum communications systems [Gisin and Thew [2007]], quantum computing [Bennett and DiVincenzo [2000]], and “completely secure” data protection [Gisin et al. [2002]; Yao et al. [2010]].

The ability for researchers to optimize optical structures is pushing the field of nanophotonics into a new age of information processing. As optic communication systems replace
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By understanding how electrons propagate as free particles in conducting lattice structures, researchers realized that light could possess similar properties in dielectric. Namely, with quantum mechanics, we discovered that electrons travel as both particles and waves, and that these waves can meet certain criteria that allow them to travel without scattering, in conventional electron-based technology, their power consumption is drastically decreased by the removal of waste heat generated by colliding electrons, their processing speed reaches the speed-of-light (and the physical speed limit of information transfer), and the number of available channels of communication is drastically increased as light-based information can be encoded into the phase of each operating wavelength [Chen et al. [2010]] and each wavelength channel can be doubled by using $x$ or $y$ polarization [Ly-Gagnon et al. [2006]]. In recent years, some fundamental stepping stones have been reached, such as the storage of coherent light up to a full minute [Heinze et al. [2013]], advancements in realizing an on-demand single photon source with good indistinguishability and collection efficiency [Somaschi et al. [2016]], and nearly threshold-less lasers operating at room temperature [Prieto et al. [2015a]].

Even with the continually improving state of nanophotonic structures, there is much room for improvement and discoveries for new science, and there are many fundamental challenges. As experimentalists push the frontier of ultra-precise microstructures, many theoretical formalisms become poor models as previously adequate approximations are rendered invalid. It is within this area of theoretical and computational nanophotonics that this thesis takes its place. Building on the success of the finite-difference time-domain (FDTD) numerical solver applied to Maxwell’s equations with open boundary conditions, we extend and exploit this method to accurately model an ensemble of quantum dots (QDs) or quantum emitters in arbitrarily shaped material structures. In particular, we numerically study photonic crystal (PC) cavity lasers, of varying lengths, with an embedded ensemble of quantum dot emitters (up to more than 24,000 QDs with statistically different properties), with a 2-dimensional (2D) FDTD algorithm. The motivation behind this, and some useful background knowledge, is presented in the following sections.
perfectly periodic lattice structures (e.g., perfect conductors). Moreover, periodic structures can be designed to prohibit the propagation of certain wavelengths, in certain directions [Joannopoulos et al. [2011]], through carefully engineered lattice structures. When a lattice prohibits propagation in all directions of a wavelength range, the material possesses a complete band gap where no electron may exist with the corresponding wavelengths. In the case of semiconductor materials, a complete band gap exists between the valence and conduction energy bands. Scattering can, however, occur by defects or impurities, which presented a major technological hurdle for solid-state device application in the mid-20th century; but once researchers reduced unwanted impurities to a manageable level, the transistor was born, sparking our information revolution and changing the world. Defect scattering is not always unwanted, adding useful functionality when applied correctly.

In the exact same way that periodic structures prohibited particular wavelengths of electrons from propagating, one is able to engineer periodic structures that prohibit light. These structures are called “photonic crystals”, and instead of having a lattice of atoms, PCs are defined by macroscopically differing dielectric structures, manufactured by material interfaces (or occurring naturally in nature, e.g., on butterfly wings [Singer et al. [2016]]). For example, Figure 1.1b depicts the top-down view of a PC slab of hexagonal lattice holes in a semiconductor substrate. Such a structure has a complicated bandstructure, seen in Figure 1.1a, which depends on the slab’s height $h$, refractive index $n$, and hole radius $r$, usually given in units of $a$ the lattice constant. The grey shaded region of the bandstructure is the cut-off for electromagnetic modes that are no longer confined within the PC slab. This interface is commonly referred to as the “light line”. A narrow in-plane band gap exists for a triangular slab, at specific hole radii; however, it does inhibit a larger range of transverse electric (TE) light modes. Vertical confinement of these modes is achieved by total-internal reflection of the slab, allowing completely lossless modes to exist below the light line.

A common use of the triangular lattice PC slab geometry is to introduce a defect at a single hole (e.g., a missing hole in the lattice), or a few holes along a specific row, that can trap, or guide light, respectively. With the defect, new modes present themselves, and some of these modes exist within the in-plane band gap, though they can leak out vertically. These defect modes are special, in that they exist within the defect, but are forbidden from travelling into the homogeneous triangular lattice membrane that makes up the rest of the
1.2. PHOTONIC CRYSTALS

Figure 1.1: (a) Using MIT’s photonic crystal bandgap software (MPB), the bandgap of an air-embedded triangular lattice PC in a slab of InP was calculated (with Bloch’s boundary conditions). Operating at 1.5 µm, the refractive index of InP is roughly 3.17. The other PC parameters were set to: \( a = 438 \text{ nm}, \ r = a/4, \) and \( h = 250 \text{ nm}. \) These inputs generated the PC slab bandstructure, which show a bandgap of 30 THz between 185.75 - 216.58 THz. (b) Top-down view of a triangular lattice slab PC, where the dark circles represent etched holes, filled with air, and the grey background is the homogeneous substraight material, with refractive index \( n \neq 1. \)

PC. In this way, researchers can create optical cavities, whereby light becomes trapped inside a finite length defect, and can only escape via vertical scattering events (as they can couple to radiation modes above the light line). Figures 1.2a and 1.2b depict such cavity structures, where the cavity is a single defect (meaning a single hole is removed), or 3 in a row. On the other hand, when an entire row of the triangular lattice holes are removed, one creates a waveguide structure, as seen in Figures 1.2c and 1.2d. The waveguide is capable of guiding specific frequencies of light, as well as slowing light down for interactions with other photonic structures [Yao et al. [2010]], and even changing the direction of the light without loss [Zimmermann et al. [2004]].

Optical structures made from PC slabs are well regarded for their “on-chip” compatibility [Yao et al. [2010]], ease of manufacturing, and high degree of tunability [Joannopoulos et al. [2011]]. Unfortunately, even the most current and advanced manufacturing techniques are not perfect, especially when operating on the nano-scale, manifesting in fabrication disorder that may play a significant role. Indeed, unavoidable disorder-induced losses will
always exist in real-world nano systems, which impose an upper limit to many device efficiencies. These losses are mainly the result of surface roughness, or inexact periodic lattice structures. In the past, these fabrication imperfections were seen as a nuisance, and great lengths were taken to minimize them as much as possible [Wiersma [2008]]. However, in recent years, researchers have discovered that disorder can also lead to novel properties that can be useful to the functionality of its host device. For instance, some solar cell researchers are actively pursuing how best to disorder their structure’s nominal order in hopes of improving light collection efficiency and increased absorption [Seassal et al. [2014]]; and how novel localized modes with small volumes can be made to lase [Liu et al. [2014a]], and in some cases reduce the lasing threshold [Fujii et al. [2012]]. In this thesis, disorder will also be modelled, and assessed for its influence on PC cavity lasers.

1.3 Lasers

The laser is perhaps one of quantum mechanic’s greatest triumphs (certainly in the field of optics), and includes an interesting chapter of history. Stimulated emission, the required mechanism for lasing, was first predicted in 1916 by Albert Einstein. In 1951, stimulated emission was proposed as an amplification source for microwave radiation by Joseph Weber, and in 1953 Charles Hard Townes produced the first microwave amplifier based on principles similar to a laser. This Microwave Amplification by Stimulated Emission of Radiation (MASER) was incapable of continuous output at the time, and it was Nikolay Basov
and Aleksandr Prokhorov of the Soviet Union who worked out the problem of continuous emission by using more than two energy levels to achieve continuous population inversion (that is, having more carriers in an excited state than in the ground state, which is a requirement for continuous lasing). In 1957, Townes and Arthur Leonard Schawlow began to study optical amplification by stimulated emission of radiation at Bell Labs, which they termed “an optical-maser”. This poor choice for the device’s name would prove costly, as in 1959, Gordon Gould published a paper [Gould [1959]] that first coined the word “LASER”. Gould filed a patent under this more fitting description, with his notes on the laser concept and multiple applications such as spectrometry, interferometry, radar, and nuclear fusion. The U.S. Patent Office denied his claims, and instead awarded Bell Labs with the invention in 1960, which started a twenty-eight-year lawsuit between the two parties. Interestingly, apparently neither side were the first to create a working laser, as Theodore H. Maiman was cited to be the first in 1960 using a ruby crystal to produce red laser light. In 1964, C. H. Townes, N. Basov, and A. Prokhorov shared the Nobel Prize “for fundamental work in the field of quantum electronics, which has led to the construction of oscillators and amplifiers based on the maser-laser principle”. Since the early 1960’s, the laser has become the most widely applied application of quantum mechanics, with research efforts continuously increasing as we push forward into the 21st century, which is very much a photonics world.

The basic properties of the conventional laser have not changed since it was first demonstrated with a ruby crystal. To achieve a working laser, two things are needed: some method of trapping light, with a small aperture to let light escape, and some material capable of coherently amplifying the trapped light, which is referred to as the gain medium, or simply the gain. In most laser systems, the trapping of light is actually quite necessary, and not simply done to save on the size of lasers. Stimulated emission is more coherent than regular gain emissions, and so allowing light to build up over multiple round trips increases the overall coherence of the laser output. In comparison with traditional light sources, such as incandescent or fluorescent sources which use heat and fluorescence respectively to emit light, lasers are hundreds-of-thousands of times more coherent, which has allowed for a wide range of remarkable research in recent years. Such research includes incoherent optics, quantum optics [Fox [2006]], attosecond pulse generations [Krausz [2016]] allowing researchers to image molecular dynamics in real time, and the detection of gravitational waves [Abbott
et al. [2016]) (which has opened the door to a completely new way of viewing our universe). Usually, light trapping is done with simple mirrors [Milonni and Eberly [2010]], but as technology continues to shrink, PC cavities become a natural replacement, as the trapped light interacts with the cavity edges in much the same way as it would with mirrors, with the benefit of bandwidth, smaller size, and flexibility in the design. However, many traditional gain substrates, such as gas lasers (e.g., mixes of HeNe, N, Ar, CO, CO$_2$, or metal vapours), liquid dyes, and certain crystals typically doped with rare-earth ions (e.g., Nd, Yb, Er) or transition metal ions [Hecht [1992]], are not compatible with the solid-state design of PCs. The best methods of including an active medium (another term for gain medium) are through semiconductor QDs, or quantum wells, which are much more efficient and practical than bulk semiconductors. In this thesis, we choose to model QDs, which are described in detail in the next section, as they have superior room temperature operation [Bimberg and Pohl [2011]], tunability [Schliwa et al. [2014]], and excellent temporal and spatial stability [Borri et al. [2001]].

1.4 Quantum Dots

The term “quantum dot” was coined in 1988 in the abstract of [Reed et al. [1988]], in reference to a semiconductor quantum well confined in all three dimensions. A quantum well is a semiconductor structure where the electronic density of states (DOS) of its charge carriers are spatially confined in one direction, thus leading to energy quantization. This confinement is typically on the scale of 2-100 nm [Tartakovskii [2012]], which is the same order of magnitude as the conduction band electron de Broglie wavelength (and smaller than the Bohr radius of electron-hole pairs), removing the periodicity previously used by the electron wave, thus trapping it. As the dimensionality of the confinement increases from 1D to 3D, the DOS quantization becomes more isolated in frequency, which is shown in Figure 1.3a, until full energy gaps appear like an artificial atom. The 3D DOS in Figure 1.3a is predicted by assuming a cubic confinement, and illustrates one of the most important attributes of QDs, namely their temperature stability. While bulk material charge carriers are continuously distributed to greater energy states as the temperature increases, the same is not necessarily true for QDs. If the excited states lie sufficiently above the ground state,
1.4. QUANTUM DOTS

then many carriers contribute to lasing regardless of the operating temperature (up to a point) [Bimberg and Pohl [2011]]. The quantized nature of the Coulombically-coupled electron-hole pair (referred to as an exciton) energy levels is what makes QDs gigantic “artificial atoms”. Figure 1.3b depicts this discretized energy level diagram, where an example photon with energy greater than the gap energy $E_G$ knocks an electron from the valence band, into an excited state that quickly decays with lifetime $\tau$ down to the lowest conduction band energy level, from which it recombines with the hole to emit a photon near energy $E_G$.

![Energy Level Diagram](image)

Figure 1.3: (a) Reduced dimensionality effect on DOS of QDs, from [Bimberg and Pohl [2011]]. The charge carriers are confined in red, while the bulk semiconductor is in blue. (b) Simple energy level schematic of a QD, where the filled circles represent electrons, and the empty circle represents a hole. When an electron drops down into the valence band, it combines with the available hole, and emits a photon of energy $E_G$.

From their inception, it took almost a full decade for QDs to realize their superior lasing properties, as compared with state-of-the-art quantum well lasers [Bimberg and Pohl [2011]], and much of this success is built upon the success of the Stranski-Krastanow (SK) grown technique, which lead to easy fabrication of defect-free QDs [Bimberg and Pohl [2011]]. For this technique, a thin “wetting layer” of semiconductor is grown onto of a slightly different crystalline structure, and this lattice mismatch causes strain in the deposited layer, preventing uniform distribution. Instead, the wetting layer finds stability by forming little
islands of coalesced clusters, where the thickness exceeds several atomic layers [Tartakovskii [2012]]. The SK growth technique creates QDs with much greater lateral dimensions compared to their height, which causes vertical energy levels to be spaced so greatly, that they are effectively frozen out. The exact energy levels of each QD is largely dependant on the specific dot parameters [Jacak et al. [2013]]. These QDs are said to be self-assembled, in that their formation is a random physical process, and so their position, and exact size is stochastic in nature, although the variance of the QD size can be controlled to some degree. This variance introduces a spreading of the single-dot lineshapes, which is referred to as inhomogeneous broadening, and is typically greater than 50 meV [Bimberg and Pohl [2011]], and temperature dependant. An SEM image of a QD grown in GaAs is shown in Figure 1.4a, where the dot’s radius is around 5 nm. In Figure 1.4b, we find an SEM image of a QD ensemble, with an average dot (in-plane) radius of approximately 7.5 nm.

By merging the high DOS of QDs with PC cavities, one can create a semiconductor laser. This is an ideal application between two massive feats of optical engineering; both PCs and QDs have a high degree of tunability that allows for enhanced coupling, and both are made of fundamentally similar material, making for seamless integration. Quantum dot ensembles are generally excited incoherently with an optical pump (or an electrical pump), injecting radiation from above the cavity [Xue et al. [2016a]], which stimulates the QDs into higher energy levels that quickly relax to their more stable excited state. It is this picture of QDs that we wish model in this thesis: the ensemble statistics of randomly placed QDs, all with slightly different energy lineshapes that lead to an inhomogeneously
broadened gain spectra, within a PC cavity structure capable of trapping the emitted light, and subsequently lasing.

1.5 Layout of the Thesis

Over the past few decades, various computational techniques, such as the FDTD method, have been developed to solve the set of coupled electromagnetic equations that make up Maxwell’s equations, in the presence of arbitrary media. In this thesis, we use FDTD to solve the geometry of a PC cavity made in etched hexagonal lattice holes, in a real (i.e. not complex or lossy) dielectric substrate, with open boundary conditions, including disorder and embedded gain materials. The active region requires a robust model of QDs.

In Chapter 2, we will derive the necessary equations used throughout the thesis for both analyzing Maxwell’s equations, and implementing QD gain. We start by introducing classical electromagnetic theory, and discussing the various ways of solving these equations within an arbitrary cavity structure with open boundary conditions. We also introduce the general idea of cavity modes and Green function solutions and expansion in terms of these modes. Next, we introduce the basic theory of lasers, and how QDs can be made to lase by modelling them as effective two-level atoms via quantum mechanics density matrix analysis. In the subsequent Chapter 3, we describe the FDTD method, and the considerations made by this thesis specifically, to ensure physically meaningful results were obtained. In Chapter 4 we outline how our QD model is self-consistently incorporated within the FDTD scheme, and how we modelled the QD ensemble statistics. In Chapter 5 we present a recently completed paper [Cartar et al. [2017]], in manuscript form, co-authored by Jesper Mørk at the Technical University of Denmark, and Stephen Hughes at Queen’s University, discussing the threshold behaviour of QD PC cavity lasers, using self-consistent Maxwell Bloch modelling in the form of a QD ensemble. There are four appendices included that cover: the basics of Green function solutions to differential equations, A; the homogeneous free space solution to the photonic Green function in 2D and 3D, B; code excerpts from the C++ plugin class created for this research, C; and additional figures for the submitted paper discussed in Chapter 5, D. Finally, we conclude this thesis in Chapter 6 and discuss some areas for future work.
Chapter 2

Theory

In this chapter, we describe the general light-matter interaction theory associated with PCs, as well as the basic quantum electronic theory of QDs, as modelled by a two-level atom (TLA). Starting from Maxwell’s equations, we show how the photonic Green function (GF) can be used to extract fundamental light-matter interaction properties, and include various ways of calculating the GF. We then discuss the fundamental models used to describe TLAs, and derive the Maxwell-Bloch equations to be numerically implemented in Chapter 4. Using a simple rate equation approximation, we probe some basic features of the model, and compare the findings to alternative rate equations for semiconductor lasers.

2.1 Classical Electromagnetic Theory

To solve the response of Maxwell’s equations given some initial source, in the presence of an arbitrary medium, the frequency domain often provides simpler solutions. Most notably, GF solutions are readily found given the initial source can be modelled as a dipole. Before introducing the photonic GF, let us discuss where electromagnetic mode solutions originate. Working in the frequency domain, and using $J$ as the current density, and $\rho_c$ as the charge
density, we write Maxwell's equations as

\[ \nabla \times \mathbf{E}(r; \omega) = i \omega \mathbf{B}(r; \omega), \] (2.1a)
\[ \nabla \times \mathbf{H}(r; \omega) = -i \omega \mathbf{D}(r; \omega) + \mathbf{J}(r; \omega), \] (2.1b)
\[ \nabla \cdot \mathbf{D}(r; \omega) = \rho_c(r; \omega), \] (2.1c)
\[ \nabla \cdot \mathbf{B}(r; \omega) = 0, \] (2.1d)

where \( \mathbf{E} \) and \( \mathbf{B} \) are the electric and magnetic fields, related to \( \mathbf{D} \) and \( \mathbf{H} \), which are the auxiliary fields for the electric displacement and \( \mathbf{H} \) field,

\[ \mathbf{D}(r; \omega) = \varepsilon_0 \varepsilon(r; \omega) \mathbf{E}(r; \omega), \] (2.2a)
\[ \mathbf{H}(r; \omega) = \mu_0^{-1} \mu^{-1}(r; \omega) \mathbf{B}(r; \omega), \] (2.2b)

where \( \varepsilon \) and \( \varepsilon_0 \) are the relative material and free space permittivity and \( \mu \) and \( \mu_0 \) are the relative material and free space permeability. Note we have neglected spatial dispersion and assume linear media for now [Novotny and Hecht [2012]]. We have also assumed isotropy for the relative permittivity and permeability, however anisotropy can easily be added by substituting the tensor permittivity and permeability values. The two equations in 2.2 are referred to as the constitutive relations, as they relate information about the material substrate to the electromagnetic fields travelling through. Substituting equations (2.2a), and (2.2b) into equation (2.1b), we find

\[ \nabla \times \left( \mu_0^{-1} \mu^{-1}(r; \omega) \mathbf{B}(r; \omega) \right) = -i \omega \varepsilon_0 \varepsilon(r; \omega) \mathbf{E}(r; \omega) + \mathbf{J}(r; \omega), \] (2.3)

which can be simplified further using equation (2.1a):

\[ \nabla \times \left( \mu_0^{-1} \mu^{-1}(r; \omega) \nabla \times \mathbf{E}(r; \omega) \right) - \omega^2 \varepsilon_0 \varepsilon(r; \omega) \mathbf{E}(r; \omega) = i \omega \mathbf{J}(r; \omega). \] (2.4)

Now, rather than working with a current source, we wish to work with polarization sources. By introducing a polarization source into the system with polarizability \( \alpha(\omega) \), and source volume \( \Delta V \) where

\[ \mathbf{J}(r; \omega) = -i \frac{\omega}{\Delta V} \varepsilon_0 \alpha(\omega) \mathbf{E}(r; \omega), \] (2.5)

with polarization

\[ \mathbf{P}(r; \omega) = \frac{\alpha(\omega)}{\Delta V} \mathbf{E}(r; \omega), \] (2.6)
we arrive at a wave equation of the form:

\[
\left[ \nabla \times \mu^{-1}(r;\omega) \nabla \times - k_0^2 \epsilon(r;\omega) \right] E(r;\omega) = k_0^2 P(r;\omega),
\] (2.7)

where \( k_0 = \frac{\omega}{c} \) is the wavevector in vacuum and \( c \) is the speed of light. Assuming we have a non-magnetic \((\mu = 1)\) lossless \((\text{Im}[\epsilon] = 0)\) system, which is generally the case for PC dielectric media, we have a simplified Helmholtz equation given by

\[
\left[ \nabla \times \nabla \times - k_0^2 \epsilon(r;\omega) \right] E(r;\omega) = k_0^2 P(r;\omega).
\] (2.8)

### 2.1.1 Mode Expansion of the Photonic Green Function

Usually, an optical cavity structure of interest is dominated by one of a few resonant cavity modes. These modes are defined by their solutions to the source free Helmholtz equation, and the boundary conditions (BCs) used to normalize the modes. Assuming we are working within a structure with nondispersive permittivity, the homogeneous solution to our Helmholtz equation 2.8, is written as

\[
\nabla \times \nabla \times f_\lambda(r) = \frac{\omega^2}{c^2} \epsilon(r)f_\lambda(r),
\] (2.9)

where \( f_\lambda(r) \) are the resonant modes labelled by \( \lambda \), and we have kept our harmonic dependence. Since equation 2.9 is Hermitian [Sakoda [2004]; Joannopoulos et al. [2011]], we have

\[
\int_V g \cdot \nabla \times \nabla \times f = \int_V f \cdot \nabla \times \nabla \times g,
\]

where \( V \) is integrated over all space. Note that this property of \( f \) is only true if our modes are well behaved at the boundary as \( V \to \infty \); that is, the solution is non-divergent. Given this property, it is easily seen that

\[
(\omega_\lambda^2 - \omega_{\lambda'}^2) \int_V \epsilon(r)f_\lambda(r) \cdot f_{\lambda'}(r)dr = 0,
\] (2.10)

by using \( \int_V f_\lambda \cdot \nabla \times \nabla \times f_{\lambda'} = \int_V f_{\lambda'} \cdot \nabla \times \nabla \times f_\lambda \), and \( \int_V f_\lambda \frac{\omega^2}{c^2} f_{\lambda'}(r)dr = \int_V f_{\lambda'} \frac{\omega^2}{c^2} f_\lambda(r)dr \) on equation 2.9 after premultiplying by \( \int_V drf_{\lambda'} \). In this way, we arrive at the orthonormality relation

\[
\langle \tilde{f}_\lambda | \tilde{f}_{\lambda'} \rangle = \lim_{V \to \infty} \int_V \epsilon(r)f_\lambda(r) \cdot f_{\lambda'}(r) = \delta_{\lambda,\lambda'},
\] (2.11)

where \( \partial V \) denotes the border of volume \( V \) and the limit of \( V \to \infty \) is calculated by increasing the volume to obtain convergence. Note, our normalized modes capture the spatial confinement of the light they describe by the mode’s effective volume \( V_{\text{eff}} \), defined
by
\[ V_{\text{eff}} = \int_V \frac{\epsilon(r)|f_\lambda(r)|^2}{\epsilon(r_c)|f_\lambda(r_c)|^2} dV, \]  
(2.12)
where \( r_c \) is the peak cavity field volume at the anti-node position.

In addition, we can derive the completeness relation for these modes by expanding an arbitrary field \( g \) in terms of \( f \) such that
\[ g(r) = \sum_\lambda f_\lambda(r) \int_V \epsilon(r')f_\lambda^*(r') \cdot g(r') \]
\[ = \int_V \left( \sum_\lambda f_\lambda(r)\epsilon(r')f_\lambda^*(r') \right) \cdot g(r'), \]  
(2.13)
thus requiring that
\[ \epsilon(r) \sum_\lambda f_\lambda(r)f_\lambda^*(r') = \bar{I}\delta(r - r'), \]  
(2.14)
where the sum over \( \lambda \) includes all mode solutions (e.g., both transverse and longitudinal) [Sakoda [2004]].

From this point, since we know \( \{f_\lambda\} \) make up a complete basis, we could describe our electric field by defining \( E = \sum_\lambda C_\lambda f_\lambda \cdot f_\lambda^* \), and try to find solutions to our inhomogeneous Helmholtz equation 2.8, but such an analysis is greatly simplified by using a photonic GFs \( \bar{G}(r, r'; \omega) \), where we assume that the initial source in our system can be modelled as a point dipole. With this assumption, we are able to replace the polarization by a Dirac delta function in the inhomogeneous Helmholtz equation, allowing us to use the completeness relation in place of the polarization. The GF is a tensor (3x3 matrix) defined by a source location \( r' \) and response location \( r \), giving us the 9 matrix elements in 3D Cartesian coordinates. Since the GF is defined at all possible source and response locations, it describes all scattering events, for frequencies \( \omega \), making it a very powerful tool. Following the same arguments outlined in appendix A, which describes GF solutions to inhomogeneous differential equations, we define our photonic GF from
\[ \left[ \nabla \times \nabla \times - k_0^2 \epsilon(r; \omega) \right] \bar{G}(r, r'; \omega) = k_0^2 \bar{I}\delta(r - r'), \]  
(2.15)
where \( \delta(r - r') \) is the Dirac delta function, \( \bar{G}(r, r'; \omega) \) is a dyad field solution that depends on the position of \( r' \) of the inhomogeneity \( \delta(r - r') \), and \( \bar{I} \) is the unit dyad. Note that our GF includes an additional factor \( k_0^2 \) relative to other common sources such as [Novotny and
2.1. CLASSICAL ELECTROMAGNETIC THEORY

Hecht [2012]; Knöll et al. [2001]. The reason for this is our $\bar{G}$ is in units inverse volume, and is consistent with the GF from a dipole source solution to the full Maxwell equations, thus being more suited for numerical calculations of arbitrary structures [Angelatos [2015]]. The tensor $\bar{G}$ has matrix elements $G_{i,j}$ where $i$ and $j$ span $x, y$, and $z$; columns are responsible for the response field due to source points defined in the $x, y$ or $z$ directions.

Now we can derive the mode expansion form of our GF, assuming $\bar{G} = \bar{G}^T$ is the transverse solution; we start with $\bar{G} = \sum_\lambda C_\lambda f_\lambda \cdot f_\lambda^*$ where $C_\lambda$ is an unknown prefactor to be determined, and we only use the transverse modes in the sum; combining equations 2.9, 2.14, and 2.15, while using our expanded GF in the $\{f\}$ basis, we get

$$\left[ \nabla \times \nabla \times -\frac{\omega^2}{c^2} \epsilon(r) \right] \sum_\lambda C_\lambda f_\lambda \cdot f_\lambda^* = \frac{\omega^2}{c^2} \epsilon(r) \sum_\lambda f_\lambda(r) f_\lambda^*(r'),$$

(2.16)

$$\sum_\lambda C_\lambda \left( \frac{\omega_\lambda^2}{c^2} - \frac{\omega^2}{c^2} \right) \epsilon(r) f_\lambda(r) f_\lambda^*(r') = \sum_\lambda \frac{\omega^2}{c^2} \epsilon(r) f_\lambda(r) f_\lambda^*(r'),$$

(2.17)

denote therefore

$$C_\lambda = \frac{\omega^2}{\omega_\lambda^2 - \omega^2},$$

(2.18)

and

$$\bar{G}(r, r'; \omega) = \sum_\lambda \frac{\omega^2 f_\lambda(r) \cdot f_\lambda^*(r')}{\omega_\lambda^2 - \omega^2}.$$

(2.19)

Finally, using the source term in equation 2.7 as a superposition of point sources, we can find solutions to equation 2.7 with source term $P(r'; \omega)$ contained in a volume $dV'$ as

$$E(r; \omega) = \int_V \bar{G}(r, r'; \omega) \cdot P(r'; \omega) dV'.$$

(2.20)

The usual cavity mode solution to our GF in equation 2.19 does not account for the true leaky nature of open cavity systems. As such, the mode solutions we have presented here describe systems without loss, such as waveguide modes along a line defect in a PC, generated by periodic boundary conditions and confined by total internal refraction. In contrast, cavity structures do not have normal modes, e.g. they have out-of-plane scattering and emit radiation vertically. These modes can be modelled more correctly by open boundary conditions, and are inherently leaky in nature. Because of the leakage, the modes are termed quasinormal modes (QNMs), which are characterized by complex frequencies and divergent modes in space. The complex frequencies $\tilde{\omega} = \omega - i\Gamma$ all have a negative
imaginary component, that transform to complex wave vectors $\tilde{k}$ with positive imaginary components. As such, the far-field solutions are inherently divergent in nature, and the outgoing BCs are only physically meaningful near the structure of interest. This divergence, in addition to the complex nature of QNMs, posses a rather cumbersome challenge to their normalization. In 1994, Leung et al. proved that QNMs are complete and orthogonal in 1D [Leung et al. [1994]], and in 2012 Kristensen et al. expanded that normalization to 3D, showing that QNM could be used to correctly describe the leaky nature of 3D cavities [Kristensen et al. [2012]] using the following normalization

$$\left\langle \tilde{f}_\lambda | \tilde{f}_\lambda' \right\rangle = \lim_{V \to \infty} \int_V \epsilon(r) \tilde{f}_\lambda(r) \cdot \tilde{f}_\lambda'(r) dr + i \frac{\sqrt{\epsilon c}}{\tilde{\omega}_\lambda + \tilde{\omega}_\lambda'} \int_{\partial V} \tilde{f}_\lambda(r) \cdot \tilde{f}_\lambda'(r) d\mathbf{r} = \delta_{\lambda,\lambda'},$$

where $\tilde{\omega}_\lambda = \omega_\lambda - i \Gamma_\lambda$. Although the divergent-volume integral components increase, additional surface integral components counterbalance the divergence. Though some care is needed in obtaining there normalized QNMs [Kristensen et al. [2015]], the GF can also be expanded in their basis via [Ge et al. [2014]],

$$\tilde{G}(r, r'; \omega) = \sum_\lambda \frac{\omega^2 \tilde{f}_\lambda(r) \tilde{f}_\lambda(r')} {2 \tilde{\omega}_\lambda (\tilde{\omega}_\lambda - \omega)}. \quad (2.22)$$

Another usefulness of QNMs, is that one can correctly model the asymmetric spectral response often found in complex, open boundary problems (especially with plasmonic resonators) with only one or a few modes, comparing extremely well to full-dipole calculations [Ge et al. [2014]; Ge and Hughes [2016]; Kristensen et al. [2015]; Ge et al. [2015]]. Finally, the mode volume calculation for QNMs is also changed slightly, but to an unambiguous form, now given by

$$\frac{1}{V_{\text{eff}}} = \text{Re} \left[ \frac{1}{V_Q} \right], \quad V_Q = \frac{\left\langle \left\langle \tilde{f}_c \right| \tilde{f}_c \right\rangle}{\epsilon(r_c) \tilde{f}_c^2(r_c)}. \quad (2.23)$$

This QNM correction is more important for low $Q$ resonances, and the normal mode approach with a phenomenological decay is a reasonable approach as long as one defines the volume integral to a reasonably finite size [Kristensen et al. [2012]; Mann et al. [2013]].

### 2.1.2 Applying and Computing the Photonic Green Function

Before discussing how to compute the photonic GF, let us see how to apply it. As previously mentioned, the GF includes information about all possible linear scattering events in the
propagation of light, and as such, many useful properties of a system can be found such as mode coupling, the light emission spectrum, the spontaneous emission enhancement factor, and the photonic local density of states (LDOS) [Fox [2006]]. In this work, we are also interested in understanding the impact of disorder in PC cavity light-matter interactions. As such, the LDOS $\rho_n(r; w)$, or the local number of states per interval of energy for photons, is a fundamental tool in our analysis. The projected LDOS is readily obtained directly from the imaginary part of the GF [Novotny and Hecht [2012]], by projecting the GF along a dipole unit direction $\mathbf{n}$ at position $r$, thus defining a projected LDOS as

$$
\rho_n(r; w) = \frac{6}{\pi \omega} \frac{\text{Im}[\mathbf{n} \cdot \mathbf{G}(\mathbf{r}, \mathbf{r}; \omega) \cdot \mathbf{n}]}{\text{Im}[\mathbf{n} \cdot \mathbf{G}^b(\mathbf{r}, \mathbf{r}; \omega) \cdot \mathbf{n}]} \tag{2.24}
$$

where $\mathbf{n}$ is the emitters unit vector, and $\mathbf{G}^b$ is the homogeneous background GF, which is derived to be $\mathbf{G}^b(\mathbf{r}, \mathbf{r}; \omega) = \left[ i \sqrt{\epsilon \omega / 6 \pi c^3} \right] \mathbf{I}$ in appendix B (for 3D space). In equation 2.24, we divide by the homogeneous GF so that our LDOS is in the same units as the Purcell factor (PF), which is a measure of the enhancement of the spontaneous emission rate felt by an excite two-level atom (or single quantum emitter). The PF, when typically applied to cavities, is directly proportional to the ratio of a cavity modes quality-factor $Q$ (which measures how quickly energy is lost from a mode), to the mode volume, given by [Purcell [1946], Rao and Hughes [2007]]

$$
\text{PF} = \frac{3}{4\pi^2} \left( \frac{\lambda_c}{n} \right)^3 \frac{Q}{V_{\text{eff}}}, \tag{2.25}
$$

where $\lambda_c$ is the cavity modes wavelength, $n = \sqrt{\epsilon}$ the refractive index, and the emitter is assumed to be at the field antinode and aligned with the cavity field polarization.

The GF’s relationship to the LDOS also allows us to relate it to the spontaneous emission rate, or radiative decay rate $\Gamma$ (assuming weak coupling). In its formal derivation, found in [Novotny and Hecht [2012]], one starts with Fermi’s golden rule and finds that $\Gamma$ is proportional to the LDOS, which we just saw is also proportional to the imaginary part of the GF. In fact, the two equations are similar, as the spontaneous emission rate is given by

$$
\Gamma(r) = \frac{2}{\hbar \epsilon} \left| \mathbf{d} \cdot \text{Im}\{\mathbf{G}(\mathbf{r}, \mathbf{r}; \omega)\} \cdot \mathbf{d} \right| \tag{2.26}
$$
where $d^1$ is the dipole moment of the quantum emitter, at position $r$.

To calculate the GF using a QNM expansion, one needs to know each complex eigen-frequency $\tilde{\omega}_\lambda$ and associated eigenmode profile $\tilde{f}_\lambda(r)$ for a given cavity structure. Measuring the complex eigenfrequency requires knowledge of the $Q$-factor by definition, since $\Gamma_\lambda = \omega_\lambda / 2Q_\lambda$, which is not always easy to obtain accurately. This is because many PC cavity structures have inherently large $Q$-factors, which means the electric field time signal takes a very long time to decay, and thus simply using a Fourier transform on the time signal is an impractical method for measuring large $Q$, as the resulting spectra may contain oscillation artefacts from the abrupt end of the time signal. These ripples drastically reduce the accuracy of the $Q$-factor measurement, and specific $Q$-analysis tools such as Harminv [Harminv] or the built in $Q$-Analysis function from Lumerical [QualityFactorCalculations] must be used to fit the decaying time signal to its decaying eigenfrequency. These tools will be compared and discussed in Chapter 3. If using FDTD, once a mode eigenfrequency is known, measuring the spatial mode profile is simply a matter of using a discrete Fourier transform profile monitor, at the specified $\omega_\lambda$.

To check the accuracy of the GF QNM expansion technique, “exact” (or full dipole) numerical calculations of the GF are performed by rearranging equation 2.20 for $\tilde{G}$. Assuming there is no initial field in the structure, the electric fields response at $r$ to a point dipole at location $r'$ is found. Knowing both the electric field and polarization time response, the GF can easily be found as [Van Vlack [2012]]

$$G_{ij}^{tot}(r, r'; \omega) = \frac{E_i(r; \omega)}{P_j(\omega)} = \frac{FT[E_i(r; t)]}{FT[P_j(t)]},$$

(2.27)

where $FT[\ ]$ represents a Fourier transform, and $E_i$, $i = x, y, z$ is the response to an oscillating polarized dipole source $P_j$, $j = x, y, z$. Thus, we have a direct numerical method of checking our theoretical GF solutions. Unfortunately, such direct numerical techniques are computationally expensive, since each simulation only defines a single GF matrix element, at a specific $r$ and $r'$, and also requires the electric field time response to decay long enough such that we remove any numerical ripple artefacts.

---

1Equation 2.26 assumes that $d$ is real, otherwise one needs a more general form [Young et al. [2015]]
2.1.3 Bloch Mode Limitations

Another common method for solving Maxwell’s equations, in the presence of a PC structure, is to utilize the periodic nature of the structure and assume the mode intensity is also periodic. However, the electromagnetic fields may have a phase component that is not periodic, preventing the use of periodic boundary conditions. The periodic fields are known as Bloch modes, and require Bloch’s boundary conditions that allows for phase shifts between unit cells. The basics of Bloch mode numerical techniques frequently rely on formulating Maxwell’s equations into a matrix eigenvalue problem where the solution provides the eigenvalues and eigenvectors for each $k$ point in reciprocal lattice space, defined by the structure being analyzed. This analysis is very good at calculating band structures, group velocities, and eigenmodes of any structure that can be well modelled using Bloch boundary conditions. A common tool for implementing Bloch mode analysis of PCs is the open source, plane wave expansion software known as MIT Photonic Bands (MPB) [MPB], or using FDTD with Bloch’s BC. In MPB, Maxwell’s equations are solved for $H$ through the eigenvalue problem

$$\nabla \times \frac{1}{\epsilon(r)} \nabla \times H(r; \omega) = \frac{\omega^2}{c^2} H(r; \omega),$$

which is formulated by equations (2.1a), the curl of (2.1b), and the constitutive relations 2.2.

By defining $\epsilon(r)$ within a single unit cell, Bloch’s theorem can be used whereby $H(r; \omega) = h_k(r)e^{ik \cdot r}$. This unit-cell function can be represented by a superposition of plane waves $h_k(r) = \sum_m c_{k,m} e^{G_m \cdot r}$, where $\{G_m\}$ is the set of reciprocal lattice vectors defined by the given PC structure. This summation can be recognized as a spatial Fourier transform of the plane wave amplitudes $\{h_{k,m}\}$, allowing equation 2.28 to be recast into a matrix eigenvalue problem that is easily solved for $H$, given a specified wave vector $k$ [Patterson [2009]]. Given $H$, the electric field $E$ is readily found using equation (2.1b).

MPB is a very effective tool for calculate band structures, normally performed along the boundary of the irreducible Brillouin zone, offering computation speeds orders of magnitude more efficient than FDTD [Patterson [2009]]. However, due to the intrinsically lossy behaviour of modes above the light line, MPB is only able to calculate modes below the light line, which is why the band structure of Figure [1.1a] is shaded above the light line. In addition, modelling an open system such as a PC cavity requires a very large unit cell,
known as a supercell, to prevent evanescent coupling between structures, as Bloch boundary conditions will place infinitely many structures above one another, and side-by-side in both \(x\) and \(y\) directions. The increased size of the super cell drastically reduces MPB’s computational efficiency, and thus limits the usefulness of such a computational method in the context of PC cavities. In addition, to implement the additional equations, e.g., to model gain, it is not possible. Combining all of these issues together limits our use of MPB to a tool that is used to identify bandgaps of PC structures and lossless modes, as is shown in Figure 1.1a.

2.2 Laser Physics

Now that we have introduced some key numerical tools to capture the optical properties of PCs, we are faced with the task of understanding how to modify the structure such that it accurately models an amplifying medium. To do this, let us first understand the basic classical picture of an atom interacting with an electric field. Consider the force \(\mathbf{F}\) exerted on a particle with charge \(e\), velocity \(\mathbf{v}\) by an electromagnetic field \(\mathbf{E}\) and \(\mathbf{B}\):

\[
\mathbf{F} = e(\mathbf{E} + \mathbf{v} \times \mathbf{B}).
\]

(2.29)

Assuming the nucleus is stationary as compared to the electron’s position, such that its equation of motion can be neglected, one can use center-of-mass coordinates for the electron-nucleus system and define \(\mathbf{r}\) to be the electron coordinates relative to the nucleus. Thus the equation of motion for the electron becomes

\[
m \frac{d^2 \mathbf{r}}{dt^2} = e\mathbf{E}(\mathbf{R}, t) + \mathbf{F}_{e,n}(\mathbf{r}),
\]

(2.30)

where \(\mathbf{R}\) is the center of mass for the system, \(\mathbf{F}_{e,n}\) is the force exerted on the electron by the nucleus, and we have dropped the magnetic force term by assuming our electron is not travelling at relativistic speeds. Now, to deal with \(\mathbf{F}_{e,n}\), we employ the \textit{ad hoc} hypothesis proposed by H. A. Lorentz around 1900 [Milonni and Eberly [2010]], stating that electrons respond to its atom as if they were held together by a spring \(\mathbf{F}_{e,n}(\mathbf{r}) = -k_s \mathbf{r}\), such that

\[
\left( \frac{d^2}{dt^2} + \frac{k_s}{m} \right) \mathbf{r} = \frac{e}{m} \mathbf{E}(\mathbf{R}, t),
\]

(2.31)
which is the differential equation for an oscillating mass. This theory was proposed before atoms were understood to have a nucleus, and clearly, this hypothesis goes against our understanding of Bohr’s model of the atom which accounts for the quantized orbital motion of electrons. In addition, we know that electrostatic forces are quadratic in nature, not linear. Despite these shortcomings, the electron oscillator model, also known as the Lorentz oscillator model agrees with the correct quantum mechanically derivation for a weakly excited two-level atom [Milonni and Eberly [2010]], given that the atom stays in its ground state. That is, if an atom is weakly excited by an electric field, its response is to oscillate.

So our picture is set, electrons do not orbit their atoms in the presence of electromagnetic waves, they oscillate. Now recall that a system's polarization $\mathbf{p}$ is defined as $\mathbf{p} = e \langle \mathbf{r} \rangle$, where $\langle \rangle$ denote an average. This means that an electric field, even a weak electric field, will alter the polarization since $\langle \mathbf{r} \rangle$ will change in its presence. This in turn will modulate the electric field through the wave equation 2.7. Thus, we have a rather complicated feedback loop where the electric field modulates itself by interacting with atoms. To fully understand this process, we will need to employ a semi-classical analysis where we treat our atoms quantum mechanically, while keeping our electric fields classical. This has the unfortunate consequence of missing some of the desired physics. For instance, to get the physics of spontaneous emission correct, one requires a quantized picture of light [Allen and Eberly [2012]]. However, as long our system has many more photons than unity [Allen and Eberly [2012]], we can safely ignore many of these subtleties (and, as we will show later, spontaneous emission can be modeled semi-classically via “radiation reaction”, e.g., in FDTD).

2.2.1 Quantum Dots as effective Two-Level Atoms and the Optical Bloch Equations

So far, we have only understood an electric field classically interacting with electrons while they interact with their nucleus by a spring like force. In the real world, matter is much more complicated than this. Indeed, lasers can be made by lots of different media including crystals, various gas mixtures, and a variety of solid state structures and materials [Milonni and Eberly [2010]]. The gain medium we wish to model is an ensemble of semiconductor QDs, which can be modeled as effective two-level atoms (TLAs) as indicated in Figure
2.2. LASER PHYSICS

2.1. Traditionally, TLA models were used to understand the interactions between nearly monochromatic light fields and matter. The TLA was a poor gain model because most lasing media operate on more than two energy levels. That is, for a laser model to achieve amplification, positive inversion is required. Inversion is the difference in population between the excited state $|1\rangle$, and the ground state $|0\rangle$. If more atoms are in the ground state than the excited state, then radiation at the lasing frequency will be absorbed, pumping electrons out of the ground state into the excited one. If more atoms are in the excited state, then more photons are emitted than are absorbed, and we achieve light amplification. Thus, positive inversion is required for lasing, which is described later in this chapter. At our level of modelling, only by including more than two energy levels is it possible to have positive inversion\(^2\). Typically, this is done by having a higher energy level above $|1\rangle$, which has a very quick relaxation period down to $|1\rangle$; or by having the lower energy level of a TLA resonance not the true ground state. Assuming our QD system is not excited with too large of a pump field, it is a good assumption that the majority of our electrons will recombine with holes from their respective ground states, thus leaving us with a valid (effective) TLA model, as seen in Figure 2.1. That is, if excited to higher energies, our electrons (or electron-hole pairs) have very fast decay rates into their ground state, where they then recombine with the available hole to emit light with a frequency equal to the energy difference of the energy gap between the electron’s ground state, and that of the hole’s ground state.

A TLA is a simple concept, yet it is able to describe a remarkably rich variety of quantum physics such as photon echoes, self-induced transparency, mode locking, and optical nutation [Allen and Eberly [2012]]. Since the physics of a TLA is contained within two levels, the equations describing a TLA are very similar to a spin-one-half particle in a magnetic field. As such, it follows that the spin vector formalism used by Bloch to describe magnetic resonance, is directly applicable to optical resonance. The equations of motion describing optical resonance or near-resonance are called the optical Bloch equations (OBEs).

To derive the OBEs, we start with the TLA system Hamiltonian $\mathcal{H}$, which consists of two terms. First is the energy difference between $|0\rangle$ and $|1\rangle$; second is the interaction

\(^2\)note, some quantum optical models that can achieve inversion with phonons or quantized cavity models [Hughes and Carmichael [2013, 2011]]
between the electric field and our atom, so that

\[ H = \frac{\hbar \omega_0}{2} \sigma_z - \hbar \chi(t)(\sigma^+ + \sigma^-), \tag{2.32} \]

where \( \omega_0 \) is the energy difference between the ground and excited states, and \( \chi(t) = \frac{d(t)E(t)}{\hbar} \) describes the field interaction between the dipole moment \( d \) associated with our TLA, and the electric field \( E \), and \( \sigma_z \) is the usual Pauli Matrix, while \( \sigma^+ \) and \( \sigma^- \) are the raising and lowering operators of our TLA, defined as

\[ \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}; \quad \sigma^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = (\sigma^-)^\dagger; \quad \sigma^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = (\sigma^+)^\dagger. \tag{2.33} \]

From equation 2.32, equations of motion are readily derived using a density matrix \( \rho \), (i.e., \( \langle \mathcal{O} \rangle = \text{Tr}[\rho \mathcal{O}] \)). The density matrix is a key tool of quantum mechanics that allows us to directly connect quantum mechanics with statistical mechanics. The density matrix is defined as

\[ \rho = \sum_j P_j |\psi_j\rangle \langle \psi_j|, \tag{2.34} \]
where $P_j$ is the probability amplitudes associated with mixed state $j$. Given that our Hamiltonian is a system of only two states, our density matrix is defined by

$$\rho = \begin{pmatrix} \rho_{11} & \rho_{10} \\ \rho_{01} & \rho_{00} \end{pmatrix},$$

(2.35)

where $\rho_{11}$ and $\rho_{00}$ are probabilities associated with the excited and ground states respectively. As such, we can define inversion as $\rho_{11} - \rho_{00}$, and we can connect the two probabilities by $\rho_{11} + \rho_{00} = 1$. This equation holds phenomenologically, since the total population probabilities must equal 1, but it also holds by definition of the density matrix. Namely, the sum of the diagonal elements of the density matrix is unity by definition. The off-diagonal elements $\rho_{10}$ and $\rho_{01}$ relate to the coherence of the system. Since the density matrix is Hermitian [Fox [2006]], we have $\rho_{10} = \rho_{01}^*$. Using the quantum Liouville equation $\dot{\rho} = -i\hbar [\mathcal{H}, \rho]$, we can find equations of motion for our coherence and population levels, but before we do this, it is necessary to identify the dissipative nature of the systems we will be describing. Namely, our TLA will be interacting within an open system PC environment, where various collisions destroy the coherence of our TLAs, and lead to radiative and non-radiative decay process. To incorporate such dynamics, it is common practice to use the Lindblad superoperator $\mathcal{L}$. For an operator $\mathcal{O}$, the Lindblad superoperator acts on $\rho$ by

$$\mathcal{L}(\mathcal{O})\rho = \mathcal{O}\rho\mathcal{O}^\dagger - \frac{1}{2} (\mathcal{O}^\dagger \mathcal{O}\rho + \rho \mathcal{O}^\dagger \mathcal{O}).$$

(2.36)

Traditionally, when a TLA interacts with a bath (or reservoir) with many degrees of freedom, e.g., photons, phonons, other collective modes, molecular vibrations, rotations, and translations, it experiences a broadening of its absorption linewidth directly proportional to the total dephasing time [Skinner and Hsu [1986]]. This broadening has two main contributions, an inherent relaxation rate $\Gamma_R$ determined by the TLA’s cavity environment ($\Gamma_R \propto Q/V_{\text{eff}}$, as shown in equation 2.26), and a pure dephasing rate $\gamma'$ which is typically dominated by phonon effects and also depends on the temperature. Both of these relaxation rates can be phenomenologically included in our system Hamiltonian via the Lindblad superoperator $\gamma'\mathcal{L}(\sigma^+\sigma^-)$, and $\Gamma_R \mathcal{L}(\sigma^-)$.

Finally, to account for the multi-level nature of our TLA, we require an incoherent pump rate $P$, that acts to model an external optical pump, which raises electrons to a
higher energy level than $|1\rangle$, but quickly decay, as depicted in Figure 2.1. To this end, we add a Lindblad pump term $\mathcal{P}\mathcal{L}(\sigma^+)$. Thus, our quantum master equation becomes

$$\frac{d\rho}{dt} = -\frac{i}{\hbar} [\mathcal{H}, \rho] + \mathcal{P}\mathcal{L}(\sigma^+)\rho + \Gamma R\mathcal{L}(\sigma^-)\rho + \gamma'\mathcal{L}(\sigma^+\sigma^-)\rho . \quad (2.37)$$

The first term in equation 2.37 can be simplified to

$$[\mathcal{H}, \rho] = \begin{pmatrix} \frac{\hbar\omega_0}{2} & -\hbar\chi(t) \\ -\hbar\chi(t) & -\frac{\hbar\omega_0}{2} \end{pmatrix} \begin{pmatrix} \rho_{11} & \rho_{10} \\ \rho_{01} & \rho_{00} \end{pmatrix} - \begin{pmatrix} \rho_{11} & \rho_{10} \\ \rho_{01} & \rho_{00} \end{pmatrix} \begin{pmatrix} \frac{\hbar\omega_0}{2} & -\hbar\chi(t) \\ -\hbar\chi(t) & -\frac{\hbar\omega_0}{2} \end{pmatrix} ,$$

and for the incoherent pump term:

$$\mathcal{P}\mathcal{L}(\sigma^+)\rho = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \rho_{11} & \rho_{10} \\ \rho_{01} & \rho_{00} \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} - \frac{P}{2} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \rho_{11} & \rho_{10} \\ \rho_{01} & \rho_{00} \end{pmatrix} + \begin{pmatrix} \rho_{11} & \rho_{10} \\ \rho_{01} & \rho_{00} \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} , \quad (2.38)$$

which simplifies to

$$\mathcal{P}\mathcal{L}(\sigma^+)\rho = P \begin{pmatrix} \rho_{00} & -\frac{\rho_{10}}{2} \\ -\frac{\rho_{01}}{2} & -\rho_{00} \end{pmatrix} ; \quad (2.40)$$

while the remaining two Lindblad superoperators simplify to

$$\Gamma R\mathcal{L}(\sigma^-)\rho = \Gamma R \begin{pmatrix} -\frac{\rho_{11}}{2} & -\frac{\rho_{20}}{2} \\ -\frac{\rho_{01}}{2} & \rho_{11} \end{pmatrix} , \quad (2.41)$$

and

$$\gamma'\mathcal{L}(\sigma^+\sigma^-)\rho = \gamma' \begin{pmatrix} 0 & -\frac{\rho_{10}}{2} \\ -\frac{\rho_{01}}{2} & 0 \end{pmatrix} . \quad (2.42)$$

Combining equations 2.37, 2.38, 2.40, 2.41, and 2.42, we find equations of motion for $\rho_{11}$ and $\rho_{01}$,

$$\frac{d\rho_{11}}{dt} = -i\chi(\rho_{10} - \rho_{01}) + P\rho_{00} - \Gamma R\rho_{11} , \quad (2.43)$$
\[ \frac{d\rho_{01}}{dt} = i\chi(\rho_{11} - \rho_{00}) + i\omega_0\rho_{01} - \frac{P + \Gamma_R + \gamma'}{2}\rho_{01}, \]  

which together, form the OBEs. We have no need for \( \dot{\rho}_{00} \) or \( \dot{\rho}_{10} \) since they are directly related to \( \dot{\rho}_{11} \) and \( \dot{\rho}_{01} \) through \( \rho_{00} = 1 - \rho_{11} \) and \( \rho_{10} = \rho_{01}^* \). Using these relations, we can simplify the OBEs to a more compact form,

\[ \frac{d\rho_{11}}{dt} = -i\chi(\rho_{01}^* - \rho_{01}) + P(1 - \rho_{11}) - \Gamma_R\rho_{11}, \]  

\[ \frac{d\rho_{01}}{dt} = i\chi(2\rho_{11} - 1) + i\omega_0\rho_{01} - \frac{P + \Gamma_R + \gamma'}{2}\rho_{01}. \]

From these equations, we can clearly see that our Lindblad superoperators achieved their purpose. Our incoherent pump rate \( P \) will continuously add electrons to the excited state \( \rho_{11} \) until completely saturated. Our radiative relaxation rate \( \Gamma_R \) acts to oppose the pump \( P \) and destroys coherence along with the pure dephasing rate \( \gamma' \); all the while our electric field is driving the coherence dynamics (through \( \chi \)) and in turn the inversion levels.

It is worth noting that this form of the OBEs is nearly identical to the one derived in many texts [Milonni and Eberly [2010]; Allen and Eberly [2012]], however, because we have not assumed any information about the electric field, it has not yet been possible to make the rotating wave approximation, which changes \( \omega_0 \rightarrow \omega_0 - \omega = \Delta \) such that it is possible to ignore rapidly oscillating terms in the equations of motion.

### 2.2.2 Maxwell Optical Bloch Equations

Now that we know how an arbitrary electric field interacts with our effective TLAs dipole moment through \( \chi \), it is time to see how this information can be used to influence the electric field. That is, we need to determine how the change to our density matrix impacts our atoms expectation value for \( \langle r \rangle \). To begin, let us define our TLA wavefunction as

\[ \psi(r, t) = \sum_{n=0}^{1} a_n(t)\phi_n(r), \]

where \( a_n(t) \) are the probability amplitudes associated with the time independent wave function \( \phi_n(r) \). In this basis, where \( \psi(r, t) = \langle r | \psi(t) \rangle \), and our density matrix elements are
defined as
\[ \rho_{m,n} = \langle \phi_m | \rho | \phi_n \rangle = \langle \phi_m | \sum_j P_j(t) | \psi_j(t) \rangle | \psi_j(t) \rangle | \phi_n \rangle = \langle a_m(t) a_n^*(t) \rangle. \]  

By definition, the expectation value of \( \mathbf{r} \) is given by
\[ \langle \mathbf{r} \rangle = \int \mathrm{d} \mathbf{r} \psi^*(\mathbf{r},t) \mathbf{r} \psi(\mathbf{r},t), \]

\[ \langle \mathbf{r} \rangle = \int \mathrm{d} \mathbf{r} \sum_{m=0}^1 a_m^*(t) \phi_m^*(\mathbf{r}) \mathbf{r} \sum_{n=0}^1 a_n(t) \phi_n(\mathbf{r}), \]

\[ \langle \mathbf{r} \rangle = \sum_{m=0}^1 \sum_{n=0}^1 a_m^* a_n \mathbf{r}_{m,n}, \]

where \( \mathbf{r}_{m,n} = \int \mathrm{d} \mathbf{r} \phi_m^*(\mathbf{r}) \phi_n(\mathbf{r}) \), and we have dropped the time dependence for simplicity (although it remains). Notice that \( \mathbf{r}_{m,m} = \mathbf{r}_{n,n} = 0 \) since we would be integrating an odd function \( \mathbf{r} \) times an even function \( |\phi(\mathbf{r})|^2 \). Thus, only two of the four terms in our double summation survive giving us
\[ \langle \mathbf{r} \rangle = a_1^* a_0 \mathbf{r}_{1,0} + a_0^* a_1 \mathbf{r}_{0,1}, \]
or, in terms of our density matrix elements, we have
\[ \langle \mathbf{r} \rangle = \rho_{10} \mathbf{r}_{10} + \rho_{01} \mathbf{r}_{01}. \]

Therefore, the average position of the electron depends solely on the off diagonal terms of the density matrix. Thus, if we assume \( \mathbf{r}_{mn} = \mathbf{r}_{nm} = \mathbf{r} \), we can see that
\[ \mathbf{p} = e \mathbf{r} (\rho_{01} + \rho_{01}^*) = 2e \mathbf{r} \mathcal{R}[\rho_{01}], \]

where \( \mathcal{R}[\rho_{01}] \) is the real component of \( \rho_{01} \), and that the polarization density \( \mathbf{P} = N \mathbf{p} \), is
\[ \mathbf{P} = 2e \mathbf{r} \mathcal{R}[\rho_{01}], \]

where \( N \) is the density of TLAs in our system. Finally, let us use the wave equation 2.7 in the time domain, relating the change in polarization to the electric field:
\[ \nabla \times \nabla \times \mathbf{E} = -\mu_0 \frac{\partial^2}{\partial t^2} (\epsilon_0 \mathbf{E} + \mathbf{P}), \]
\[ \left( \nabla \times \nabla \times + \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \right) E = -\frac{2dN}{\epsilon_0c^2} \frac{\partial^2 R[\rho_{01}]}{\partial t^2}, \]  

where \( d = e r \) is the dipole moment associated with our artificial atom, assuming our dipole moment is equally strong in all directions.

When equation 2.57 is combined with the OBEs 2.45 and 2.46, we arrive at a set of three coupled equations collectively known as Maxwell Bloch (MB) equations. Before we continue, let us pause here to better appreciate the possible numerical challenge we have constructed. Firstly, we must solve Maxwell’s equations in a PC cavity (or arbitrarily shaped cavity structure), which also requires open boundary conditions to model field decay, thus eliminating the numerically efficient Bloch boundary conditions. In addition, we have to self-consistently solve Maxwell’s equations with an ensemble of (up to many thousands) TLAs. Finally, we also want the system to include structural disorder, not as a perturbation, but as a real scattering effect, since we have no guarantee that perturbation theory will work with these (high \( Q \)) systems. To accomplish this computational task, Lumerical’s FDTD software provides an extension in the form of a “plugin”, which allows the user to define an arbitrary polarization felt by the numerically updated electric field. In addition to the flexibility of Lumerical’s plugin, the FDTD method is arguably the most rigorous technique we have for solving Maxwell’s equations in an arbitrary medium. The next two chapters will describe in detail the numerical methods used to implement this approach, as well as the various tests used to make sure the simulations were providing sensible results.

We note that this simple description of a laser does not take into account the quantum nature of light, and thus cannot model spontaneous emission as a quantum effect, nor can it get the full physics of stimulated emission correct. With these limitations in mind, our simulations will need some “seed radiation” to give the system an initial kick to start lasing; despite the complexity and limits, this MB approach is remarkably powerful as radiation reaction can model radiation decay and dipole-coupling in a fully self-consistent way. Note also, although we are primarily interested in the behaviour of QD ensembles, one could easily apply the same technique to study ensembles of atoms or molecules, by connecting to the appropriate polarizability model for the point dipole OBEs that are implemented in the plugin.
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2.2.3 Rate Equation Limit

Coherent optical effects such as optical nutation and self-induced transparency only occur if time scales associated with interaction of the radiation field of the atom is shorter than the relaxation times [Allen and Eberly [2012]]. Thus, we can make a rate equation approximation, by assuming $\gamma'$ is very large (and thus, the pure dephasing lifetime very short - e.g., valid at room temperatures), such that $\rho_{01}$ reaches a quasi-steady state $\frac{d}{dt}\rho_{01} = 0$, while $\frac{d}{dt}\rho_{11} \neq 0$. To implement this approximation more easily, we will split up the real $\mathcal{R}[\rho_{01}] = \rho_{01}^{\text{Re}}$ and imaginary $\mathcal{I}[\rho_{01}] = \rho_{01}^{\text{Im}}$ parts of $\rho_{01}$. Doing so, we arrive at

$$\frac{d\rho_{11}}{dt} = -2\chi\rho_{01}^{\text{Im}} + P(1 - \rho_{11}) - \Gamma_R\rho_{11}, \quad (2.58)$$

$$\frac{d\rho_{01}^{\text{Re}}}{dt} = -\omega_0\rho_{01}^{\text{Im}} - \frac{P + \Gamma_R + \gamma'}{2}\rho_{01}^{\text{Re}}, \quad (2.59)$$

$$\frac{d\rho_{01}^{\text{Im}}}{dt} = \omega_0\rho_{01}^{\text{Re}} - \frac{P + \Gamma_R + \gamma'}{2}\rho_{01}^{\text{Im}} + \chi(2\rho_{11} - 1), \quad (2.60)$$

and we let $\partial\rho_{01}^{\text{Re}}/\partial t = \partial\rho_{01}^{\text{Im}}/\partial t = 0$, such that

$$\rho_{01}^{\text{Im}} = \frac{\beta\chi(2\rho_{11} - 1)}{\beta^2 + \omega_0^2}, \quad (2.61)$$

where $\beta = \frac{P + \Gamma_R + \gamma'}{2}$, and

$$\rho_{01}^{\text{Re}} = \frac{-\omega_0\chi(2\rho_{11} - 1)}{\beta^2 + \omega_0^2}, \quad (2.62)$$

which gives

$$\frac{d\rho_{11}}{dt} = -2\Gamma_R I \frac{\beta^2}{\beta^2 + \omega_0^2}(2\rho_{11} - 1) - \Gamma_R\rho_{11} + P(1 - \rho_{11}), \quad (2.63)$$

where $I = \chi^2/\beta\Gamma_R$. Equation 2.63 is easily solvable given the initial condition $\rho_{11}(t = 0) = 0$, yielding

$$\rho_{11}(t)|_{\rho_{11}(0)=0} = \frac{C\Gamma_R + P}{2C\Gamma_R + \Gamma_R + P} \left[1 - e^{-(2\Gamma_R + \Gamma_R + P)t}\right], \quad (2.64)$$

where $C = 2I\frac{\beta^2}{\beta^2 + \omega_0^2}$. The practice of eliminating the coherence in the OBEs is referred to as an adiabatic elimination. This simple analysis is able to predict some interesting results, namely, stronger dipole interactions from a larger $\chi$, causes inversion levels to be driven to equilibrium, or zero. This is seen in Figure 2.2b, where the larger dipole moment curves are
driven to zero, while the value of $P$ determines if inversion will be driven below or above zero.

![Graph](image)

Figure 2.2: (a) Inversion dynamics of equation 2.64 for various dipole moments ($D = \text{Debye}$), while keeping all other parameters constant, and $P = 0$. Positive inversion is not possible, regardless how large the dipole moment is made. (b) Inversion dynamics of equation 2.64, for various incoherent pump rates $P = 1e9, 1e10, 1e11 \text{ s}^{-1}$ in the solid, dashed, and dot-dashed lines respectively, for dipole moment magnitudes: $d = 5 \text{ D}$ and 10 D, in red and blue, respectively. Strong coherent fields drive the inversion to zero, while the value of $P$ determines if inversion will be driven just below, or above zero.

Equation 2.64 is not very interesting on its own. For instance, we would like to know how $\rho_{11}$ impacts our electric field $E$ through equation 2.57, but to accomplish that, we also need to know some information about electric field. Let us assume a very simple scenario, without a PC, and assume our electric field is a 1D plane wave, travelling in the $x$-direction given by

$$E(t, x) = \mathcal{E}(t, x)e^{-i\omega(t-x/c)}\hat{u},$$  

(2.65)

where $\mathcal{E}(t, x)$ is our unknown fields amplitude, $e^{i\omega(t-x/c)}$ is the carrier wave, and $\hat{u}$ is the unit vector assumed to be in the same direction as the displacement $\langle r \rangle$ of our TLA system. Given that this field is transverse, the left-hand side of our wave equation 2.57 can be simplified using the vector identity $\nabla \times (\nabla \times G) = \nabla(\nabla \cdot G) - \nabla^2 G$, since $\nabla \cdot G$ is zero if $G$ is to be a transverse field [Milonni and Eberly [2010]]. Thus our LHS of equation 2.57
becomes
\[ \nabla^2 \mathbf{E} - \frac{1}{c^2} \frac{\partial^2 \mathbf{E}}{\partial t^2} = \left[ \frac{\partial^2 \mathbf{E}}{\partial x^2} + 2i \frac{\omega}{c} \frac{\partial \mathbf{E}}{\partial z} - \frac{\omega^2}{c^2} \mathbf{E} - \frac{1}{c^2} \left( \frac{\partial^2 \mathbf{E}}{\partial t^2} - 2i \omega \frac{\partial \mathbf{E}}{\partial t} - \omega^2 \mathbf{E} \right) \right] e^{-i\omega(t-x/c)} \mathbf{\hat{u}}, \]
(2.66)

\[ \nabla^2 \mathbf{E} - \frac{1}{c^2} \frac{\partial^2 \mathbf{E}}{\partial t^2} \approx 2i \frac{\omega}{c} \left( \frac{\partial \mathbf{E}}{\partial z} + \frac{1}{c} \frac{\partial \mathbf{E}}{\partial t} \right) e^{-i\omega(t-x/c)} \mathbf{\hat{u}}, \]
(2.67)

where we have used the slowly-varying-envelope approximation to remove the higher order derivatives. We thus have
\[ 2i \frac{\omega}{c} \left( \frac{\partial \mathbf{E}}{\partial z} + \frac{1}{c} \frac{\partial \mathbf{E}}{\partial t} \right) e^{-i\omega(t-x/c)} = \frac{-2dN \frac{\partial^2 \mathcal{R}[\rho_{01}]}{\partial t^2}}{\epsilon_0 c^2}. \]
(2.68)

However, this equation is incomplete since it does not include any information about how the polarization changes in response to the electric field. To work this out, we would have to re-derive our TLA Hamiltonian in the presence of our defined electric field, which is somewhat involved and laid out in Chapter 9 of [Milonni and Eberly [2010]]. The only change to our polarization is
\[ p = d(\rho_{01} + \rho_{01}^*) \rightarrow d(\rho_{01} e^{-i\omega(t-x/c)} + \rho_{01}^* e^{i\omega(t-x/c)}). \]
That is, our polarization now oscillates with both the coherence, and the electric field envelope function. Now we can recalculate \( \partial^2 \mathbf{P}/\partial t^2 \) as
\[ \frac{\partial^2 \mathbf{P}}{\partial t^2} = dN \frac{\partial^2}{\partial t^2} \{ [\rho_{01}^{\Re} + i\rho_{01}^{\Im}][\cos(\omega(t-x/c)) - i \sin(\omega(t-x/c))] + \}
\[ [\rho_{01}^{\Re} - i\rho_{01}^{\Im}][\cos(\omega(t-x/c)) + i \sin(\omega(t-x/c))]) \mathbf{\hat{u}}, \]
(2.69)

and since \( \rho_{01} \) varies much more slowly than \( e^{-i\omega t} \), we can make the approximation that
\[ \frac{\partial^2 \mathbf{P}}{\partial t^2} \approx -2dN \omega^2 [\rho_{01}^{\Re} \cos(\omega(t-x/c)) + \rho_{01}^{\Im} \sin(\omega(t-x/c))]) \mathbf{\hat{u}}. \]
(2.70)

Using this expression in our wave equation 2.68, we arrive at:
\[ \frac{\omega}{c} \left( \frac{\partial}{\partial z} + \frac{1}{c} \frac{\partial}{\partial t} \right) \mathbf{E} = \frac{dN \omega^2}{\epsilon_0 c^2} \rho_{01}^{\Im}. \]
(2.71)

Finally, we replace \( \rho_{01}^{\Im} \) with its steady state approximation equation 2.61 and multiplying both sides by \( \left( \frac{\partial}{\partial t} \right)^2 \frac{\epsilon}{\beta \Gamma_R} \), we arrive at
\[ \left( \frac{\partial}{\partial x} + \frac{1}{c} \frac{\partial}{\partial t} \right) I = \frac{\omega N d^2}{\epsilon_0 c h} \frac{\beta}{\beta^2 + \omega_0^2} (2\rho_{11} - 1) I, \]
(2.72)

where \( I = \chi^2/(\beta \Gamma_R) = \left( \frac{\partial \mathbf{E}}{\partial t} \right)^2 / (\beta \Gamma_R) \), as in 2.63. In this way, we have coupled the electric
field intensity $I$ to the TLA inversion.

It is clear from equation 2.72 that unless $\rho_{11} \geq 0.5$, the electric field intensity will decrease in intensity or be absorbed. Thus, we can make the crude assumption that pump threshold $P_{th}$ occurs once $\rho_{11} = 0.5$ in the long time limit. Using this limit in equation 2.64, we find that

$$\rho_{11}(t \to \infty)\big|_{P \to P_{th}} = 0.5 = \frac{cT_R + P_{th}}{2cT_R + T_R + P_{th}},$$

or

$$P_{th} = T_R \propto \frac{Q}{V_{eff}}.$$  \hfill (2.73)

Thus, from this very naive rate equation approximation, for a 1D plane wave travelling through a TLA resonant medium, we expect that the pump threshold for an individual QD be proportional to the radiative decay rate. That is, the larger the decay rate, the larger the pump rate is needed to be to ensure positive inversion is met. This is to be expected, as positive inversion can only be met when the pumping rate is greater than the excitation losses. The pump threshold in equation 2.74 does not shed light into the pump threshold of an ensemble of QDs embedded in a PC cavity, as the cavity physics is completely neglected in this analysis (along with dipole-dipole coupling). In cavity structures, the larger the PF, the longer light is trapped (through the increased $Q$), which allows for better stimulated emission processes; at the same time, radiative decay processes are increased, thus increasing the minimum pump rate to ensure positive inversion. As a final complexity, the PF is highly dependant on position, which makes determining the pump threshold of a QD ensemble virtually impossible through analytic techniques alone.

2.2.4 Semiconductor Rate Equations

Alternatively, rate equations can be described in the language of semiconductor physics where carrier density dynamics are used to understand when lasing occurs. Much of the literature [Nomura et al. [2006]; Matsuo et al. [2013]; Prieto et al. [2015a]] obtains semiconductor rate equations from [Coldren et al. [2012]], including different parameters depending on their system specifications. The general form of these rate equations consider how an excited carrier density $N$ populates a photon density $P$, through the two coupled differential
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The equations

\[
\frac{dN}{dt} = R_p - \frac{N}{\tau_r} - \frac{N}{\tau_{nr}} - g\frac{c}{n_{eff}}(N - N_{tr})P,
\]
(2.75)

\[
\frac{dP}{dt} = \Gamma g\frac{c}{n_{eff}}(N - N_{tr})P + \Gamma \beta \frac{N}{\tau_r} - P \tau_c,
\]
(2.76)

where \(\tau_r\) and \(\tau_{nr}\) are radiative and non-radiative lifetimes respectively, \(\Gamma\) is the confinement factor describing the spatial and spectral overlap of the mode and gain medium, \(\beta\) is the spontaneous emission coupling factor usually input as a fitting parameter, \(g\) is the gain coefficient, \(\tau_c\) is the photon cavity lifetime, \(N_{tr}\) is the transparency density referring to the point where optical pumping shifts a semiconductor from an absorber to an emitter [Coldren et al. [2012]], and \(n_{eff}\) is the effective refractive index defined as

\[
n_{eff}^2 = \frac{\int_V n(r)^2 f(r)^2 dV}{\int_V f(r)^2 dV}.
\]
(2.77)

To account for the mode’s interaction with underlying gain, a spatial confinement factor \(\Gamma\), comparing the active region to the spatial profile of the optical mode, is used. The non-uniform behaviour of a QD active medium, requires us to define \(\xi_{spec}\) as the spectral matching factor, giving us

\[
\Gamma = \xi_{spec} \Gamma_{spec},
\]
(2.78)

where

\[
\Gamma_{spec} = \frac{\int_{active} n_a(r)^2 \tilde{f}^2 dV}{\int_{cavity} n(r)^2 \tilde{f}^2 dV},
\]
(2.79)

where \(n_a\) is the active region refractive index and \(n\) is the refractive index of the host material.

Finally, using these rate equations, the lasers pumping threshold rate \(R_{p,th}\) is estimated in steady state through [Prieto et al. [2015a]]

\[
R_{p,th} = (1 - \beta) \frac{N_{th}}{\tau_r} + \frac{N_{th}}{\tau_{nr}},
\]
(2.80)

where \(N_{th}\) is the carrier density

\[
N_{th} = \frac{1}{\tau_c \Gamma \frac{g}{n_{eff}^2}} + N_{tr}.
\]
(2.81)

Many of the parameters defined in equation 2.80 are uniquely defined for different PC
cavity structures; some are readily connected to theory, such as $\tau_r$ and $\tau_\text{c}$; others are usually obtained through experimental fits, such as $\beta$ and $N_{\text{tr}}$. These equations are commonly used by experimental groups to extract meaningful data after measuring their system characteristics (e.g., see references Prieto et al. [2015a], Altug and Vučković [2005], Xue et al. [2016a]); whereas we will attempt to model the key light-matter interactions self-consistently with MB in FDTD simulations. For a more detailed rate equation analysis, see e.g. [Coldren et al. [2012]].
Chapter 3

Basic FDTD Techniques for Solving Maxwell’s Equations

The finite-difference time-domain (FDTD) method was developed by Kane S. Yee in the 1960’s, far before computers became the standard in numerical analysis implementation. His remarkable idea was to combine the central difference approximation with a staggered grid composed of Yee Cell’s that achieved second-order accuracy for the dynamic solution to time-dependent partial-differential equations. Rather than using mathematical transforms or ad hoc assumptions and initial conditions, the FDTD method relies on real time steps on spatially defined grid points to solve Maxwell’s equations. Initial conditions are required of course to define the simulation region, as well as boundary conditions (BCs), initial source terms, and field monitors, but the dynamics of the system are solved with phenomenal accuracy given that no information is assumed about the structure’s optical properties.

The power of the FDTD method is inherent in the Yee cell, which is specially designed to solve the curl components in Maxwell’s equations, ensuring that the curl is approximated on the same plane as the relevant vector component. The use of Cartesian coordinates also allows for straightforward parallelization of the algorithm, which is crucial for numerically intensive simulations.

However, the FDTD method is not without its limitations. Most notable, is the computational cost, which is often many orders of magnitude larger than alternative numerical methods used for simplified geometries (e.g., in the frequency domain with periodic or fixed
BCs). When solving for the optical properties of lossless materials such as photonic band-
structure, or the resonant mode eigenfrequencies and eigenmodes, it is often preferred to use
these alternative techniques that allow for easier parameter sweeps and faster optimizing
routines simply by saving numerical effort. However, these simulations are often incom-
plete, and no physical structure is truly lossless or perfectly periodic. To make matters
worse, many of the alternative numerical methods require very large simulation regions to
remove artefacts such as super-cell effects, which increases numerical run time thus dimin-
ishing the usefulness compared with the FDTD method. Also, adding realistic structural
disorder to the simulated structures increases their dissipative nature, and subsequently
their reliance on the FDTD method to accurately solve the optical properties. Finally, as
computation power steady increases, the FDTD method’s greatest inhibitor becomes less
of an issue, and many FDTD solvers can nicely exploit HPC architecture as the algorithm
is “embarrassingly parallizable”.

However, great care is needed in setting up high-Q cavity simulations, as the slightest
change to their environment can have a large impact on their performance. In the re-
mainder of this chapter, we will introduce the FDTD scheme implemented by Lumerical
[Lumerical], and discuss its many features such as perfectly-matched layer (PML) bound-
ary conditions, conformal-mesh technology, and high-Q analysis technique; all of which help
improve accuracy, and decrease numerical costs.

3.1 The Finite-Difference Time-Domain Method

The FDTD method uses a central difference approximation in both its temporal and spatial
updates, where the $E$ and $D$ fields are updated along integer space steps and half-integer
time steps, while the $B$ and $H$ fields are updated along half-integer space steps and integer
time steps. This spacial gridding is depicted in Figure 3.1, where the $E/D$ fields are
calculated along the edge of the Yee cell, and $B/H$ are shifted by a half step and calculated
along the faces. The advantage of such a scheme is immediately obvious when numerically
calculating equations 2.1a or 2.1b. Take for instance $B_x$, which would be calculated as

$$-\frac{\partial}{\partial t} B_x(r,t) = \frac{\partial}{\partial y} E_z(r,t) - \frac{\partial}{\partial z} E_y(r,t),$$

(3.1)
3.1. THE FINITE-DIFFERENCE TIME-Domain METHOD

from equation 2.1b. Discretizing (in scaled units) \( r = [i, j, k] \), we see that \( B_x \) is updated at location \( r = [i, j + \Delta y/2, k + \Delta z/2] \), where \( \Delta x, \Delta y, \Delta z \) are the dimensions of the Yee cell in the \( x, y, z \) direction respectively. More importantly, we see the central difference approximations for each expression in 3.1 is given as

\[
\frac{\partial}{\partial t} B_x(i, j + \Delta y/2, k + \Delta z/2, t) = \frac{B_x(i, j + \Delta y/2, k + \Delta z/2, t + \Delta t) - B_x(i, j + \Delta y/2, k + \Delta z/2, t)}{\Delta t}, \tag{3.2}
\]

\[
\frac{\partial}{\partial y} E_z(i, j + \Delta y/2, k + \Delta z/2, t + \Delta t) = \frac{E_z(i, j + \Delta y, k + \Delta z/2, t + \Delta t) - E_z(i, j, k + \Delta z/2, t + \Delta t)}{\Delta y}, \tag{3.3}
\]

\[
\frac{\partial}{\partial z} E_y(i, j + \Delta y/2, k + \Delta z/2, t + \Delta t) = \frac{E_y(i, j + \Delta y/2, k + \Delta z, t + \Delta t) - E_y(i, j + \Delta y/2, k, t + \Delta t)}{\Delta z}, \tag{3.4}
\]

and by combining equations 3.2-3.4 with equation 3.1, and making the approximation \( E(r, t + \Delta t) \approx E(r, t + \Delta t/2) \) since our \( E \) field is only updated on the half-integer time steps, we arrive at

\[
B_x(i, j + \Delta y/2, k + \Delta z/2, t + \Delta t) = B_x(i, j + \Delta y/2, k + \Delta z/2, t) + \frac{\Delta t}{\Delta y} [E_z(i, j + \Delta y, k + \Delta z/2, t + \Delta t/2) - E_z(i, j, k + \Delta z/2, t + \Delta t/2)]
- \frac{\Delta t}{\Delta z} [E_y(i, j + \Delta y/2, k + \Delta z, t + \Delta t/2) - E_y(i, j + \Delta y/2, k, t + \Delta t/2)], \tag{3.5}
\]

which is to say \( B_x(r, t + \Delta t) \) is updated by the previous time steps value in combination with the 4 field components nearest and within the same plane. This is what provides the FDTD method with its second order accuracy, but also prevents any field vector from being known exactly at any one point in space. Instead, one must interpolate the adjacent field components to get near-exact results; however, in practice this requirement is not very strict since our fields are usually slowly varying over a few Yee cells leaving interpolation as an unnecessary step. In principle, the FDTD method can model any finite-sized structure
3.1. THE FINITE-DIFFERENCE TIME-DOMAIN METHOD

Figure 3.1: An FDTD Yee cell, taken from reference [Van Vlack [2012]], with the associated \( \mathbf{E} \) and \( \mathbf{H} \) fields identified for the Yee cell indexed by \([i, j, k]\).

(given sufficient computational resources), making it a very powerful numerical solver; and although it is numerically intensive, the algorithm scales with \( N \), the number of unit cells, rather than \( N^2 \), e.g., as required for matrix diagonalization techniques implemented in alternative linear algebra techniques.

Once every field point in our simulation domain is known for \( \mathbf{B} \), we can use the constitutive relation 2.2b to relate \( \mathbf{B} \) to \( \mathbf{H} \) and then update our \( \mathbf{D} \) field using equation 2.1b. Then using the constitutive relation 2.2a, we relate \( \mathbf{D} \) to \( \mathbf{E} \), and step forward in time to repeat the process once more. At the beginning of the simulation, the FDTD grid is defined by the user’s input mesh requirements, and in addition to system “monitors” that capture the dynamic outputs of the FDTD algorithm, source “objects” create structures and add initial radiation to the simulation as needed. At the very start of each simulation, FDTD is set up as a source free environment, but that quickly changes once the predefined source begins to emit. Since we have complete control over the source term’s time signal, we can introduce an impulse with a very large bandwidth, or a continuous-wave signal with only a single frequency component. In either case, FDTD naturally handles the evolution of such light-matter interactions.
Unfortunately, finite-sized simulations have boundaries, and these boundaries can be challenging to model with a discretized grid of space points. Next, we will introduce the absorption boundary conditions used to model an open system, and the conformal mesh technology used to model interfaces within the simulation region.

3.2 Open Boundary Conditions in FDTD

The FDTD algorithm relies on neighbouring Yee cell data to accurately update, so how do we deal with the edge of a simulation? One option is to model boundaries as perfect reflectors, known as metal or conducting BCs, but this is obviously not going to model an open system. Similarly, periodic, or Bloch BCs do not allow for radiation to escape naturally, and thus are not good at modelling open systems either. This issue of modelling open systems was well known and initially studied in the 1970’s [Kunz and Lee [1978]]; and in 1981, Mur proposed the first absorbing BC to be stable and efficient in FDTD [Mur [1981]], thus mimicking the behaviour of an open system. In 1994, the concept of absorbing BCs was improved one step further by Bérenger’s PML [Berenger [1994]], which are now the industry standard in open BCs. They are “perfectly matched” in that they suppress reflection into the physical domain by matching the computational domains gridding, and they are layered in their implementation. Namely, PML BCs have a finite size to them, determined by the number of layers specified. The more layers, the better the absorption at the boundary. The need for layers arose from a limitation of PML to only perfectly reflect an exact continuous wave equation. Since FDTD implements a discretized version of the wave equation, small numerical reflections do exist, and to minimize the numerical reflections, the PML coefficients are turned on gradually via layers with polynomial fits [Lumerical]. In addition to these small numerical reflections, it is possible for the PML BC to become unstable and exhibit exponential growth, rather than decay.

In spite of PML’s limitations, Lumerical has developed some highly-stable settings that minimize numerical reflection and maximize performance. When implementing PML BCs in Lumerical, there are 6 parameters that need to be set: the unitless parameter $\kappa$ that sets the source free stretched coordinate metric coefficient [Gedney and Zhao [2010]], the absorption coefficient $\sigma$, the complex frequency shift parameter $\alpha$, 2 polynomial fits for
grading the parameters $\kappa$ and $\sigma$ or $\alpha$, and finally the number of layers that specify the thickness of the PML. In most cases, choosing the PML pre-setting “standard” offered by Lumerical is sufficient for accurate, and fast simulations; however, it is not uncommon for 3D simulations to sometimes experience unexpected exponential growth for high-$Q$ cavities. In these instances, custom PML settings are needed to remove the divergence. The most common fix is done with two actions: (i) increase the ratio of $\alpha/\sigma$, which increases the stability of the PML layers at the cost of reducing the absorption characteristics of $\alpha$; (ii) increase the number of layers (always to an even integer for easier numerical integration) to compensate for the lost effectiveness of $\alpha$. The overall cost of these actions is to increase the simulation run time, since additional layers increases the overall simulation domain.

### 3.2.1 Example for a 3D PC cavity

As a final note on high-$Q$ cavity boundary conditions, one must take great care in defining the simulation region size to ensure the PML BCs do not interact with the modelled PC cavity dynamics. In our study of high-$Q$ cavities, we simulate multiple cavity lengths, and need to be sure each simulation has PML BCs that meet this criteria, while creating a simulation domain as small as possible to minimize numerical requirements. The characteristic most affected by domain size is the measured $Q$-factor of the cavities, which is a crucial input for QNM calculations, as it defines the imaginary part of the eigenfrequency.

To test the convergence of our $Q$-factor on the FDTD simulations, we gradually increase the simulation size until convergence is met across all cavity lengths. We increase the simulation size by factors of $a$, in both the $x$ and $y$ direction, while keeping the size of the simulation constant in $z$. The $z$-span of the simulations is set to half a wavelength (i.e., the peak wavelength of the optical source) of dissipation on either side of the cavity, which provides optimal absorption. In addition, the BC in the $z$ direction can be set to “symmetric”, due to the symmetry of our cavity structure, which effectively cuts the simulation run times in half, and is shown in Figure 3.2d. Figure 3.3 depicts the effect of increasing the domain size, measured as the number of lattice constants past the edge of the cavity (thus the total width of the domain is the cavity length, plus twice the number of lattice constants past the cavity edge). The number of PML layers used was determined as the lowest power with a base of 2 that did not suffer from any numerical divergences. The
number of layers in the $x$ and $y$ directions was set to 32, while in the $z$ direction it was set to 16. Using more layers than this did not significantly alter the measured $Q$-factors, while it did increase the run times. Based on this figure, $9a$ was the determined length between a cavity edge and the simulation domain.

Figure 3.2: (a-c) Simulation screen shot of the simulation with PML $5a$, $7a$, and $9a$ from the cavity edge for figures (a-c) respectively. (d) Symmetric boundary conditions used and the $z$-span of the 3D simulations, which gave half a wavelength on either side of the cavity before hitting PML.

Figure 3.3: Simulation domain testing for 3D PC cavities (see Figure 3.2), where $Q_0$ is determined as the largest $Q$ measured for any given cavity length (e.g., for $L7$, $Q_0 \approx 1e5$), and the values are given in the inset. The simulations are scaled in both the $x$ and $y$ directions, and the total width of the domain is the cavity length, plus twice the number of lattice constants past the cavity edge. The number of PML layers is set to 32 in the $x$ and $y$ directions, and 16 in the $z$ direction. Example screen shots of half the simulation region (that includes the dipole source), are shown in Figures 3.2a - 3.2c, for the distances of 5, 7 and 9, respectively.
3.3 Conformal Mesh

In addition to the simulation boundaries, object interfaces within the simulation region must be treated with care to avoid numerical artefacts. Since the FDTD method uses a Cartesian coordinate system, curved objects are not easily modelled and can lead to artefacts such as staircase interfaces, since the curved surface permittivity appears as a staircase. To deliver subcell accuracy to the electromagnetic fields, Lumerical implements a conformal mesh technology (CMT) along curved dielectric interfaces. In general, this method accounts for subcell features by solving Maxwell’s integral equations along the Yee cell’s of an object boundary [Lumerical]. As an example, Figure 3.4a shows the Yu-Mittra method, a form of conformal meshing for perfect electrical conductors (PECs). However, the simulations performed in this work do not use PECs, and instead uses a different CMT algorithm designed for non-metal interfaces called “Conformal variant 0” [Lumerical], although the basic idea remains the same; use the information on the edge of the Yee cell to derive a field update algorithm, bypassing the area and volume calculations [Yu and Mittra [2001]] of many legacy CMTs.

To ensure all etched holes in the triangular lattice membrane of our PC cavities are the same (when modelling a perfect lattice), we define an additional mesh lattice within our simulations determined by our triangular lattice structure. Having uniform meshing across each PC hole is necessary to ensure numerical stability, as shown in Figure 3.5, where the electric field of a PC cavity simulation (measured at the cavity center), with and without uniform meshing is shown. Since our triangular lattice has a unit cell of $a$ in the $x$-direction, and $\sqrt{3}/2 a$ in the $y$-direction, the new mesh steps $dx$ and $dy$ are defined by $a/N_x$ and $\sqrt{3}/2 a/N_y$ respectively, where $N_x$ and $N_y$ are the number of mesh steps in the $x$ and $y$ direction. This step is critical in any FDTD simulation to ensure all curved dielectric objects are created identical by Lumerical, as shown in Figure 3.4b.
3.3. CONFORMAL MESH

Figure 3.4: (a) Conformal mesh method introduced by Yu and Mittra [Yu and Mittra [2001]] to provide greater accuracy at curved object interfaces. (b) Consistent mesh implemented in FDTD for a triangular lattice (without disorder).

Figure 3.5: Passive L15 simulation with $E_0 = 1e9$, and a run time of 250 ps, comparing the electric field time signal with and without uniform meshing. The points-per wavelength for both meshing algorithms is greater than 35 in both the $x$ and $y$ directions, where $\lambda$ is 1587 nm (190 THz).
3.4 Harminv Versus Lumerical Numerical $Q$-Factor Extraction

One potential downside to the FDTD method (or any time-space-dependent Maxwell solver) is that high $Q$-factor structures require a long simulation run time to decay to a measurable level. That is, if we try to measure $Q$ of a high-$Q$ cavity in the usual way, where the full-width half-max (FWHM) of the spectral response is compared with the resonant frequency, then we must run the simulation long enough for the Fourier transformed spectra of the time signal to not be affected by a cut-off in the time domain. This run time quickly becomes unrealistically long, as larger cavities with larger simulations domains, also have larger $Q$-factors. Thus, practically we must fit the slowly-dying time signal to a sum of decaying exponential solutions, one for each resonant mode present, of the form

$$A \cdot e^{-i(2\pi f_{Hrm}t - \phi)} - \gamma_{Hrm} t,$$

where $f_{Hrm}$ is a modal peak frequency, $\gamma_{Hrm}$ is the decay constant, $A$ is the modes amplitude, and $\phi$ is a phase shift. Both $A$ and $\phi$ are generally less accurate than $f_{Hrm}$ and $\gamma_{Hrm}$ [Harminv], however this is of no concern since only $f_{Hrm}$ and $\gamma_{Hrm}$ are used to measure $Q$. To accomplish this task, two analysis methods readily exist: Harminv [Harminv], which is an external application written in C++ for Unix-like operating systems by MIT, and Lumerical’s built in $Q$-analysis group [QualityFactorCalculations]. Harminv was our research group’s standard in fitting high-$Q$ time signals for eigenvalue extractions, as it pre-dates Lumerical’s analysis tool by almost a decade, but Lumerical’s $Q$-factor analysis has many reasons for now being the superior method.

The most obvious reason why Lumerical’s built in $Q$-analysis is better than Harminv is that it cuts down on on the time required to analyze the structure of interest. With Harminv, simulated time-domain data needs to be sent from Lumerical to Matlab so it can be prepared in the correct data structure before being sent to the terminal for execution by Harminv. Then the output of Harminv must be loaded into Matlab, to extract the $Q$-factor. All of these steps are avoided with Lumerical’s built in analysis. The less obvious, and more important reason for choosing Lumerical over Harminv is that the required time-signal length for Lumerical’s analysis is substantially less than Harminv. Figures 3.6a and
3.4. HARMINV VERSUS LUMERICAL NUMERICAL Q-FACTOR EXTRACTION

3.6b demonstrate this superior performance, by comparing the change in Q-factor as the time signal is reduced for both methods. Clearly, as the time signal is reduced, the measured Q-factor becomes increasingly worse in comparison with the original (true) measurement. Remarkably, this behaviour occurs a full order of magnitude lower in Lumerical than in Harminv, making it the obvious choice. This improved performance is the result of newer algorithms that use better windowing functions, and multiple time signal inputs from a cluster of time monitors that make up the analysis group, rather than a single time signal, which is all that can be sent to Harminv. Thus, not only is Lumerical simpler to use, but it is also drastically more efficient.

![Figure 3.6: Comparison between Harminv and Lumerical’s Q-factor accuracy as a function of decreasing signal length. (a) Lumerical is highlighted with dots, while Harminv tracks its trends. (b) Lumerical is shown to have consistent accuracy a full order of magnitude lower than Harminv.](image)

The one downside to using Lumerical’s analysis over Harminv is a strange artefact in the measurement of the peak frequency of the fitted mode. Namely, when 20 disordered simulations were performed, a discretized behaviour was found in the peak frequency measurements as shown in Figure 3.7b. For comparison, the same data is run through Harminv in Figure 3.7a, demonstrating that these disordered instances did indeed possess unique frequencies. However, the Q-factor measurements performed by Lumerical’s analysis group did not show any such discretized nature, which is the more important measurement.
3.5 FDTD Simulation of Disordered PC Cavities

To model fabrication (and structural) disorder in our FDTD simulations, the center of each etched hole is shifted by a random amount $\Delta r$ characterized by the standard deviation $\sigma_{\text{Dis}}$ of a random number generator. The direction of each hole’s shift is also randomized, characterized by $\theta$, with equal probability to be shifted in any direction, which is simply a random number chosen between $-\pi$ and $\pi$. To map this random shift of each hole into FDTD, we give each hole’s $x$ and $y$ location an additional term of $\Delta x$ and $\Delta y$ defined as

$$\Delta x = \Delta r \cos(\theta), \quad \Delta y = \Delta r \sin(\theta).$$

These random shifts in the lattice are exaggerated for an example L5 cavity shown in Figure 5.3b.

The amount of disorder characterized by $\sigma_{\text{Dis}}$ in a 2D simulation is not equal to the same 3D simulation (which has out of plane decay), given that both structures have similar $Q$-factors. This is shown in Figure 5.4d, which compares the statistical average and variance of the disordered L15 cavity 3D simulations to varying amounts of disorder for the corresponding 2D simulation. Only a single disorder value $\sigma_{\text{Dis}} = 0.005a$ is used in the 3D simulations since this value is shown to capture recent experimental inherent disorder well [Mann et al.
Taking the normal definition of our $Q$-factor to be $Q = \frac{\omega}{2\Gamma}$, we can capture the disorder statics using $\Gamma$, as $\omega$ is roughly constant with increasing disorder. Defining $\Gamma = \Gamma_0 + \Gamma_{\text{Dis}}$, where $\Gamma_0$ is the ideal structure’s broadening and $\Gamma_{\text{Dis}}$ is additional broadening due to disorder (which can sometimes be negative), we plot $\langle \Gamma_{\text{Dis}}/\Gamma_0 \rangle$ for 20 instances of 3D data and compare it to 100 instances of 2D simulations with $\sigma_{\text{Dis}}/a = [0.0025, 0.005, 0.01, 0.02]$ (400 simulations total). Thus demonstrating our effective 2D simulations, intrinsic disorder is best modelled by $\sigma_{\text{Dis}} = 0.01a$.

Figure 3.8: (a) Disorder statistics of $\Gamma_{\text{Dis}} = \Gamma - \Gamma_0$, for the L15 cavities of varying amounts of 2D disorder, referenced to the 3D intrinsic disorder of $\sigma = 0.005a$. (b) Schematic of the disordered cavity simulation with the disordered holes (red circles) over-top the ideal air holes (black holes), and the background slab (gray).
Chapter 4

Development of a TLA Polarization Plugin Tool for Lumerical’s FDTD

Modelling nonlinear materials is a particular challenge for commercial software due to the flexibility required, and it would take a vast amount of work to rewrite a full FDTD solver in-house to handle various types of nonlinear models. The difficulties for commercial software arise because nonlinear material models differ in both the nonlinearity being implemented, and the approximations used. As such, it is not possible to have a universal material extension that will fit the needs of all users. Instead Lumerical has recently introduced a user defined polarization plugin written in C++ that allows users to implement their own material models, specific to their research. This drastically improves Lumerical’s FDTD software as users can define cutting-edge material responses by themselves, such as novel negative-index material, time-dependant index material, or whatever polarization model best describes the research being done, without being dependant on Lumerical. However, Lumerical is still a black box in many respects, and as such, when a user creates a new material, Lumerical offers substantial assistance to resolve any technical issues that may arise.

In this chapter, we will describe how this plugin tool works with Lumerical’s FDTD
software, and implement optical Bloch equations using a Runge-Kutta (RK4) numerical analysis to form a powerful set of Maxwell Bloch equations (MBEs). We will then verify the plugin tool works as it should by comparing against some known physics models, and learn how to implement a new material as a single quantum dot (QD) within the simulation.

4.1 Lumerical’s Plugin Implementation

The plugin tool allows a user to implement a custom material with desired polarization $P^n$, at time $n\Delta t$, by altering the electric field components $E^n$ with the following equation

$$U^n E^n + \frac{P^n}{\epsilon_0} = V^n,$$  \hspace{1cm} (4.1)

where $U^n$ and $V^n$ are inputs defined, and provided within Lumerical’s algorithm. In this way, the plugin tool acts as Lumerical’s application programming interface, since all algorithms not defined in calculating $P^n$ are still unknown to the plugin, and cannot be altered. However, the plugin class has read access to $E^n$, $U^n$, and $V^n$. The only return parameter of the plugin class is $E^n$, which is altered by the user defined $P^n$, via equation 4.1. Each direction of $E$ can be defined differently by the vector components of $P$.

For example, in the trivial case of adding a nondispersive linear material, where $P^n = \chi E^n$, one would simply return the following equation

$$E^n = \frac{V^n}{U^n + \chi}.$$  \hspace{1cm} (4.2)

The usefulness of $U$ and $V$ is to allow our added material to be combined with any desired base material, offered by Lumerical.

The C++ code for Lumerical’s plugin is implemented as a class, which is compiled and added to Lumerical’s directories as outlined in appendix C, and various online resources are made available by Lumerical [FlexibleMaterialPluginFrameWork] to help researchers learn the basics of the plugin tool. Careful note should be taken if a user wishes to run FDTD simulations on a remote super computer clusters, as mentioned in appendix C.
4.2 Implementation and Discretization of the Bloch Equations

Lumerical has developed an example laser material model for a four-level two-electron scheme, based on S. Chang and A. Taflove’s 2004 paper [Chang and Taflove [2004]] on implementing gain within the FDTD method. This model is good for many laser systems, but is not appropriate for a quantum dot gain ensemble, which is effectively a two-level system as described in Chapter 2. By reducing our system to a two-level model, we reduce the computational cost of the plugin by having fewer storage fields to update and keep track of. In addition, the four-level two-electron model relies on the rate equation approximation, which ignores the coherent state of the electrons, and we would rather not have to do that. Given all of these considerations, we have developed our own Maxwell Bloch plugin, which connects the Optical Bloch equations 2.45 and 2.46 to polarization modulation 2.55, derived in Chapter 2, which is returned by the plugin.

To implement the OBEs in a plugin tool, we need to discretize equations 2.45 and 2.46, and update the fields with a stable numerical method. After testing various difference approximations, we decided to implement the RK4 method to update our density operator, as it proved to be the most stable and numerically accurate. The trade-off of course is computational cost, as RK4 takes many more lines to implement than a standard central-difference approximation. The Runge-Kutta scheme is a differential equation of the form

\[
\frac{d\sigma_1}{dt} = F(\sigma_1, \sigma_2, \sigma_3),
\]

discretized with time steps \( \Delta t \) and updated by

\[
\sigma_1^{n+1} = \sigma_1^n + \frac{\Delta t}{6}(K_1 + 2K_2 + 2K_3 + K_4),
\]

(4.3)

where

\[
K_1 = F(\sigma_1, \sigma_2, \sigma_3),
\]

\[
K_2 = F\left(\sigma_1 + \frac{\Delta t}{2}K_1, \sigma_2 + \frac{\Delta t}{2}L_1, \sigma_3 + \frac{\Delta t}{2}M_1\right),
\]

\[
K_3 = F\left(\sigma_1 + \frac{\Delta t}{2}K_2, \sigma_2 + \frac{\Delta t}{2}L_2, \sigma_3 + \frac{\Delta t}{2}M_2\right),
\]

\[
K_4 = F(\sigma_1 + \Delta tK_3, \sigma_2 + \Delta tL_3, \sigma_3 + \Delta tM_3),
\]

(4.4)

where \( L_i \) and \( M_i \) have similar equations to \( K_i \) for their respective differential equations.
4.2. IMPLEMENTATION AND DISCRETIZATION OF THE BLOCH EQUATIONS

involving $\sigma_2$ and $\sigma_3$:

\[
L_1 = G(\sigma_1, \sigma_2, \sigma_3),
\]

\[
L_2 = G \left( \sigma_1 + \frac{\Delta t}{2} K_1, \sigma_2 + \frac{\Delta t}{2} L_1, \sigma_3 + \frac{\Delta t}{2} M_1 \right),
\]

\[
L_3 = G \left( \sigma_1 + \frac{\Delta t}{2} K_2, \sigma_2 + \frac{\Delta t}{2} L_2, \sigma_3 + \frac{\Delta t}{2} M_2 \right),
\]

\[
L_4 = G(\sigma_1 + \Delta t K_3, \sigma_2 + \Delta t L_3, \sigma_3 + \Delta t M_3),
\]

\[\text{(4.5)}\]

and

\[
M_1 = H(\sigma_1, \sigma_2, \sigma_3),
\]

\[
M_2 = H \left( \sigma_1 + \frac{\Delta t}{2} K_1, \sigma_2 + \frac{\Delta t}{2} L_1, \sigma_3 + \frac{\Delta t}{2} M_1 \right),
\]

\[
M_3 = H \left( \sigma_1 + \frac{\Delta t}{2} K_2, \sigma_2 + \frac{\Delta t}{2} L_2, \sigma_3 + \frac{\Delta t}{2} M_2 \right),
\]

\[
M_4 = H(\sigma_1 + \Delta t K_3, \sigma_2 + \Delta t L_3, \sigma_3 + \Delta t M_3).
\]

\[\text{(4.6)}\]

In the RK4 algorithm, $K_1, L_1,$ and $M_1$ are calculated first, followed by $K_2, L_2,$ and $M_2$, and so on. Recall the form of our OBE (e.g., equations 2.45 and 2.46) as

\[
\frac{d\rho_{01}^{\text{Re}}}{dt} = -\omega_0 \rho_{01}^{\text{Im}} - \frac{P + \Gamma + \gamma'}{2} \rho_{01}^{\text{Re}} = F(\rho_{01}^{\text{Re}}, \rho_{01}^{\text{Im}}, \rho_{11}),
\]

\[\text{(4.7)}\]

\[
\frac{d\rho_{01}^{\text{Im}}}{dt} = \omega_0 \rho_{01}^{\text{Re}} - \frac{P + \Gamma + \gamma'}{2} \rho_{01}^{\text{Im}} + \chi(2\rho_{11} - 1) = G(\rho_{01}^{\text{Re}}, \rho_{01}^{\text{Im}}, \rho_{11}),
\]

\[\text{(4.8)}\]

\[
\frac{d\rho_{11}}{dt} = -2\chi \rho_{01}^{\text{Im}} + P(1 - \rho_{11}) - \Gamma \rho_{11} = H(\rho_{01}^{\text{Re}}, \rho_{01}^{\text{Im}}, \rho_{11}),
\]

\[\text{(4.9)}\]

where $\chi = d(t) \cdot E(t)/\hbar$, and $E$ at time step $n\Delta t$ is given to the plugin script when it is called.

Substituting these OBE into our RK4 scheme, we arrive at the code seen in appendix C, which updates $\rho_{01}^{\text{Re}}, \rho_{01}^{\text{Im}},$ and $\rho_{11},$ and returns a polarization defined by equation 5.11.
4.3 Set up of Simulation Analysis

To verify the plugin tool was working correctly, initial tests were performed to confirm basic properties of the Maxwell Bloch equations for a TLA, such as Rabi flopping, pulse reshaping, pulse absorption, coherent decay, and mode frequency shifts when the plugin material is present in a cavity structure. As a final check in the next section, radiative decay will be computed and compared to analytic theory to ensure FDTD is interacting with the TLA correctly.

To test the majority of the plugin’s basic features, a simple 2D simulation was set up where an incident total-field scattered-field (TFSF)₁ pulse, polarized in the z-direction, travels through a rectangular slab of the plugin material, 20 µm long (except for the pulse reshaping simulation, which was 240 µm long) and 2 µm wide. This simulation can be seen in Figure 4.1.

By driving the plugin material with a resonant pulse, starting with the TLA in the ground state, we can achieve Rabi-flopping given that the pulse area is a multiple of 2π. This resonant behaviour is clearly seen in Figure 4.2a, where the temporal behaviour of the coherence \( \rho_{01}^{\text{im}} \) is compared to the electric field, and the inversion \( 2\rho_{11} - 1 \), which clearly “flops” from the ground state to the excited state, and back down again. The basic properties are verified as the pulse travels without backscattering, preserving its shape, and becoming essentially transparent, as shown in Figure 4.2b. In comparison, a 0π pulse has a long temporal response, determined by the oscillatory behaviour of the TLA with the natural decay of its environment, which is shown in Figure 4.3a. Finally, we demonstrate pulse reshaping, which is a phenomenon that occurs as the front 2π area of a 4π pulse experiences no backscattering, thus separating itself from the full pulse area and creating two individual 2π pulse packets (temporal solitons). This phenomenon is clearly shown in Figure 4.3b.

Recall in Chapter 2 we approximated the influence of a TLA on a 1D plane wave using a rate equation approximation. In this approximation, we found intensity of our plane wave

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₁A TFSF is an optical source with two regions: one, a defined space where the source propagation is defined and constrained to (referred to as the total-field); two, the remainder of the simulation space where any scattering light may propagate, but not the initial source (referred to as the scattered-field).
4.3. SET UP OF SIMULATION ANALYSIS

Figure 4.1: Example of Lumerical’s FDTD 2D simulation set up, which is 2 µm wide, and 20 µm long (except for the 4π pulse simulation, which was 240 µm long). The white rectangle denotes the total-field scattered-field propagation region while the red rectangle contains the gain plugin (without any dielectric mismatch, to better explore the features of the OBEs). The blue arrows depict the polarization of light and the yellow strips indicate electric field-time monitors capturing both the pulse propagation as well as the material plugin storage fields.

To obey equation 2.72, which gives us an absorption coefficient $\alpha$ of the form

$$\alpha = \frac{\omega N d^2}{\epsilon_0 c \hbar} \frac{\beta}{\beta^2 + \omega_0^2},$$

(4.10)

where it has been assumed that $\rho_{11} \approx 0$, such that we are in the absorbing regime. Using this equation to predict the absorption of our initial 2D TFSF pulse (which is essentially a 1D simulation), we find good agreement with simulation time monitors as seen in Figures 4.4a and 4.4b, which show the absorption after 8 µm and 22 µm of penetration for various plugin dipole magnitudes $d$, holding $N$ constant. Notably, as the dipole moment strength increases, the absorption spectra becomes asymmetric as FDTD captures nonlinearities.
4.3. SET UP OF SIMULATION ANALYSIS

Figure 4.2: (a) Single Rabi flop (solid line) for a $2\pi$ pulse (dot-dashed line), with the coherence $\rho_{01}^{\text{in}}$ included (dotted line) similar to the results found in [Hughes [1998]]. (b) The time domain evolution of a $2\pi$ pulse, with a full structure length of 20 $\mu$m. The CW normalization referees to Lumerical’s continuous wave normalization, which is described in detail on their webpage [Lumerical].

Figure 4.3: (a) The time domain evolution of a $0\pi$ pulse (i.e., low intensity or linear), with a full structure length of 20 $\mu$m. Interference is clearly visible between the incident pulse and backscatter, even though there is no background index difference between the two regions. (b) Time domain evolution of a $4\pi$ pulse, with a full structure length of 240 $\mu$m.

excluded from our analytic model, likely due to a breakdown of the slowly-varying envelope approximation in space.
Figure 4.4: (a) Absorption profile, through a simple plane wave 2D simulation, at $z = 8 \, \mu m$. (b) Absorption profile, through a simple plane wave 2D simulation, at $z = 22 \, \mu m$. The approximate analytic result (Eqn. 4.10) is also shown, which fails for increasing dipole moments.

To ensure the pure dephasing rate $\gamma'$ was performing as expected, we sent $0\pi$ (namely, linear or low intensity) pulses into the 2D material with varying amounts of pure dephasing $\gamma'$, and measured the temporal decay rates. The resulting decay curves are shown in Figure 4.5a, where the theoretical half-lifes $\tau = \ln(2)/\gamma'$ are highlighted for comparison with the simulations. Finally, we expect the response of MBE’s to shift the frequency of resonant modes in cavity simulations. To confirm this, a uniform sheet of absorbing plugin material is embedded throughout a 2D L5 cavity simulation, and a weak pulse is injected into the simulation to measure the resonant mode response in the spectral domain. This response is shown in Figure 4.5b, where the mode’s eigenfrequency real and imaginary parts are clearly seen to shift.
4.4. Modelling the Optical Properties of Simple Quantum Dots

To model QDs in FDTD, one must carefully consider the Yee cell, which is the smallest spatial grid unit allowed in simulations. Even if a material is specified at a single field point such as $E_y$, with dimensions much smaller than the Yee cell, the effective volume of that material is still the size of a Yee cell. As such, one must reduce the mesh spatial steps to a sufficient size, as the QDs density $N$ will be given by $N^{-1} = \Delta x \Delta y \Delta z$ [Schelew et al. [2016]], where $\Delta x$, $\Delta y$, and $\Delta z$ are the mesh-steps in the $x$, $y$, and $z$ directions, respectively.

To implement a material at a single location, we simply add a rectangular material centred at the field point of interest. Since our cavities are TE modes, with lasing in the $E_y$ direction, we set our QDs to be centred at $E_y$ update points. This can be seen in Figure 4.6c, for a 2D QD. To model QDs randomly throughout the simulation, as would occur naturally when growing a QD gain ensemble, we randomly select grid points to contain QDs. The inputs for this random process are the experimental QD density $N$, and the simulated QD’s area defined by $\Delta x$, $\Delta y$. Using these parameters, we define the total percentage of field
points within a plane that should contain a QD $P_{QD}$ as

$$P_{QD} = N\Delta x \Delta y,$$  \hspace{1cm} (4.11)

which clearly indicates a lower limit to $N$, defined by $\Delta x \Delta y$, since $P_{QD} \leq 1$. This makes sense, since a very large QD density is only achievable if the QD’s size is small enough such that the dots are not touching.

With $P_{QD}$, we randomly identify 2D grid points by requesting Lumerical to generate a random 2D matrix with dimension proportional to the number of grid points in the $x$ and $y$ direction, for the defined gain region. This random matrix contains real numbers from 0-1, such that any matrix point with a value less-than, or equal-to $P_{QD}$ should be given a QD. However, this poses a problem in that QDs can be side-by-side. To circumvent this issue, we use “if statements” to ensure no QD’s can be nearest neighbours (NN) in the $x$ or $y$ direction. These “if statements” reduce the overall number of QDs in our simulation, to a density less than what we initially wanted. To overcome this issue, we calculate the percent chance that any NN will be a QD $P_{NN}$, and define the percentage of QDs lost due to our NN requirement as $P_{NN}P_{QD}$. Then, we must add this lost percentage to $P_{QD}$, to arrive at the correct percentage of mesh points that will contain a QD $P_{Tot}$, given that no NN QDs are allowed, then

$$P_{Tot} = P_{QD}(1 + P_{NN}),$$

where

$$P_{NN} = 1 - (1 - P_{QD})^4,$$  \hspace{1cm} (4.13)

since there are 4 NNs for every grid point. In testing the number of QDs generated by this algorithm, we find that using $P_{Tot}$ creates a stochastic number of QDs within 5% of the theoretical value, while $P_{QD}$ is only within 25%, given that both algorithms are subjected to the NN restriction. The resulting (non resonant) QD ensemble can be seen in Figure 4.6a.

Each QD field location is given a background index that matches the substrate material, which is a good approximation since the QD material has an index very near the homogeneous structure. To ensure that no QD is created within the etched holes of the PC, a mesh order is assigned to the QDs to be the second last material added to the system, with
etching having the final say in the index at an given location (so any QD dipoles within the holes are ignored). This is verified by the index monitor, displayed in Figure 4.6b.

![Figure 4.6: Screen shots from Lumerical’s GUI, where x and y are horizontal and vertical, respectively. (a) Randomly positioned QDs with no NN algorithm, given a density of 5.4e14 m\(^{-2}\). (b) Highlighted QDs (light blue) via index mismatching (which is not be the case when simulations are run) against dark blue etched holes and homogeneous background in red, for a QD sheet density of 5.4e14 m\(^{-2}\). (c) QD set up, located at \(E_y\) along the Yee cell. The QD is effectively the same size as the Yee cell.](image)

One aspect of QDs that cannot easily be directly captured by this FDTD method is the slight variations in size, which ultimately leads to nonuniform emission lines and inhomogeneous broadening. In this way, the overall polarization density of the QD ensemble is due to many different natural frequencies, which is possible to incorporate in our model. The broadened QD spectra is an averaged quantity defined by the individual linewidths of each QD, that are characterized by the temperature of the QDs environment. At room temperature, QDs are dominated by pure dephasing \(\gamma'\), defined as 1.5 THz (or 6 meV) [Borri et al. [2001]], and the overall inhomogeneously broadened spectra is roughly 10 THz (or 40 meV), as shown by the QD ensemble electroluminescence [Semenova et al. [2014]]. Thus, we assign each QD a resonant frequency that is selected randomly from a Gaussian distribution modelled after experimental linewidth of QD electroluminescence. This model is shown in Figure 4.7, where the Gaussian distributions average is zero, and \(\sigma = 6.6\) THz. In this way, both position, and resonant frequency are stochastically modelled.

As a final test of our plugin, we compute the radiative decay experienced by a single QD on resonance with the fundamental frequency of an L5 cavity. Recall from equation
4.4. MODELLING THE OPTICAL PROPERTIES OF SIMPLE QUANTUM DOTS

Figure 4.7: Modelled QD ensemble (dashed and dot-dashed lines) for 10 (green-chain) and 10,000 (magenta-dashed) QDs, for typical room temperature inhomogeneous broadening. The individual QD lineshape is given by the orange (light) line, with $\gamma' = 1.5$ THz. The y-label is a normalized photoluminescence (PL) for individual (solid) and ensembled (dashed or dot-dashed) QDs.

Fermi’s golden rule gives us radiative decay rate as

$$\Gamma(r) = \frac{2}{\hbar \varepsilon_0} \{ \mathbf{d} \cdot \text{Im}[\mathbf{G}(\mathbf{r}, \mathbf{r}; \omega)] \cdot \mathbf{d} \}, \quad (4.14)$$

where $\mathbf{d}$ is the dipole moment and $\mathbf{G}$ is the Green function tensor, with $\mathbf{d}$ pointed in the dominant field direction (in our PC cavities, that is the $y$-direction). This definition of radiative decay assumes we are in 3D space, and our GF has units of inverse volume ($\text{m}^{-3}$), while the dipole moment has units Coulomb meter ($\text{Cm}$), and the overall decay rate has units of inverse seconds ($1/\text{s}$). However, our cavity simulations that include QDs are performed in 2D, thus we have the following problem: modelling a 3D radiative decay lifetimes using a 2D FDTD solver. In equation 4.14, we see that $\hbar$, $\varepsilon_0$, and $\mathbf{d}$ do not change in magnitude from 3D to 2D, and as such, we must introduce a length $l_z$ to help convert $\Gamma_{2D}$ to $\Gamma_{3D}$, since our goal is to model 3D space (and dipoles) as accurately as possible.

The Green function for homogeneous medium $\mathbf{G}^{\text{Hom}}$ allows us to match our 2D decay to an effective 3D rate. In 2D, we derive $\text{Im}[\mathbf{G}^{\text{Hom}}_{2D}] = \frac{1}{8} \frac{\omega^2}{c^2}$ in appendix B, as equation B.23, while in 3D, we derived equation B.12 with the result $\text{Im}[\mathbf{G}^{\text{Hom}}_{2D}] = \frac{n}{6\pi} \frac{\omega^3}{c^2}$. Matching
these GF solutions such that $\Gamma_{2D,\text{FreeSpace}}/l_z = \Gamma_{3D,\text{FreeSpace}}$, we find

$$l_z = \frac{3\pi c}{4n\omega}, \quad (4.15)$$

and the effective 3D radiative decay rate given a 2D GF $\Gamma_{2D,\text{eff}}$, is determined by

$$\Gamma_{2D,\text{eff}}(\mathbf{r}) = \frac{2}{\hbar\epsilon_0}\{\mathbf{d} \cdot \text{Im}[\bar{G}_{2D}(\mathbf{r}, \mathbf{r}; \omega)] \cdot \mathbf{d}\} \frac{4n\omega}{3\pi c}. \quad (4.16)$$

To verify this model works, we scale our QD density $N$ by $l_z$ in equation 4.15, such that $N^{-1} = dx dy l_z$, arriving at $N = 1.743e22$ m$^{-3}$, since $dx = 16.8462$ nm, $dy = 14.5892$ nm, and $\omega = 190$ THz. To test this fit, we follow the procedure outlined in reference [Takeda and John [2011]], where we insert our plugin material to a single Yee cell, and give it an initial polarization to simulate a dynamical decay from a radiation reaction (which is known to give the same decay as from vacuum fluctuations). From this simulation, we find excellent agreement between theory and simulation, where the GF of our cavity simulations are defined using quasi-normal mode (QNM) theory, which shows excellent agreement with numerically exact full-dipole simulations. This is confirmed by comparing the LDOS spectra of both methods, seen in Figure 4.8a.

![Figure 4.8](image-url)

**Figure 4.8:** (a) Fundamental mode comparison between full-dipole expansion and QNM theory for low Q-cavity, seen in (b). The projected LDOS along the $y$ direction (the vertical direction in (b)) has been normalized to represent PF. (b) 2D simulation set up, with a low Q-factor of 430, to avoid strong coupling with a reasonable dipole moment (magnitude). The QD is located at the cavity center.

To initially ensure we are not near the strong-coupling regime (where Fermi’s golden
4.4. MODELLING THE OPTICAL PROPERTIES OF SIMPLE QUANTUM DOTS

rule breaks down), we set up our 2D cavity to have a low Q-factor, by having a shortened PC membrane (compared to the 3D ones) on either side of the cavity edge (seen in Figure 4.8b). Once we have the GF, we insert a single QD PI defined to be the size of a single Yee cell (seen in Figure 4.6c), at the center of the cavity.

To fit our simulations of $\Gamma_{\text{Num}}$ with $\Gamma_{2D,\text{eff}}$, we simply match decay lifetimes as seen in Figure 4.9a. Note, the initial decay of $\rho_{11}$ is nonexponential because its inversion level is positive, thus the electric field emitted grows in magnitude. Once our QD becomes an absorber once more ($\rho_{11} < 0.5$), we have our expected exponential decay shape. Finally, we see in Figure 4.9b, that when we restore our 2D cavities to their usual high $Q$ values (now in the strong coupling regime), we get the semi-classical analogue of vacuum Rabi oscillations.

![Figure 4.9: (a) $\rho_{11}$ dynamics within an L5 low Q-factor ($\approx 400$) PC cavity, seen in Figure 4.8b, solved by MBE without any phenomenological decay terms. The analytic solution is determined by $\Gamma_{2D,\text{eff}}$, calculated by a QNM GF. (b) Comparison of high and low Q cavities for the 2D L5 cavity structure, which were 47,000 and 430, respectively. All other parameters are kept equal in this comparison. In the high Q Case, we observe the remarkable analogue of “vacuum Rabi oscillations”.](image-url)
Chapter 5

Manuscript: Self-consistent Maxwell Bloch modelling of the threshold behaviour of quantum dot photonic crystal cavity lasers

In this chapter, we present our recently completed paper, that will shortly be submitted to Physical Review A: “Self-consistent Maxwell Bloch modelling of the threshold behaviour of quantum dot photonic crystal cavity lasers”, co-authored by Dr. Jesper Mørk at the Technical University of Denmark, and Dr. Stephen Hughes at Queen’s University. Jesper Mørk’s data and analysis paper published last year in Physical Review Letters [Xue et al. [2016b]] motivated the research, and he contributed towards the understanding of the results as well as the limitations of the current rate equation models. Stephen Hughes provided necessary guidance of the theory being implemented, realistic parameters to be used, and carried out various edits to the paper. All versions of the paper and numerical simulations were carried out by William Cartar.

Using the theory outlined in Chapter 2, and numeric techniques described in Chapters 3 and 4, quantum dot ensembles were used to determine the threshold behaviour of PC cavity lasers, of varying lengths. Indeed, much of the previous work in this thesis has lead to the
analysis presented in this chapter. However, the work done in previous chapters is more
general, and can be applied as a model for individual QDs, a few QDs, or an ensemble,
which makes the groundwork done here widely applicable to many future projects. In
demonstrating our ability to connect with experimental data, we hope to encourage further
application of the Maxwell Bloch plugin tool for QD systems.

Finally, in appendix D, additional figures are presented for some claims made in the paper, which were simply taken to be true.

5.1 Abstract

We present a powerful numerical model to investigate QD gain threshold behaviour from
an ensemble of more than 20,000 randomly positioned two-level atoms in photonic crystal
cavities, which are defined by a system of optical Bloch equations (OBEs) that are solved
self-consistently with Maxwell’s equations using a finite-difference time-domain (FDTD)
technique. Phenomenological pure dephasing and incoherent pumping rates are added to
the OBEs to allow for continuous lasing dynamics, but the precise radiative dynamics
of each QD is naturally obtained within the model. These Maxwell Bloch equations are
implemented by Lumerical’s flexible material plugin tool, which allows a user to define
nonlinear polarizations media, that can be added to the standard FDTD method as optical
objects embedded in the existing infrastructure of Lumerical’s FDTD solver. We implement
the gain ensemble within triangular lattice photonic crystal cavities of various length, N
(where N refers to the number of missing holes), with open boundary conditions, and
investigate the cavity mode characteristics and the pump threshold lasing as a function
of cavity length. We develop effective 2D model simulations which are modelled after
studying the passive 3D structures by matching the cavity quality factors and resonance
properties. We also demonstrate how to obtain the correct point-dipole radiative decay
rate from Fermi’s golden rule, which is captured by the FDTD method. Our numerical
simulations predict that pump threshold plateaus around lengths greater than N = 9,
which we identify as a consequence of the radiative dynamics between the QD ensemble.
This behaviour is not expected from simple rate equation analysis commonly adopted in
the literature, but is in qualitative agreement with recent experiments. Single and multi-
mode lasing is observed, depending on the spectral peak of the QD ensemble. We also
investigate the role of structural disorder on both the passive cavity and QD-cavity laser,
where the latter show a general increase in the pump threshold for cavities lengths greater
than $N = 7$. In addition, we show the breakdown of a simple rate equation model and
showcase the generality of our model in its ability to simulate thousands of QDs coupled to
nanophotonic cavity structures with and without structural disorder.

5.2 Introduction

Microcavity photonic crystals (PCs) are a natural advancement to mirror-based feedback
systems as many technologies continually shrink to the nanoscale. In 1989, the vertical
cavity surface emitting laser (VCSEL) was demonstrated [Jewell et al. [1991]], with a host
of applications in telecommunication systems, optical interconnects, spectroscopic sensing
and optical image processing. In 1994, Dowling et al. proposed a 1D PC operating near the
photonic band edge [Dowling et al. [1994]], making use of slow light modes to increase the
power emitted by these lasers—which had been one of the limitations of microcavity lasers
[Droulias et al. [2014]]. Experimentally, slow-light band edge lasers have been demonstrated
in both 2D [Meier et al. [1999]; Imada et al. [1999]; Riechel et al. [2000]; Ryu et al. [2002];
Kwon et al. [2003]; Wu et al. [2004]; Raineri et al. [2005]; Karnutsch et al. [2007]; Luo et al.
[2009]], and 3D [Xue et al. [2016b]; Cao et al. [2002]; Park et al. [2004]] architectures, while
over the past decade, significant progress has been made in the optimization of these lasers
[Park et al. [2004]; Noda et al. [2006]; Atlasov et al. [2009]; Matsuo et al. [2010]], allowing
for the investigation of new operation regimes such as single emitter lasing [Nomura et al.
[2010]] and ultrahigh speed modulation [Mørk et al. [2014]]. Many VCSELs now use 2D
PC arrays to improve the vertical power output and overall efficiency.

To directly model the optical properties of open-system microcavity structures, finite-
difference time-domain (FDTD) analysis is often employed, since open cavities support
quasi-normal modes that have a finite lifetime due their coupling to a continuum of modes
with outgoing boundary conditions [Kristensen and Hughes [2013]]. Quasinormal modes
are the mode solutions to the Helmholtz equation with open boundary conditions [Ching
et al. [1998]], resulting in a complex eigenfrequency for each cavity mode. To numerically model a gain medium within the cavity, various techniques have been implemented ranging from the simple inclusion of a negative imaginary component in the refractive index [Fujii et al. [2012]], to including rate equations embedded in the FDTD algorithm [Droulias et al. [2014]; Shi and Prather [2007]; Fang et al. [2010]], or finite element method [Fietz and Soukoulis [2012]]. It is also common to adopt simple rate equations for the population density of carriers and photon flux [Prieto et al. [2015b]; Altug and Vučković [2005]], which can quickly connecting to experimental data. It is, however, a major challenge to model arbitrarily shaped gain materials coupled to arbitrarily shaped cavity structures, which is desired for many quantum dot (QD) microcavity structures, especially as the modal properties of the laser cavity change drastically as a function of position (which results in spatially dependent radiative decay dynamics). Semiconductor QDs are increasingly used as the underlying gain material in microcavity lasers, due to their superior room temperature operation [Bimberg and Pohl [2011]], tunability [Schliwa et al. [2014]], unique atom-like density of states and carrier dynamics [Markus et al. [2003]], and excellent temporal and spatial stability [Borri et al. [2001]; Bimberg and Pohl [2011]]; to develop a theoretical model of the light-matter interactions, one would like to model their collective gain more appropriately as an ensemble of effective two-level atoms (TLAs) [Stievater et al. [2001]; Zrenner et al. [2002]; Reithmaier et al. [2004]].

The simplest implementation of a TLA coupled to electromagnetic fields is achieved with the optical Bloch equations (OBEs), which add linear and nonlinear interactions between the dipole-induced polarization and electric field, giving rise to the Maxwell-Bloch (MB) equations when combined with the Maxwell equations. Using an effective TLA, positive populations inversion can be achieved, e.g., by a phenomenological incoherent pump rate that mimics ultrafast relaxation rates from higher lying level to the lasing exciton state, thus eliminating the need for additional energy levels (that can be effectively adiabatically eliminated). This simple model of an artificial atom gain, implemented with the full Maxwell equations, has the distinct benefit of allowing researchers to study general light-matter interactions without using either of the rotating-wave approximation or slowly-varying-envelope approximation, which have already lead to a number of new effects such as the dynamic nonlinear skin effect [Forysiak et al. [1996]] and carrier-wave Rabi flopping [Hughes
even using simple 1D equations of motion. Moreover, when studying quantum information systems that are dominated by radiative decay, it is critical to preserve the coherent radiative contributions that a MB analysis provides [Takeda and John [2011]], without recourse to adding in phenomenological damping constants. Otherwise, if non-radiative processes dominate, a more straightforward MB formalism may be used, in which phenomenological damping terms like pure dephasing are implemented [Ziolkowski et al. [1995]; Slavcheva et al. [2002]].

In many nanophotonic cavity structures, it is critical to go beyond 1D models and simple rate equation analysis; in addition, many of the decay processes are affected by unavoidable fabrication disorder, even with state-of-the-art manufacturing techniques, and these minute levels of disorder can play a role in understanding the rich physics of slow light systems [Hughes et al. [2005]; Mazoyer et al. [2009]; Patterson et al. [2009]; Le Thomas et al. [2009]; Sapienza et al. [2010]; O’Faolain et al. [2010]; Liu et al. [2014b]]; indeed, it is even possible for disorder to be added extrinsically (i.e., deliberately) to a system to gain access to novel effects such as reduced laser thresholds in random laser systems [Fujii et al. [2012]], brought on by Anderson localization [Anderson [1958]] (i.e., isolated modes due to multiple scattering events that randomly localizes the mode instead of scattering the light out of the PC). Modelling such features in the presence of gain is clearly a major computational challenge.

With this current trend of miniaturized semiconductor laser systems, there is now a need for more sophisticated models of PC lasers beyond the simple rate equation picture [Prieto et al. [2015b]; Altug and Vučković [2005]], where the emitters’ coherence is assumed to be in steady-state or adiabatically eliminated, leading to coupled equations between the available energy levels without any information regarding the system coherence. In many cases, this may fail to describe emerging experiments. For example, a recent investigation of lasing threshold as a function of band-edge proximity, performed by increasing a triangular lattice PC cavity length, found counter intuitive results [Xue et al. [2016b]]: rather than a decreasing gain threshold for increasing cavity length, which is predicted by simple laser theory, there existed a threshold minimum around the L8-L9 cavities, where LN denotes a cavity of length N (missing holes in the lattice), and cavity lengths ranging from L3-L20 where created. These cavities have fundamental modes (M1, M2, ...) confined within the
5.2. INTRODUCTION

Figure 5.1: Top down view region of an L5 (a) and L7 (b) PC slab cavities. (c) First fundamental mode (M1) profile $|E(r)|$, inside an L5 cavity, computed by 3D FDTD simulations. The circle outlines where etched holes exist within the homogeneous background material, which has an index of refraction of $n = 3.17$ in 3D simulations. The two white lines in the $x-z$ spatial profile represent the characteristic length $l_{z,V}$ we use to relate 2D mode volumes to 3D calculations (see Sec. 5.3). The slab has properties of lattice pitch $a = 438$ nm, radius $r = a/4$, and height $h = 250$ nm. The mode profile measured at the center of the 3D slabs (in the $z$-direction) is very similar to an effective 2D mode profile with the same properties, except $n = 2.54$ (see text).

cavity region, as shown in Fig. 5.1c for an L5 cavity. In the theoretical analysis of a 2D square based PC microcavity laser, a similar trend is observed, but only for systems with low optical density of states (DOS) [Droulias et al. [2014]]. Since the DOS of band-edge cavities are so high, the results of Ref. [Xue et al. [2016b]] were partly explained by a heuristic model of disorder-induced backscattering and out scattering of the Bloch mode into modes above
the light line (which is known to occur in longer length PC waveguides). In such a model, disorder shifts some of the lasing mode near the band-edge into the regime where it is no longer confined to the cavity structure, and this shift is felt more strongly by longer cavity modes (thus slower light is more sensitive to disorder), which exist deeper in the slow-light regime, thus creating an optimal pump threshold by minimizing both reflection losses, and backscattering losses. To model a PC “cavity mode” as a Bloch mode, one assumes that there is a trapped W1 Bloch mode inside an effective Fabry-Perot (FP) resonator, where the cavity edges model reflective mirrors. This modelling technique has had good agreement between theory and experiment for cavities down to a single hole [Sauvan et al. [2005]], and has been used to optimize the Purcell factors of various cavity configurations [Lalanne and Hugonin [2003]]. However, in Refs. [Sauvan et al. [2005]; Lalanne and Hugonin [2003]], Bloch modes are used to analyze the quality factor ($Q$) and effective mode volumes ($V_{\text{eff}}$) of cavities, while Ref. [Xue et al. [2016b]] modelled the lasing characteristics of their cavity modes. In Ref. [Xue et al. [2016b]], a simple FP model is employed and theoretical trends generally match experimental data; however, the disorder parameters required to achieve this fit were not related to the measured disorder of the structures, and it is not known if the models of disorder-induced scattering in PC waveguides are appropriate for smaller LN cavity structures, which are in general quite robust to disorder unless they have extremely high quality factors. It is also not really known to what extent one can adopt simple rate equation analysis for lasers structures that couple complex PC cavity modes to an ensemble of QDs, where there is clearly a nonuniform profile for gain and radiative dynamics, as well as a variety of potential cavity modes involved in the light-matter interactions. It is not known to what extent one can use the passive ($Q$) as input for a realistic laser model in such structures.

In this paper, we present a systematic numerical study of a QD ensemble in triangular lattice PC cavities, and explore the lasing threshold behaviour as a function of PC length as well as explore the role of structural disorder on the PC cavity modes. We closely follow the designs and recent experiments of Xue et al. [Xue et al. [2016b]], and explore the role of disorder on lasing threshold in PC cavities, which were credited to be likely responsible for the unusual gain threshold dependence on cavity length. Our results provide fresh insights into these observations. Using Lumerical’s FDTD material plugin tool,
which allows a user to include unique polarizations in simulation objects [Lumerical], we investigate the gain and lasing behaviour of effective 2D cavity laser structures, modelled after full passive 3D simulations. Though we use Lumerical FDTD, the general technique can naturally be adopted with any general FDTD solver. The user-controlled plugin tool returns MB dynamics by solving the OBE (for each QD), and includes radiative decay and QD-QD coupling that is captured by the FDTD method, as well as pure dephasing included as a phenomenological decay rate, and an incoherent pump term which effectively models a 3-level gain system for each QD. The OBE plugin has the distinct advantage of being completely general, solving lasing dynamics with zero a priori knowledge (other than inherent properties of the QDs), when compared to traditional rate equations. Indeed, we are able to easily model more than 20,000 unique QDs in a self-consistent way. Rate equations are a reasonable starting point to fit experimental data that occurs on time scales much longer than relaxation times [Prieto et al. [2015b]; Altug and Vučković [2005]], but they do not account for the coherent nature of a QD gain ensemble. To accurately model lasing in a time dependant simulation, one is reliant on building up the lasing mode with as few assumptions as possible, to ensure the system evolves naturally. Our polarization plugin is able to capture a wide range of complex effects described by a TLA, such as self-induced transparency, pulse-reshaping, mode pulling, power broadening, and hole burning. In addition, because the plugin is implemented in FDTD, it is able to model QDs by existing only on individual Yee-cells, which are defined to have similar dimensions to experimental QDs [Semenova et al. [2014]]. Both single-mode, and multi-mode lasing is found to exist within these cavities, and in general, we find a plateauing of the pump threshold around L9, for the single-cavity laser. These simulations are compared to a single plugin material modelling the QD ensemble with inhomogeneous broadening and pure dephasing, characterized by the same distribution used to select the QDs center frequency. The plateauing behaviour is diminished when we use a “sheet” of gain material, demonstrating the importance of nonuniform gain coupling. The role of radiative decay, which is captured self-consistency by the MB approach, is also probed by including a (dominant) phenomenological decay rate to the OBEs, which is clearly shown to destroy the plateauing nature of the pump threshold all-together, showing the need to have a multi-QD self-consistent solution with as few assumptions as possible. Fabrication disorder is also modelled and is found to slightly
increase the pump threshold for cavities greater than $L_7$. Finally, we briefly study the cre-
ation of localized modes via increasing the amount of disorder beyond what would normally be found due to manufacturing imperfections.

The remainder of our paper is organized as follows: In Sec. 5.3, we introduce the cavity specification and model the basic cavity properties of the 2D simulations after obtaining the results for passive 3D (slab) structures. In addition, we investigate the role of fabrication disorder, and model 2D after 3D simulations once more. In Sec. 5.4, we introduce our OBEs, and discuss their implementation within the plugin tool as a source for nonlinear polarization. In Sec. 5.5, we discuss the dipole moment used in our simulations and explain how to obtain the correct radiative decay of a point dipole in a 2D model. In Sec. 5.6, we discuss the implementation of QDs in the FDTD method, and model our radiative decay after 3D values by including a characteristic length $l_z$. In Sec. 5.7, we outline and discuss the results of including an active QD ensemble (which include $14,000 - 24,000$ randomly positioned QDs) to various cavity lengths, extracting pump thresholds, and investigating different models of the plugin. We also connect our results to recent experiments of Xue et al. [Xue et al. [2016b]], and provide fresh insights into the gain threshold dependence on cavity length. Finally, we summarize in Sec. 5.8.

5.3 Passive Cavity Simulations: Effective 2D Simulations and Role of Fabrication Disorder

Full 3D simulations of passive PC slab structures (i.e., with no gain material) are an appropriate starting point to model planar PC slabs with no QDs, as they produce the same mode characteristics and allow for additional measurements such as $Q$, $V_{\text{eff}}$, and LDOS at any point in the cavity structure. However, 2D simulations take significantly less time to run, and can be modelled after 3D simulations to capture PC slab modes with similar peak properties, such as mode frequency (shown in Fig. 5.2a) and $Q$-factors (studied later), at a fraction of the computational cost (see Fig. 5.2b). This is important for developing effective 2D models for the full Maxwell-OBEs with gain materials and thousands of OBEs (i.e., one OBE set for each QD). It should also be noted that Fig 5.2b is obtained for passive simulations only, and to accurately include QD dipoles in our simulation, we require a finer
5.3. PASSIVE CAVITY SIMULATIONS: EFFECTIVE 2D SIMULATIONS AND ROLE OF FABRICATION DISORDER

spatial mesh of more than twice what is used in passive simulations. As such, the simulations performed with a QD ensemble require significantly longer to run than is represented in Fig. 5.2b, so that the lasing dynamics may eventually reach steady state (SS). For example, each of our 2D L15 lasing simulations (shown below) takes roughly 20 hours to run, given 16 cores are used with 1024 Mb of memory. This increased run time is roughly 400 times the passive simulations shown in Fig. 5.2b. As such, we chose to develop an effective 2D FDTD method when using the OBEs, which makes it easier to carry out a systematic sweep of various system parameters such as cavity length and pump powers, especially for high $Q$ cavity modes which take a long time to reach SS.

(a) Cavity mode frequencies

(b) Quality factor of M1

Figure 5.2: Passive cavity simulations for an LN cavity in a triangular PC cavity with lattice pitch $a = 438$ nm, radius $r = a/4$, height $h = 250$ nm (in 3D), and refractive index $n = 3.17$ or 2.54 for 3D and 2D simulations respectively. (a) Comparison of the fundamental mode’s peak frequency as a function of cavity length, for 2D and 3D simulations, with experimental data points from [Xue et al. [2016b]] for reference. (b) Run time requirements using 16 cores with 1024 Mb of memory, for a single passive 2D or 3D simulation, without QD mesh requirements, as a function of cavity length (see text).

In order to introduce an accurate effective 2D cavity simulations similar to the PC cavity experiments of Xue et al. [Xue et al. [2016b]], we first capture the basic cavity physics using passive 3D slab simulations. The cavities are made of InP, with a standard hexagonal latticed PC cavities, without any hole shifts or modifications to optimize the cavity $Q$. The lattice pitch is $a = 438$ nm, with hole radius $r = a/4$, slab height $h = 250$ nm, and refractive index $n = 3.17$ [Xue et al. [2016b]]. The PC bandgap (TE-like) is roughly 185-215 THz, and the QDs are made of InAs. Our simulations are run using Lumerical’s [Lumerical] FDTD
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software, with open boundary conditions via perfectly matched layers (PMLs).

An LN cavity refers to a cavity of length N, where an L5 cavity is displayed in Figs. 5.1c and 5.3b. We simulate cavity lengths ranging from L5-L15 skipping even cavity lengths, and measure the resulting Q-factors for all fundamental modes observed in the simulations. The cavity modes are excited by a dipole source defined by a fixed carrier frequency with a Gaussian envelope, located along the center axis of the cavity, shifted off the central y-axis to avoid emitting at the anti-node of even cavity modes (i.e., M2, M4, etc.). To capture the modal properties of each cavity, two simulations are run; the first simulation uses an electric-field time monitor to measure the first few dominant modes eigenfrequency \( \tilde{\omega}_\mu = \omega_\mu - i\Gamma_\mu \), where \( \omega_\mu \) is the peak frequency, and \( \Gamma_\mu = \frac{\omega_\mu}{2Q_\mu} \) is defined by the modes broadening and the cavity quality factor Q; the second simulation measures each modes spatial profile \( \tilde{f}(r) \) using a discrete-Fourier transform (DFT) monitor. Typically, 3-5 modes are measured in the frequency range of interest, depending on the cavity length—as longer cavities have stronger higher order modes, and more frequencies within the simulations bandwidth.

Using the cavity mode profiles and their corresponding eigenfrequencies, we calculate the cavity Green function (GF) using a quasi-normal mode (QNM) expansion [Ge et al. [2015]]

\[
G(r, r'; \omega) = \sum_\mu \frac{\omega^2 \tilde{f}_\mu(r) \cdot \tilde{f}_\mu(r')}{2\tilde{\omega}_\mu(\tilde{\omega}_\mu - \omega)}, \tag{5.1}
\]

where \( \mu \) uniquely identifies each mode, and the modes are normalized by [Kristensen et al. [2012]]

\[
\langle \tilde{f}_\mu | \tilde{f}_\mu \rangle = \lim_{V \to \infty} \int_V \epsilon_r(r) \tilde{f}_\mu(r) \cdot \tilde{f}_\mu(r) dr + i \frac{c}{2\tilde{\omega}_\mu} \int_{\partial V} \sqrt{\epsilon_r(r)} \tilde{f}_\mu(r) \cdot \tilde{f}_\mu(r) dr = 1, \tag{5.2}
\]

where \( \epsilon_r(r) \) is the relative permittivity of the cavity, and \( \partial V \) denotes the border of volume \( V \), in the limit \( V \to \infty \) [Kristensen et al. [2015]]. With the normalized modes, we are able to calculate accurate mode volumes [Kristensen et al. [2012]], which are defined as

\[
V_{\text{eff}}^{-1} = \text{Re} \left\{ \frac{\epsilon_r(r_c) \tilde{f}_c^2(r_c)}{\langle \tilde{f}_c | \tilde{f}_c \rangle} \right\}, \tag{5.3}
\]

where \( r_c \) is an antinode point of interest within the cavity structure. Having the GF defined...
at all locations of \( r \), and \( r' \), allows us to plot the LDOS at any location (i.e., without having to do further dipole calculations), and normalizing by the free space GF defines the projected LDOS to have units equivalent to the Purcell Factor (PF), defined as [Yao et al. [2010]]

\[
PF = \frac{3}{4\pi^2} \left( \frac{\lambda}{n} \right)^3 \frac{Q}{V_{\text{eff}}} \tag{5.4}
\]

where \( \lambda \) is now wavelength, and the \( Q \) measurement is for the resonant mode of interest. This value assumes a dipole at the optical coupling point of the cavity mode, perfectly matched to the field maximum and polarization.

Next, to identify the role of fabrication or structural disorder on the passive 3D structures, we model intrinsic fabrication disorder by shifting the center of each hole by a random amount \( \Delta r \) characterized by the standard deviation \( \sigma_{\text{Dis}} \) of a random number generator. The direction of each hole’s shift is also randomized, by defining a random number between \([-\pi, \pi]\), thus giving equal probability for a shift in any direction. Figure 5.3b depicts an exaggerated disorder instance for an L5 cavity. The PC’s required numerical size (to mimic an infinite PC system) was determined by increasing the simulation’s spatial size until the largest (dominant) \( Q \)-factor’s value converged, and the simulation size increased as the cavity length increased to prevent spurious \( Q \)-factor measurements. The intrinsic disorder is set to be \( \sigma_{\text{Dis}} = 0.005a \), as determined from experimental far-field intensity spectra compared to FDTD simulated spectra for varying amounts of disorder [Mann et al. [2015]]. Figure 5.3a depicts the measured \( Q \)-factors of 20 instances of disorder at each cavity length, showing the impact of disorder is very minimal at smaller cavity lengths, and impacts the L15 \( Q \)-factor by about 15%. These disordered statistics are consistent with the other findings of similar PC cavity investigations [Minkov et al. [2013]], for the same range of \( Q \).

Given the measured eigenfrequencies and mode volumes for passive 3D simulations, effective 2D simulations are subsequently optimized to closely match the \( Q \)-factor, mode volume, and peak frequency spread of the full 3D simulations. Firstly, the 2D simulations use an effective refractive index of \( n = 2.54 \) to shift the peak frequencies to match the 3D simulations, which used \( n = 3.17 \). Fitting this effective refractive index optimized both the location, and separation between the first and second fundamental modes M1 and M2, respectively, so that any mode coupling affects would be representative of their 3D counterparts. This is mainly why Fig. 5.2a is not simply an optimized overlap between
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2D and 3D simulation trends. In addition, to account for the leakage that occurs in 3D simulations (in that case through vertical decay), the size of the 2D PC in the $x$-direction was set to allow cavity decay that was similar to the 3D leakage. This can be seen in Fig. 5.4a, where the 2D and 3D $Q$-factors are compared. In Fig. 5.4b, we compare 2D and 3D mode volumes, which requires a characteristic length scale $l_{z,V}$ to convert the 2D mode area $A_{\text{eff},2D}$ into a volume $V_{\text{eff},2D} = l_{z,V} \cdot A_{\text{eff},2D}$. This length scale is chosen to be 205 nm (see Fig. 5.1c in Sec. 5.2), which is slightly less than the height of the 3D PC cavities. We chose this length scale as it gave a reasonable $Q/V_{\text{eff}}$ fit, as shown in Fig. 5.4c, while also containing the majority of the 3D mode’s volumes (more than 85%). A larger characteristic length would have diminished the $Q/V_{\text{eff}}$ fit, while a shorter length would sacrifice meaning in 3D (e.g., less of the 3D M1 mode volume’s would actually exist within that characteristic length). Given the complexity of the calculations that follow, this seems a reasonable method of introducing an appropriate 2D model.

To appropriately model fabrication disorder in the effective 2D model, we compared the statistical average and variance of the L15’s 3D simulation to varying amounts of disorder...
for the corresponding 2D simulation. Taking the normal definition of our $Q$-factor to be $Q = \frac{\omega}{\Gamma}$, we can capture the disorder statistics using $\Gamma$, as $\omega$ is roughly constant with increasing disorder. Defining $\Gamma = \Gamma_0 + \Gamma_{\text{Dis}}$, where $\Gamma_0$ is the ideal structure’s broadening and $\Gamma_{\text{Dis}}$ is additional broadening due to structural disorder, we plot $\langle \Gamma_{\text{Dis}}/\Gamma_0 \rangle$ for the 3D data collected in Fig. 5.3a and compare it to 100 instances of 2D simulations with $\sigma_{\text{Dis}} = [0.0025, 0.005, 0.01, 0.02]$ (400 simulations total), seen in Fig. 5.4d. In our 2D simulations, intrinsic disorder is seen to be best modelled by $\sigma_{\text{Dis}} = 0.01a$.

(a) $Q$ versus PC length  (b) $V_{\text{eff}}$ versus PC length  (c) $Q/V_{\text{eff}}$ versus length  (d) Disordered broadening

![Figure 5.4: (a-c) $Q$ and $V_{\text{eff}}$ modelling of effective 2D system compared to full 3D simulations, without disorder. (d) Disorder statistics of $\Gamma_{\text{Dis}} = \Gamma - \Gamma_0$, for the L15 cavities of varying amounts of 2D disorder, referenced to the 3D intrinsic disorder of $\sigma_{\text{Dis}} = 0.005a$.](image)

5.4 Effective Two-Level Atom Model and Polarization Plugin Equations

We now describe a simple effective gain model for typical experimental QDs [Semenova et al. [2014]]. To achieve this, we assume QDs are well described as effective TLAs, where the physics of higher order energy levels is effectively ignored (or adiabatically eliminated), and we use an incoherent pump term $P$ to create a positive population inversion and thus gain. To derive the OBEs, we use a quantum master equation to solve for the density matrix of a TLA, and treat the electromagnetic field classically. Starting with the system Hamiltonian of a TLA, with a dipole moment $d$ defined by a ground state $|0\rangle$, and excited state $|1\rangle$, with energy difference, $\omega_0$, and interacting with an electromagnetic field $E$, we have the system
5.4. EFFECTIVE TWO-LEVEL ATOM MODEL AND POLARIZATION PLUGIN EQUATIONS

Hamiltonian

\[ \mathcal{H} = \frac{\hbar \omega_0}{2} \sigma_z - \hbar \chi(t)(\sigma^+ + \sigma^-), \]  

(5.5)

where \( \chi(t) = \frac{d(t) \cdot E(t)}{\hbar} \) describes the field interaction with the dipole moment, \( \sigma_z \) is the usual Pauli matrix, and \( \sigma^+ \) and \( \sigma^- \) are the raising and lowering operators of our TLA, respectively. The electric field \( E(t) \) is solved self-consistently by FDTD, while \( d \) and \( \omega_0 \) are set by the material plugin equations, which solve the OBEs derived from the quantum master equation of this Hamiltonian. Since our QDs of interest are modelled at room temperature, the dominant source of damping is due to non-radiative processes, in particular pure dephasing. The dissipative nature of our QDs environment is included phenomenologically using Lindblad superoperators, \( L \), defined to operate on our density matrix as \( L(\mathcal{O})\rho = \mathcal{O}\rho\mathcal{O}^\dagger - \frac{1}{2}(\mathcal{O}^\dagger\mathcal{O}\rho + \rho\mathcal{O}^\dagger\mathcal{O}) \). Traditionally, when a TLA interacts with degrees of freedom such as photons, phonons, other collective modes, molecular vibrations, rotations, and translations, it experiences a broadening of its absorption linewidth directly proportional to the total dephasing rate [Skinner and Hsu [1986]]. This broadening has two main contributions in QDs, an inherent relaxation rate \( \Gamma_R \) determined by the TLA’s environment \( (\Gamma_R^{-1} \propto Q/V_{\text{eff}}) \) captured by the FDTD method at all positions, and a pure dephasing rate \( \gamma' \) which is related to the temperature, and to coupling to lattice vibrations in the solid (phonons), and charge noise. We add pure dephasing phenomenologically to our system Hamiltonian via the Lindblad superoperator \( \gamma'\mathcal{L}(\sigma^+\sigma^-) \).

To achieve positive population inversion, we include the Lindblad term \( \mathcal{P}\mathcal{L}(\sigma^+) \), which is responsible for incoherently pumping the excited QD lasing state. In the usual way, we use the quantum Liouville equation \( \dot{\rho} = -\frac{i}{\hbar}[\mathcal{H},\rho] \) with the Lindblad terms to derive equations of motion for the density matrix. The master equation is now given by

\[ \frac{d\rho}{dt} = -\frac{i}{\hbar}[\mathcal{H},\rho] + \mathcal{P}\mathcal{L}(\sigma^+)\rho + \gamma'\mathcal{L}(\sigma^+\sigma^-)\rho, \]  

(5.6)

where \( \rho \) is a \( 2 \times 2 \) matrix with diagonal elements \( \rho_{11} \) and \( \rho_{00} \) associated with the probabilities of being in the excited and ground states, respectively, and off diagonal elements \( \rho_{01} = \rho_{10}^* \) associated with the system’s coherence. We define inversion as \( \rho_{11} - \rho_{00} = 2\rho_{11} - 1 \), since \( \rho_{11} + \rho_{00} = 1 \). Solving Eq. (5.6), we find equations of motion for \( \rho_{11} \) and \( \rho_{01} \) given by

\[ \frac{d\rho_{11}}{dt} = -2\chi\rho_{01}^m + P(1 - \rho_{11}), \]  

(5.7)
5.4. EFFECTIVE TWO-LEVEL ATOM MODEL AND POLARIZATION PLUGIN EQUATIONS

\[
\frac{d\rho_{01}^{Re}}{dt} = -\omega_0\rho_{01}^{Im} - \frac{P + \gamma'}{2}\rho_{01}^{Re},
\]

(5.8)

\[
\frac{d\rho_{01}^{Im}}{dt} = \omega_0\rho_{01}^{Re} - \frac{P + \gamma'}{2}\rho_{01}^{Im} + \chi(2\rho_{11} - 1),
\]

(5.9)

where we have separated \(\rho_{01}\) into its real \(\text{Re}[\rho_{01}] = \rho_{01}^{Re}\) and imaginary \(\text{Im}[\rho_{01}] = \rho_{01}^{Im}\) parts, thus leaving us with three coupled equations with only real parameters (per QD); this is done for numerical convenience. Together, these equations define the optical Bloch equations (OBEs) which describe the quantum nature of an effective TLA interacting with a completely general classical electric field via FDTD. This formalism ignores a small frequency shift from the self-field of the emitter, which arises due to the numerically divergent in-phase contribution at the location of the emitter [Schelew et al. [2016]], though this has no influence on our findings with eventual random center frequencies for each QD emitter.

In deriving Eqs. 5.7-5.9, note that we have not made any approximations other than those defined by the model itself (i.e., only two energy levels). This is unusual compared to standard textbook derivations [Milonni and Eberly [2010]; Allen and Eberly [2012]], which often invoke a rotating-wave approximation; however, this is done as a result of assuming some form for the electric field, whereas we have not assumed any information regarding our quickly varying electric field. Instead, we leave our OBEs completely general, such that the FDTD algorithm captures the light-matter physics experienced by our TLA in a self-consistent way, including radiative decay and dipole-dipole interactions between different QDs. To include the OBE in the FDTD simulations, we use Lumerical’s user-defined-material plugin tool [Lum], which allows for the creation of customized material responses, written in C++. The plugin code is called at each time step \(n\), and is used to update the electric field \(E^n\) by the polarization density \(P^n\) output by the plugin script. In general, this is written as

\[
U^n E^n + \frac{P^n}{\epsilon_0} = V^n,
\]

(5.10)

where \(U^n\) and \(V^n\) are inputs provided by Lumerical’s software, and \(E^n\) is updated along the \(x, y, \) and \(z\) axes.

To determine the polarization density \(P\) output by our OBEs, we use \(p = \epsilon r(\rho_{01} + \rho_{01}^* ) = \epsilon r(2\Re[\rho_{01}]) = \epsilon r(2\rho_{01}^{Re})\).
5.5 DIPOLE MOMENT MODEL AND OBTAINING THE CORRECT RADIATIVE DECAY FROM A DIPOLE

2erRe[ρ₀₁], such that the polarization density $P = Np$, is

$$P = 2dNRe[ρ₀₁], \quad (5.11)$$

where $er = d$ is the dipole moment associated with our atom, which assumes our dipole moment is equally strong in all directions; while $N$ is the relevant density of the QD being polarized, defined by

$$N = V_{QD}^{-1} = δ(z - z')/(ΔxΔy), \quad (5.12)$$

where $V_{QD}^{-1}$ is the inverse QD volume, and $Δx, Δy$ are the Yee cell dimensions of the FDTD simulation. Finally, to implement the OBEs numerically, we use the 4th-order Runge-Kutta method, thus storing only the previous time step values $ρ^{n}_{11}, ρ^{Im,n}_{01}$ and $ρ^{Re,n}_{01}$, when updating $ρ^{n+1}_{11}, ρ^{Im,n+1}_{01}$ and $ρ^{Re,n+1}_{01}$, and $P^n$ using Eq. 5.11.

5.5 Dipole Moment Model and Obtaining the Correct Radiative Decay from a Dipole

In the dipole approximation, where we assume that interacting electromagnetic fields have negligible variation over each quantum emitter, we define the oscillator strength $F(ω)$ of the InAs QD, as $F(ω) = Γ_{rad, hom}(ω)/Γ_{HO}(ω)$ [Stobbe et al. [2012]], where $Γ_{rad, hom}(ω)$ is the homogeneous medium’s radiative decay rate, which includes information about the excitonic degrees of freedom, and $Γ_{HO}(ω)$ is the radiative decay rate of a classical harmonic oscillator of elementary charge. This approximation is valid because of the small size of QD used, $\sim 15$ nm in diameter (and a few nm in height) [Semenova et al. [2014]]. In Ref. [Stobbe et al. [2012]], they show that $F(ω)$ is proportional to independent electron and hole envelope function $F_{e}(r_{0}, r)$, and $F_{h}(r_{0}, r)$, respectively, in the strong confinement regime, given by

$$F(ω) = \frac{E_p}{ℏω} \left| ∫ dF_e(r_0, r)F_h(r_0, r) \right|^2, \quad (5.5)$$

where $E_p$ is the Kane energy of the QD material. The wave function overlap $I_{WF} = \left| ∫ dF_e(r_0), rF_h(r_0, r) \right|^2$, is a relatively constant function with respect to QD size, and is mainly dependant on the emission energy of the QD [Stobbe et al. [2011]]. A QD emitting at 190 THz is about 0.79 eV, which has an electron-hole overlap $I_{WF} > 0.8$ [Stobbe et al. [2011]]. In addition, the Kane energy of bulk InAs to be 21.11 eV [Rosencher and Vinter [2002]]. Thus we assume QDs with an oscillator strength of roughly
17.2 when assuming a wave function overlap of 80%.

The strength of the dipole moment \( d \) of our modelled QDs can be calculated directly by the oscillator strength, given by [Andreani et al. [1999]]

\[
d^2 = \frac{e^2 \hbar}{2m\omega} F,
\]

(5.13)

where \( e \) is the elementary charge, and \( m \) is the free electron mass. Using our oscillator strength \( F = 17.2 \), we calculate a dipole moment of 43.88 D (or 0.91 \( e \)-nm).

### 5.6 Quantum Dot Modelling and Simulation Set Up

To model QDs in FDTD, the TLA plugin is implemented at a single Yee cell point with area equal to the Yee cell. We choose to implement QDs at \( E_y \) field points, seen in figure 5.5a, as our cavity modes primarily exist in this direction. To better model the QD dimensions, we reduce the mesh steps \( \Delta x, \Delta y \) to 16.85 and 14.59 nm, respectively, which is asymmetric to maintain uniform meshing across all etched holes (in a triangular lattice). The QDs are then added to our gain region randomly, with an area density \( N_{QD} \). The only restriction placed on the QD locations is that no two QDs may be side-by-side. Each QD field location is given a background index that matches the substrate material, which is a good approximation since the QD material has an index very near the homogeneous structure. To ensure that no QD is created within the etched holes of the PC, a mesh order is assigned to the QDs to be the second last material added to the system, with etching as the final material, added over-top all previous index.

An example simulation set up is shown in Fig. 5.5b, which has the following simulation features: a time monitor at its center, an index and a DFT-monitor around the cavity in yellow (inner rectangle) to capture the electric field profiles, a gain region made as small as possible (e.g., the smallest region with the same steady-state output as larger gain regions) to save meshing overhead, an incident plane wave pulse on the left, a power line monitor on the right, and PML boundary conditions all around. The plane wave is angled slightly to excite \( E_x \) and \( E_y \) field components, and the power line monitor only captures the last 10 ps of power emitted by the cavity. This is consistent across all cavity lengths simulated, while the time each cavity simulation is run for is determined by how long it takes to reach
steady-state lasing.

Since QD materials have a large fluctuation in the QD emission frequencies, each QD has its energy spacing $\omega_0$ randomly drawn from a normal distribution to better represent slight variations in the QD size that occurs in practice. Thus, non-uniform emission lines lead to inhomogeneous broadening, which can be modelled with parameters obtained from experimental data. At room temperature, InAs QDs are dominated by pure dephasing $\gamma'$, typically around 1.5 THz (or 6 meV) [Borri et al. (2001)], and the overall inhomogeneously broadened spectra is roughly 10 THz (or 40 meV), as shown by the QD ensemble electroluminescence in Ref. [Semenova et al. (2014)]. Thus, we assign each QD a resonant frequency that is selected randomly from a Gaussian distribution modelled after experimental linewidth of QD electroluminescence. This model is shown in Fig. 5.6a, where the Gaussian distributions variance is 6.6 THz, with mean $\omega_0$. In this way, both QD position, and resonant frequency are stochastically modelled.

To further connect our 2D simulations to the 3D dipole interactions, we first model

![Figure 5.5: (a) Quantum dots located at $E_y$ along the Yee cell, randomly positioned with no nearest-neighbours, with a density of 540 $\mu$m$^{-2}$. The grid dimensions are $dx = 16.8462$ nm and $dy = 14.5892$ nm, while the QD size is made smaller than this to emphasis its location at only a single grid point; however, its size is effectively $dx \cdot dy$. (b) Quantum dot gain set up: the orange boarder is PML boundary conditions, the grey bar on the left is the initial source pulse, which stimulates the optically pumped QD gain region in the center, the yellow rectangle denotes the index and DFT-monitors, the yellow cross is a time monitor, and the orange line on the right is a power line monitor that captures the average power out of the cavity, over the last 10 ps. The total number of QDs in this particular simulation is 14,029 (for reference, L15 simulations have $\approx 24,000$ QDs).](image)
radiative decay using Fermi’s golden rule in 3D, which is well known to be [Novotny and Hecht [2012]]

\[
\Gamma(\mathbf{r}) = \frac{2}{\hbar\epsilon_0} \{ \mathbf{d} \cdot \text{Im}[\mathbf{G}(\mathbf{r}, \mathbf{r}; \omega)] \cdot \mathbf{d} \},
\]

(5.14)

where \( \mathbf{G} \) is then projected in the dominant field direction (in our PC cavities, that is the \( y \)-direction), at the location of the dipole emitter. This definition of radiative decay assumes we are in 3D space, and our GF has units of inverse volume (m\(^{-3}\)), while the dipole moment has units Coulomb meter (Cm), and the overall decay rate has units of inverse seconds (1/s).

Assuming radiative decay is calculated with the same formula in 2D, it is then required to introduce an effective length \( l_z \) as our GF loses a spatial dimension from 2D to 3D. That is, we wish to define

\[
\Gamma_{2D,\text{eff}} = \Gamma_{3D},
\]

(5.15)

where \( \Gamma_{2D,\text{eff}} \) is the radiative decay rate obtained in our 2D simulations. To achieve this, we use the radiative decay rates of free space such that \( \Gamma_{2D,\text{FreeSpace}}/l_z = \Gamma_{3D,\text{FreeSpace}} \), which
defines an effective length \( l_z \) as
\[
l_z = \frac{\Gamma_{2D,\text{FreeSpace}}}{\Gamma_{3D,\text{FreeSpace}}} = \frac{G_{2D,\text{FreeSpace}}}{G_{3D,\text{FreeSpace}}}.
\] (5.16)

The free space Green function in 2D is derived as \( \text{Im}\{G_{2D}^{\text{Hom}}\} = \frac{1}{8} \frac{\omega^2}{c^2} \) (for TE modes), while in 3D we have \( \text{Im}\{G_{2D}^{\text{Hom}}\} = \frac{n}{6\pi} \frac{\omega^3}{c^3} \) [Martin and Piller [1998]]. Using these definitions in Eq. (5.16), we find that
\[
l_z = \frac{3\pi}{4n} \frac{c}{\omega},
\] (5.17)
and the effective radiative decay rate experienced in our simulations is then
\[
\Gamma_{2D,\text{eff}}(r) = \frac{8n\omega}{3\pi\hbar\epsilon_0 c} \{\mathbf{d} \cdot \text{Im}[G_{2D}(r, r; \omega)] \cdot \mathbf{d}\}.
\] (5.18)

To verify this model indeed obtains the correct radiative decay, we scale our plugin density \( N \) by \( l_z \) in Eq. (5.17), such that \( N^{-1} = \Delta x \Delta y l_z \), arriving at \( N = 1.743e4 \mu m^{-3} \) for \( \omega = 190 \) THz. We then insert our plugin material to a single Yee cell at the center of an L5 cavity, and put it in an initially excited state to measure the natural decay of the TLA, thus turning off our phenomenological decay \( \gamma' \), and incoherent pump \( P \). Thus there are no phenomenological terms in the OBE at all, either radiative or nonradiative. We set the dipole moment magnitude to 43.88 D to mirror the values that will be used in the ensemble simulations. To initially ensure we are not near the strong-coupling regime, we first set up our 2D cavity to have a low \( Q \)-factor, by shortening the PC membrane on either side of the cavity edge. We give the TLA an initial polarization to simulate a dynamical decay from a radiation reaction (which is known to give the same decay as from vacuum fluctuations). From this simulation, we find very good agreement between theory and simulation, where the GF of our cavity is calculated with Eq. 5.1, which is shown to agree with numerically exact (i.e., full-dipole) simulations in Fig. 5.6b. Importantly, this accuracy will be maintained at any spatial position within our simulation array. We also stress that the FDTD also captures QD-QD radiative interactions, which in a master equation approach would typically appear as
\[
\Gamma(r_a \to r_b) = \frac{2}{\hbar c_0} \{\mathbf{d}_a \cdot \text{Im}[G(r_a, r_b; \omega)] \cdot \mathbf{d}_b\},
\] (5.19)
and a corresponding Lamb shift [Agarwal [2013]]. Clearly including such terms in an ensemble of different QDs, in the many thousands, would be completely tedious and intractable.
(a) FDTD-captured radiative decay rate

(b) FDTD radiative decay in weak and strong coupling regimes

Figure 5.7: (a) Population $\rho_{11}$ dynamics within an L5 low $Q$-factor ($\approx 400$) cavity, solved by MBE without any phenomenological decay terms. The OBEs are given initial conditions $\rho_{11}(t = 0) = 0.95$, $\rho_{01}^{\text{Im}}(t = 0) = 0$, and $\rho_{01}^{\text{Re}}(t = 0) = \sqrt{1 - 0.95^2}/2$, such that the Bloch vector magnitude is set to unity (e.g., $\sigma_1 = 2\rho_{11} - 1$, $\sigma_2 = 2\rho_{01}^{\text{Re}}$, and $\sigma_3 = 2\rho_{01}^{\text{Im}}$ are the usual Bloch vector components with magnitude $\sigma_1^2 + \sigma_2^2 + \sigma_3^2$). The analytic solution is determined by $\Gamma_{2D,\text{eff}}$, calculated by the QNM GF seen in Fig. 5.6b. (b) Comparison of high and low $Q$ cavities for the 2D L5 cavity structure, which were 47,000 and 430 respectively. All other parameters are kept equal in this comparison.

To fit our simulations for the single dipole $\Gamma_{\text{Num}}$ with $\Gamma_{2D,\text{eff}}$, we match decay lifetimes as seen in Fig. 5.7a. Note, the initial decay of $\rho_{11}$ is non-exponential because its inversion level is positive, thus the electric field emitted initially grows in magnitude as a consequence of the initial condition. Once our QD becomes an absorber ($\rho_{11} < 0.5$), we start to recover the expected exponential decay shape of radiative decay, which eventually becomes fully exponential at $t_0$. Finally, in figure 5.7b, we compare our low $Q$ cavity to the usual high $Q$ simulation, and find the semi-classical analogue of vacuum Rabi oscillations, namely we get periodic cycles of the population at a rate given by $2g = \Omega_{\text{Rabi}}$ [Hughes and Kamada [2004]; Andreani et al. [1999]], where $g$ is the QD-cavity coupling rate (which scaled with $d^2/V_{\text{eff}}$) and $\Omega_{\text{Rabi}}$ is the width of the frequency splitting in frequency space.
5.7 Simulation Results of Gain Threshold for a QD Ensemble in PC Cavities of Different Length

5.7.1 QD Ensemble

Using the QD ensemble parameters defined above, we are now ready to simulate gain in our 2D PC cavities, in a fully self-consistent way. The simulation domain is described in section 5.6, and shown in figure 5.5b. The only parameter left undefined is the inhomogeneous ensemble’s peak frequency $\omega_0$. As the homogeneous PC has a bandgap between 185-215 THz, the peak frequency should be somewhere within this range. We define two different $\omega_0$ values to study: $\omega_1 = 187$ THz, and $\omega_2 = 197$ THz, which result in two different gain spectra from the QD ensemble, shown in Fig. 5.8b. These two values were specifically chosen as models for: single mode lasing over all cavity lengths (which was seen and reported in Ref. [Xue et al. [2016b]]) performed by $\omega_1$, as the mode nearest resonance is always the first fundamental mode; and a peak frequency determined by the electroluminescence for the QD used in Ref. [Xue et al. [2016b]], performed by $\omega_2$. Simulations with $\omega_1$ and $\omega_2$ are carried out with all other parameters equal for consistency. Figure 5.8a compares the peak frequency of the first 5 fundamental modes as a function of cavity length to the resonant frequency of the two QD ensembles from Fig. 5.8b.

Although the pumped QDs do not need any additional optical source to achieve lasing, we found SS can be reached much more quickly when an external plane-wave source (seen in Fig. 5.5b) initially excites the cavity. The downside of this approach, is that some amount of power will always be captured by the power monitor, which is discussed in the next subsection. Fortunately, lasing threshold is determined by the slope taken from simulations that are clearly lasing. The dynamics of each simulation is obviously different depending on if the cavity is below, near, or above threshold, as is shown in Fig. 5.9, where a pump rate of 0.1 ns$^{-1}$ only decays, while 1 ns$^{-1}$ increases, followed by decay as it finds its equilibrium, and 8 ns$^{-1}$ is well into lasing, finding equilibrium quickly.

The pump threshold $P_{th}$ is defined by the usual method of extending the linear region of a “light-in light-out” (LL) curve down to the $x$-axis, as shown in Fig. 5.10 for $\omega_1$ (the results for $\omega_2$ are qualitatively similar). Comparing the low-resolution transmission spectra,
Figure 5.8: (a) Dependence of the cavity mode peak frequencies, for each cavity length, to the resonant peak QD ensemble gain (or PL) spectra. (b) Visualization of the normalized inhomogeneously broadened gain spectra of the QD ensemble for $\omega_1$ and $\omega_2$ taken from Fig. 5.6a.

measured along a line at the end of the PC membrane as depicted in Fig. 5.5b, in Sec. 5.6, for the L7 and L15 cavities of these two different QD ensembles, we see that $\omega_1$ is a single-mode laser (Figs. 5.11a and 5.11b), while $\omega_2$ is multi-mode (Figs. 5.11c and 5.11d). A clear advantage of our self-consistent model is that it is able to capture all modes that appear in the light-matter coupling.
5.7. SIMULATION RESULTS OF GAIN THRESHOLD FOR A QD ENSEMBLE IN PC CAVITIES OF DIFFERENT LENGTH

Figure 5.9: Lasing dynamics of an L5 cavity given a QD ensemble with \( \omega_1 \), as measured at the center of the cavity \((x = y = 0)\). The pump rate of \( 0.1 \text{ ns}^{-1} \) does not lase and only decays, while a pump rate \( 1 \text{ ns}^{-1} \) is into the lasing regime, as it increases in amplitude, followed by decay as it finds its equilibrium, and a pump rate \( 8 \text{ ns}^{-1} \) is clearly well into lasing.

5.7.2 Role of QD Ensemble Characteristics a Spatially-Varying Radiative Decay

The pump thresholds for each cavity length were performed with multiple QD instances to check for any significant fluctuations in any of the trend lines. An example of this can be seen in Fig. 5.12a, where a large variation was seen between L13 and L15 pump thresholds. This large fluctuation is reflected in the error bar assigned to the those particular pump thresholds, where error/uncertainty is computed as the variance of the average result. All other pump threshold’s represent a single instance, due to their minimal fluctuations between different QD instances. The error/uncertainty in the computations of single instance gain threshold is determined by the maximum and minimum fitted slopes, and uncertainty in the \( y \)-intercept. There exists some uncertainty in the \( y \)-intercept due to artificial power measurements at low pump strengths, which is caused by the initial source amplitude continuing to leak into the power monitor at the end of the simulation, due to the high \( Q \)-factors of the cavities. As such, there exists a positive \( y \)-intercept for the measured power emitted.
5.7. SIMULATION RESULTS OF GAIN THRESHOLD FOR A QD ENSEMBLE IN PC CAVITIES OF DIFFERENT LENGTH

Figure 5.10: Example lasing curve, or LL graphs of the $\omega_1$ QD ensemble. The inset is a close up of the L5, L9 and L13 curves. As the power out is measured in the final 10 ps of the simulation, the power out is consistent, but arbitrary.

by the cavity, when the pump rate is set to zero. This can be seen in Fig. 5.13, which is an L9 simulation from one of the 2 QD instances for $\omega_1$ plotted in Fig. 5.12a, with an originally negative pump threshold due to this artefact. To remove the artefact, we fit the low pump data to a polynomial curve, and extract a fitted $y$-intercept, which we use to shift the original data to have a $y$-intercept of zero. The error of this fit is then added in quadrature to the slopes error. The average threshold trend is shown in Fig. 5.12a for $\omega_1$ simulations and compared to $\omega_2$ in Fig. 5.12b.

Next, focusing on the single-mode laser, we compare the QD ensemble with simulations that exclude the ensemble statistics by replacing the active gain region with a single plugin sheet that uniformly excites the various cavity modes. This “sheet” simulation has a pure dephasing value equal to the inhomogeneously broadened ensemble of 10 THz, a peak frequency of $\omega_1$, and a dipole moment $d = 5.84$ D (which was found to model the average dipole moment of the ensemble), and $N = 1.045e5 \, \mu m^{-3}$, which was used as a fitting parameter to get the L5 pump threshold in-line with the QD ensemble value. The resulting pump threshold is shown in Fig. 5.12c, compared to the average QD ensemble, which shows
Figure 5.11: (a,b) Example transmission measured at the output power DFT-monitor for lasing L7 (a) and L15 (b) cavities ($P = 8 \text{ ns}^{-1}$) the $\omega_1$ QD ensemble. (c,d) Example transmission measured with the $\omega_2$ QD ensemble.

no sign of a plateau, and certainly no sign of an increasing pump threshold for increasing cavity lengths. We can conclude that the spatial dependent coupling of radiative decay and QD-QD interactions is a qualitatively important on the gain threshold characteristics and such behaviour would be extremely difficult to capture in a simplified rate equation analysis. Moreover, our findings are consistent with the unusual experimental trends found by Xue et al. [Xue et al. [2016b]], which was attributed to structural disorder (an effect that we have not yet included in a self-consistent way, but will do so in the next subsection).

To better understand the effects of $\Gamma_{2D,\text{off}}$ as a function of cavity length, we introduce a phenomenological radiative decay rate into the OBEs, $\Gamma_R$ using the Lindblad superoperator $\Gamma_R \mathcal{L}(\sigma^-)$, and set $\Gamma_R = 0.05 \text{ THz}$, which is roughly 100 times smaller than the maximally coupled QD decay rate, averaged over all cavity lengths (seen in Fig. 5.14b). Typically,
this will now be the dominant radiative decay process in the simulation. By reducing the natural cavity length scaling of $\Gamma$ captured by the FDTD method, we see the effects of resonance more clearly, which is reflected in the pump threshold trend in Fig 5.12d. That is, the trend of $\omega_1$ now consistently decreases, as the PF increases and the resonant mode

Figure 5.12: Pump gain thresholds extracted from LL curves for various set ups. Error bars on individual instances is determined by the maximum and minimum fitted slopes, and any uncertainty in the $y$-intercept due to artificial power measurements at low pump strengths caused by early terminations of the simulations (as demonstrated in Fig. 5.13). (a) The average (dotted black line) of 2 QD instances (orange lines) of $\omega_1$. (b) A comparison of $\omega_1$ and $\omega_2$ simulations. (c) A comparison of the sheet simulation to the average QD simulations. (d) Thresholds given by simulations with a phenomenological radiative decay rate $\Gamma_R$, set to 0.05 THz, for all QDs, for both $\omega_1$ and $\omega_2$. 

5.7. SIMULATION RESULTS OF GAIN THRESHOLD FOR A QD ENSEMBLE IN PC CAVITIES OF DIFFERENT LENGTH

M1 does not change its frequency's position with respect to resonance very much; however, the trend of $\omega_2$ is clearly impacted by how close any particular mode is to resonance (e.g., highlighted by a dip in the threshold between L9 and L11, as resonance conditions are met, and a missing dip between L5 and L7, as resonance conditions are removed).

5.7.3 Failure of a Simple Rate Equation Analysis

If the effects of a semi-constant $\Gamma_R$ across all cavity lengths is to amplify resonant effects, then what happens when we let $\Gamma_R(L)$ be defined by equation 5.18, as seen in Fig. 5.14b. This then sets each TLA plugin to have the maximum radiative decay rate, usually experienced by emitters perfectly on resonance at the maximum anti-node position. For this analysis, we first work out the pump threshold for each TLA, as having $\Gamma_R$ vary with cavity length changes the minimum threshold pump at each length.

We can determine each TLA pump threshold through the adiabatic elimination of the coherence in equation 5.7, by assuming $\gamma'$ is very large (and thus, the pure dephasing lifetime very short), such that $\rho_{01}$ reaches a quasi-steady state $\frac{d}{dt}\rho_{01} = 0$, while $\frac{d}{dt}\rho_{11} \neq 0$. That is, we let $\frac{\partial \rho_{01}^{Re}}{\partial t} = \frac{\partial \rho_{01}^{Im}}{\partial t} = 0$, such that

$$\rho_{01}^{Im} = \frac{\beta \chi (2\rho_{11} - 1)}{\beta^2 + \omega_0^2}, \quad (5.20)$$
5.7. SIMULATION RESULTS OF GAIN THRESHOLD FOR A QD ENSEMBLE IN PC CAVITIES OF DIFFERENT LENGTH

where \( \beta = \frac{P + \Gamma_R + \gamma'}{2} \), and

\[
\rho_{01}^{Re} = \frac{-\omega_0 \chi (2\rho_{11} - 1)}{\beta^2 + \omega_0^2},
\]  

(5.21)

which gives us a quasi-steady state \( \dot{\rho}_{11} \) of

\[
\frac{d\rho_{11}}{dt} = -2\Gamma_R I \frac{\beta^2}{\beta^2 + \omega_0^2} (2\rho_{11} - 1) - \Gamma_R \rho_{11} + P(1 - \rho_{11}),
\]

(5.22)

where \( I = \frac{\chi^2}{(\beta \Gamma_R)} \). Equation 5.22 is easily solvable with the initial condition \( \rho_{11}(t = 0) = 0 \), and we can use this solution to determine the steady state pump threshold, assuming threshold is reached in the long time limit where \( \rho_{11} = 0.5 \). Using this limit, we find

\[
\rho_{11}(t \to \infty) \big|_{P \to P_{th}} = 0.5 = \frac{C \Gamma_R + P_{th}}{2C \Gamma_R + \Gamma_R + P_{th}},
\]

(5.23)

or \( P_{th} = \Gamma_R \), where \( C = 2I \frac{\beta^2}{\beta^2 + \omega_0} \). Thus, we define \( P_0 = \Gamma_R \) to be the minimum pump power required to achieve any lasing action, which is sensible as pumping needs to overcome losses before positive inversion is possible. It is important to note that this threshold \( P_0 \) has little to do with the actual pump threshold \( P_{th} \) of the lasing cavity, since \( P_0 \) simply denotes the minimum power required to achieve positive inversion, given that \( \Gamma_R \) is present in the OBEs.

Assuming the threshold power is inversely proportional to PF, which is consistent with FP cavity lasers where the longer the laser (or the higher the PF), the less light is lost to imperfect reflections, and the lower the threshold; thus, one can make the crude assumption that pump threshold should perhaps go as

\[
P_{th}(N) = A_0 + A_1 \frac{V_{eff}(N)}{Q(N)},
\]

(5.24)

where \( N \) is cavity length, and \( A_0 \) and \( A_1 \) are scaling factors dependent on various system parameters such as relaxation rates, polarization density, and dipole moment.

Putting all of this together, we find that a scaled \( \Gamma_R \) does not mimic the trends found in Fig. 5.12a, and instead follows a more basic laser theory curve seen in Fig. 5.14c. In this way, scaling \( \Gamma_R \) to be the same across all TLA emitters seemingly removes the coherence of the ensemble.

Other rate equation models [Xue et al. [2016b]; Prieto et al. [2015b]] include a non-radiative decay term in their population rate, to model pure dephasing. However, these
models find threshold pump scaling which simply goes as $1/Q$, which would have the same trend as equation 5.24; a continuously decreasing pump threshold as cavity length increased. Indeed it was exactly this trend that motivated the need to add additional effects of disorder-induced losses, an effect we now quantify below.

(a) With a constant $\Gamma_R(L)$ added to FDTD calculations

(b) Fit for $\Gamma_R(L)$

(c) Threshold now decreases as a function of cavity length

Figure 5.14: (a) Lasing curves for the scaled $\Gamma_R$ simulations, modelled after $\Gamma_{\text{eff,2D}}$ measurements seen in (b), with the $x$-axis shifted by $P_0$ to allow for a reasonable comparison of different cavity lengths. (b) Solution to equation 5.18 at the maximum field anti-node and resonance as a function of cavity length. This fit is used to model the scaling $\Gamma_R$ used in the simulations shown in (a). (c) Pump threshold as a function of cavity length measured from (a), compared with Eq. 5.24, where $A_0 = 1.55$ THz, and $A_1 = \left(\frac{\omega_1}{4}\right)^2$. 
5.7. SIMULATION RESULTS OF GAIN THRESHOLD FOR A QD ENSEMBLE IN PC CAVITIES OF DIFFERENT LENGTH

5.7.4 Impact of Structural Disorder

One of the last points of our investigation for this QD ensemble and pump threshold is the impact of disorder. As mentioned previously, here we are motivated by the recent experimental results from [Xue et al. [2016b]], where the prime suspect for their observed pump threshold departing from simple rate equation theory was intrinsic disorder. As mentioned in section 5.3, the intrinsic level of disorder for our effective 2D simulations is given by $\sigma_{\text{Dis}} = 0.01a$ (which mimic the same effect as full 3D slab cavities properties). To understand the effects of additional disorder, we go beyond what would be found naturally, and set $\sigma_{\text{Dis}} = 0.04a$. Instances of these two disordered simulations can be seen in Figs. 5.15a and 5.15b, where we again use $\omega_1$ as the peak frequency. A general increase to the pump threshold, which becomes more prominent beyond L7, is clearly seen. These results are indeed consistent with the experimental results from [Xue et al. [2016b]], but, as we have shown above, disorder alone is not responsible for the general plateauing regime.

Finally, we look at the influence of increased disorder on our lasing mode profiles in the possible regime of Anderson Localization, or with strongly localized modes. At L15, the M1 is the strongest mode (highest $Q$) of all the cavity lengths, and also has the longest mode profile, which makes it the best candidate for localization. Sheet gain is used in this

![Figure 5.15: Pump threshold trends for two disordered simulations: intrinsic levels $\sigma_{\text{Dis}} = 0.01a$ (a), and larger than intrinsic disorder $\sigma_{\text{Dis}} = 0.04a$ (b), demonstrating a general increase in the pump threshold predominantly for cavity lengths greater than L7.](image-url)
analysis to isolate the randomness in the systems to the disorder of the PC. Figures 5.16b-5.16d depict the localization of the fundamental mode as disorder is increased, however, the overall PF is still less than the idealized structure as shown in Fig. 5.16a. The projected LDOS is measured at the peak anti-node location for each mode, which is marked in each mode profile by a black “x” marker. This localization is random in nature, which limits the applications of such a mode, and although the mode volume is reduced, the $Q$ factor takes an even greater hit. Note, with greater disorder comes a larger $Q$ variance, as seen in Fig. 5.4d, which does mean it is possible for these localized modes to have reduced mode volume, and increased $Q$ factors. Yet, this is statistically unlikely, and many realizations would have to be created, and tested, before such a mode would be useful.
5.7. SIMULATION RESULTS OF GAIN THRESHOLD FOR A QD ENSEMBLE IN PC CAVITIES OF DIFFERENT LENGTH

(a) L15 cavity LDOS for ordered, and disordered M1 modes

(b) Ordered cavity mode profile, $f_1$ above

(c) Disordered ($\sigma_{\text{Dis}} = 0.01a$) cavity mode profile, $f_2$ above

(d) Disordered ($\sigma_{\text{Dis}} = 0.04a$) cavity mode profile, $f_3$ above

Figure 5.16: (a) Projected LDOS along the $y$ direction for the first fundamental lasing mode of the L15 cavity, for the sheet active region with peak frequency $\omega_1$, with increasing amounts of disorder. The LDOS is normalized to free space such that our $y$-axis is in units of PF. All lasing modes are measured for simulations with incoherent pump rate $P = 8 \text{ ns}^{-1}$, where the ordered simulation’s response is in black, the intrinsically disordered simulation, $\sigma_{\text{Dis}} = 0.01a$, is in orange and the additional disordered simulation $\sigma_{\text{Dis}} = 0.04a$ is in magenta. (b-d) Mode profiles of M1 for the ordered (b), intrinsic disordered $\sigma_{\text{Dis}} = 0.01a$ (c), and additional disordered $\sigma_{\text{Dis}} = 0.04a$ (d) simulations.
5.8 Conclusions

To conclude, we have developed a numerical model to describe an active QD ensemble coupled to PC cavities using Lumerical’s plugin tool within an effective 2D FDTD method, to investigate pump threshold as a function of cavity length. Both multi-mode and single-mode lasing was found, depending on the peak frequency of the QD ensemble. Studying the effects of our ensemble on the single mode lasing, we found a general plateauing of the pump threshold beyond L9, which is seemingly due to the QD coherent dynamics, as the removal of the individual QDs in the sheet simulation lead to a lesser plateau, and the inclusion of a phenomenological decay rate also destroys the plateau by preventing the QDs unique self-consistent decay. As such, we believe there is currently no suitable replacement for the self-consistent radiative decay performed by the FDTD method, when determining lasing dynamics, and, at least, a generalization of common rate equations is called for. Structural disorder was shown to generally increase the pump threshold for cavities longer than L7, which is in agreement with the experimental findings of Ref.[Xue et al. [2016b]], though it seems unlikely that disorder alone was responsible for this effect (as our simulations show). Random localization due to disorder of the lasing cavities modes is seen, which are not particularly interesting within the scope of high-Q cavity lasers, but could merit further investigation in the context of slow-light PC waveguides [Faggiani et al. [2016]; Liu et al. [2014b]]. Future works should investigate the role of radiative decay rate by performing low temperature simulations where $\gamma'$ is no longer the dominant decay mechanism, and additional simulations should be run to build up a statistical analysis of the many random processes that take place.
Chapter 6

Conclusions and Suggestions for Further Work

In this thesis, we present a thorough investigation of light-matter interactions within PC cavity structures and introduce a powerful, novel technique for modelling full QD ensembles inside such structures, using a self-consistent FDTD method. This model was able to provide fresh insights into the recently published experimental results [Xue et al. [2016b]], demonstrating a need for retaining coherence when modelling massive QD ensembles. A rate equation analysis, which is the common approach to modelling lasing dynamics [Droulias et al. [2014]; Shi and Prather [2007]; Fang et al. [2010]; Prieto et al. [2015b]; Altug and Vučković [2005]], adiabatically eliminates the coherent nature of QDs, and as such, can be a poor model in capturing the many complexities of lasing interactions. We do recognize the usefulness of rate equations for quickly connecting with experimental results, and extracting useful figures of merits from data, but feel a more complete picture is necessary to correctly optimize photonic crystal structures. In Chapter 4, we demonstrate how to correctly model QDs in the FDTD method using a self-consistent Maxwell Bloch analysis, implemented using Lumerical’s plugin tool. In the following Chapter 5, we present our recently submitted paper in manuscript form, which applies QD ensembles to photonic crystal cavities of various lengths, and measures the resulting pump thresholds to compare simulated lasing trends with the experimental results of [Xue et al. [2016b]]. We find good agreement with the recent surprising threshold trends as a function of cavity length, which we attribute to
the coherent QD ensemble dynamics solved in the presence of the PC cavity physics. Our method was easily able to capture multiple cavity mode dynamics, and the effects these modes had on the lasing threshold. Ultimately, we have shown that standard rate equation models miss too much of the complex physics present in these microcavity structures, to be used as optimizing tools.

These results were made possible with the theory developed in Chapter 2, where general classical light-matter interactions and semi-classical laser theory were discussed. The photonic Green function’s ability to determine the LDOS, Purcell factor, and radiative decay of photonic environments was necessary in correctly setting up the cavity simulations performed, and the laser theory was critical in developing a realistic model for the QD ensemble used in the simulations. In Chapter 3, we introduce and discuss some key observations of the FDTD method as it applies to high-$Q$ photonic crystal cavity systems, which can be very sensitive to both the simulation’s boundaries, and initial conditions. Throughout most of this thesis, we have tried to keep our analysis general (assuming FDTD analysis methodologies are used), such that the ideas presented here can easily be applied to other structures. We have shown powerful simplicity in our self-consistent Maxwell Bloch solver by its careful analysis of photonic crystal cavities within the FDTD domain, and useful application in the results of Chapter 5.

6.1 Suggestions for Future Work

Due to the growing popularity of QDs in many microcavity laser systems [Bimberg and Pohl [2011]; Tartakovskii [2012]], and the complete generality of both the FDTD method, and our OBE plugin material, we believe there is much more research to be done using the tools developed here, even well beyond microcavity laser structures. Using a few QDs, one could probe the effects of dipole-dipole coupling for optimizing “on-chip” photonic systems [Yao et al. [2010]], or research novel architectures that utilize specific emitter locations for enhanced or suppressed radiative decay dynamics. Alternatively, the full QD ensemble could be used to model temperature dependant simulations by decreasing the Gaussian spread used to set the inhomogeneously broadened linewidth, and the ensemble can be used in a variety of other systems such as random lasing in waveguide structures [Liu et al. [2014a]],
or solar cell structures [Nozik [2002]]. The plugin can also be used to explore the coupling nature of metallic resonators with single QDs [Chikkaraddy et al. [2016]] with the prospect of modelling SPASERS [Stockman [2008]]. Finally, the simulations carried out in Chapter 5 could be extended to 3D, if one had access to greater computer power, and researched fewer cavity lengths.
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Appendix A

An Introduction to the Green Function

In this appendix we outline the basic application of the Green function (GF) to solve a general differential equation. Let us consider a general inhomogeneous differential equation

$$\Lambda R(r) = S(r),$$

(A.1)

where $\Lambda$ is a linear operator acting on an unknown response vector field $R$, and $S$ is a known vector field source that makes the differential equation inhomogeneous. From the superposition theory, it is known that the solution to such a differential equation will consist of a homogeneous ($S = 0$) and a particular inhomogeneous solution. Assuming the homogeneous solution is known, the problem reduces to finding an adequate inhomogeneous solution. To accomplish this, one can introduce an arbitrary function that satisfies the following equation

$$\Lambda \bar{G}(r, r') = \bar{I} \delta(r - r'),$$

(A.2)

where $\delta(r - r')$ is the Dirac delta function, $\bar{G}(r, r')$ is a dyadic function that depends on both the position of interest $r$ and the location of the Dirac delta $r'$, and $\bar{I}$ is the unit dyad and the whole equation is in closed form such that $\Lambda$ acts on each column of $G(r, r')$. Assuming the solution to this simple equation is obtainable such that $G(r, r')$ is known, we can post-multiply equation A.2 by the source vector field $S$ and integrate over the volume.
V such that $S \neq 0$, and arrive at
\[
\int_V \Lambda G(r, r') \cdot S(r') dV' = \int_V S(r') \cdot \delta(r - r') dV',
\] (A.3)
which, has the right hand side simplify to $S(r)$, thus we can substitute in equation A.1 giving us
\[
\Lambda R(r) = \int_V \Lambda G(r, r') \cdot S(r') dV',
\]
\[
R(r) = \int_V G(r, r') \cdot S(r') dV'.
\] (A.4)

As the GF tensor, and the source vector field are both known at this point, the solution to this general inhomogeneous differential equation is known.
Appendix B

Homogeneous Photonic Green Function in 2D and 3D

In this appendix we introduce the homogeneous Green function (GF) solution for both 2D and 3D space, which are used throughout this thesis to normalize LDOS calculations to represent a Purcell factor. The 3D solution can be found in [Novotny and Hecht [2012]], and the extended 2D result here [Martin and Piller [1998]]. We shall start with the 3D problem, and then extend this solution to 2D by integrating over the line source which differentiates the 2D GF from its 3D counterpart.

\[ \mathbf{E}(\mathbf{r}; \omega) = i\omega \mathbf{A}(\mathbf{r}; \omega) - \nabla \phi, \]  
\[ \mathbf{B}(\mathbf{r}; \omega) = \nabla \times \mathbf{A}(\mathbf{r}; \omega). \]

Using these equations in (2.1b), for a homogeneous nonmagnetic medium (\(\mu = 1\), \(\epsilon(\mathbf{r}; \omega) = \epsilon_B\)), with the constitutive relations 2.2, we find

\[ \nabla \times \nabla \times \mathbf{A}(\mathbf{r}; \omega) = -\frac{i\omega \epsilon_B}{c^2} \{ i\omega \mathbf{A}(\mathbf{r}; \omega) - \nabla \phi \} + \mathbf{j}_s(\mathbf{r}; \omega). \]

Note that \(\mathbf{A}\) and \(\phi\) are not unique, in that we can apply an arbitrary time harmonic scalar function \(\chi\), such that \(\mathbf{A} \rightarrow \mathbf{A} + \nabla \chi\) and \(\phi \rightarrow \phi + i\omega \chi\), and generate the same \(\mathbf{E}\) and \(\mathbf{B}\) fields. As such, we choose \(\chi\) to give us a Lorenz gauge, which defines \(\nabla \cdot \mathbf{A} = i\omega \epsilon_B \phi / c^2\).
With this gauge transform, equation B.3 becomes

\[-\nabla^2 + \nabla \nabla \cdot) A(r; \omega) = -\frac{i \omega B}{c^2} \{ i \omega A(r; \omega) - \nabla \phi \} + j_s(r; \omega), \quad (B.4)\]

\[-\nabla^2 A(r; \omega) + i \frac{\omega B}{c^2} \nabla \phi = -i \frac{\omega B}{c^2} \{ i \omega A(r; \omega) - \nabla \phi \} + j_s(r; \omega), \quad (B.5)\]

\[(\nabla^2 + k^2) A(r; \omega) = -j_s(r; \omega), \quad (B.6)\]

where we started with the identity \( \nabla \times \nabla \times = -\nabla^2 + \nabla \nabla \cdot \), and \( k = \sqrt{\epsilon_0 c^2} \). Now we apply the usual GF method outlined in the last section A, defining the homogeneous GF \( \bar{G}_h \) as

\[(\nabla^2 + k^2) \bar{G}_h(r, r'; \omega) = \frac{\omega^2}{c^2} \delta(r - r'), \quad (B.7)\]

where our prefactor \( \omega^2/c^2 \) is included due to its presence in equation 2.8, and we only have one physical solution [Novotny and Hecht [2012]]

\[\bar{G}^h_A(r, r'; \omega) = \frac{\omega^2}{c^2} e^{i k R} 4 \pi R \bar{I}, \quad (B.8)\]

where \( R = |r - r'| \), and we have chosen the outward propagating solution. Since \( E(r; \omega) \) is given by

\[E(r; \omega) = i \omega \left[ \bar{I} + \frac{\nabla \nabla}{k^2} \right] A(r; \omega), \quad (B.9)\]

in the Lorenz gauge, we can immediately construct \( \bar{G}^h \) for \( E \), using our solution for \( \bar{G}_h^h \)

\[\bar{G}^h(r, r'; \omega) = \frac{\omega^2}{c^2} \left[ \bar{I} + \frac{\nabla \nabla}{k^2} \right] e^{i k R} 4 \pi R. \quad (B.10)\]

Equation B.10 is the general solution for 3D homogeneous space; however, we are mostly interested in the GF solution where \( r = r' \) so we may normalized LDOS calculations to the expected free space calculation, giving the LDOS in Purcell factor units. To do this, we first apply the Laplacian

\[\bar{G}^h(r, r'; \omega) = \frac{\omega^2}{c^2} 4 \pi R \left[ \left( 1 + \frac{ikR - 1}{k^2 R^2} \right) + \left( \frac{3 - 3ikR - k^2 R^2}{k^2 R^2} \right) \left( \frac{r - r'}{R^2} \right) \right] \bar{I}, \quad (B.11)\]
and noticing \( r = r' \) will diverge, we take the limit \( r \to r' \), and find

\[
G^h(r, r'; \omega) |_{r \to r'} = \frac{\omega^2}{4\pi c^2} \left[ \frac{2}{k^2 R^2} + \frac{1}{R} + \frac{2i}{3} + \ldots \right] \bar{I},
\]

\[
G^h(r, r'; \omega) |_{r \to r'} = \left[ \infty + i \frac{\sqrt{\epsilon_B} \omega^3}{6\pi c^3} \right] \bar{I}.
\] (B.12)

To extend our result B.8 to 2D, we first consider that the Green’s tensor in a 2D system represents the field generated in an observation plane \( z = \text{const} \) by an infinite line source, extending in the \( z \) direction, with an \( e^{ikz} \) dependence [Martin and Piller [1998]]. As such, can remove the \( z \) dimension of equation B.8 by integrating over this line source

\[
\bar{G}^h_{A,2D}(r, r'; \omega) = \int_{-\infty}^{\infty} dz' \frac{e^{ik\sqrt{x'^2 + y'^2 + (z-z')^2}}}{4\pi \sqrt{x'^2 + y'^2 + (z-z')^2}} e^{ikz'} \bar{I},
\] (B.13)

where we are assuming the line source is located at \( x' = y' = 0 \). The integral of equation B.13 can be done with the help of Eq. (3.876) in [Gradshteyn and Ryzhik [2014]], giving us

\[
\bar{G}^h_{A,2D}(r, r'; \omega) = \frac{i}{4} H_0(kR) e^{ikz} \bar{I},
\] (B.14)

where \( k \) is the wave vector defined for only \( x \) and \( y \) space, \( R = (x - x', y - y') \), and \( H_i \) is notation for the Hankel function of the first kind \( H^{(1)}_i \). Using equation B.14 in place of \( \bar{G}^h_A \) in equation B.10, we define

\[
\bar{G}^h_{2D}(r, r'; \omega) = \frac{i\omega^2}{4c^2} \left[ \bar{I} + \nabla \nabla \frac{k^2}{k^2} \right] H_0(kR) e^{ikz},
\] (B.15)

which is carried out at \( z = 0 \), and gives the general Green’s tensor solution for an infinite homogeneous 2D system. This tensor still has 9 components, yet we are only interested in the \( yy \) component \( (G^h_{yy,2D}) \) since our 2D cavity simulations are TE modes dominated in the \( y \) direction, which is given analytically by [Martin and Piller [1998]]

\[
G^h_{yy,2D}(r, r'; \omega) = \frac{i\omega^2}{4c^2} \left[ \cos^2(\theta)H_0(kR) - \frac{\cos(2\theta)}{kR} H_1(kR) \right],
\] (B.16)

where \( \theta \) is the angle of incidence for a propagating field into the \( x,y \) plane (with \( \theta = 0 \) travelling into the plane, and \( \theta = \pi/2 \) travelling parallel to the plane) and \( G^h_{xx,2D}(R) \) is given by a similar equation. Modes that are TE have \( \theta = 0 \), and thus are solved by

\[
G^h_{yy,2D}(r, r'; \omega) = \frac{i\omega^2}{4c^2} \left[ H_0(kR) - \frac{1}{kR} H_1(kR) \right].
\] (B.17)
To evaluate B.17 at the location of an emitter ($\mathcal{R} = 0$), we will need to apply L'Hopital’s Rule, as the second term currently diverges in the limit $R \to 0$. Before applying L'Hopital’s Rule, we note
\[ \frac{d}{dz} H_1(z) = \frac{1}{2} (H_0(z) - H_2(z)), \quad (B.18) \]
which is evaluated with the help of [WolframAlpha]. Thus, if we use L'Hopital’s Rule on the second term in equation B.17, we find that
\[
G_{yy,2D}(r, r; \omega) \bigg|_{\lim R \to 0^+} = \frac{i\omega^2}{4c^2} \left[ H_0(kR) - \frac{1}{2} (H_0(kR) - H_2(kR)) \right], \quad (B.19)
\]
\[
G_{yy,2D}(r, r; \omega) \bigg|_{\lim R \to 0^+} = \frac{i\omega^2}{8c^2} \left[ H_0(kR) + H_2(kR) \right], \quad (B.20)
\]
where
\[
\lim_{R \to 0^+} H_0(kR) = 1 - i\infty, \quad (B.21)
\]
and
\[
\lim_{R \to 0^+} H_0(kR) = -i\infty, \quad (B.22)
\]
where both limits have been evaluated with the help of [WolframAlpha]. Thus, we arrive at
\[
G_{yy,2D}(r, r; \omega) = \infty + \frac{i\omega^2}{8c^2}. \quad (B.23)
\]
Appendix C

Polarization Plugin Code Excerpts

In this appendix we present example code used to implement our optical Bloch equation plugin Tool for Lumerical software, and describe how to add the C++ class to Lumerical. The basic idea for the plugin is to create a class in a C++ header that has access to: \( E^n \), \( U^n \), \( V^n \), can store as many fields update parameters as specified (in our case, 3, as seen in the line “size_t storageSizeE() const {return3;}” in Figure C.1), has user defined inputs specified in the graphic user interface (GUI) (7 in our case from “static const char* names[8];”, seen in Figure C.1, since the 8th element of “names” is a zero, indicating the end), and has various constant values that are defined in the main function, which are used to carry out the desired polarization calculation. Note, to properly compile the header file shown in Figure C.1, you need to have Lumerical’s “imaterialplugin.h” header in the same folder, and each new material must have its own Globally Unique Identification (GUID), created by a GUID generator. The line “const char* name() const {return ‘optical Bloch Equation’;}” is where the name of this plugin is defined, as it appears in the GUI.

The main script is where most of the action takes places, and it has many parts. First, the plugin must be initialized by the user defined parameters: “w0”, “Gamma”, “gamma”, “Pump”, “Initial Inversion [rho22]”, “Dipole Moment [Debye]”, “N Density”. These parameters are loaded into “parameters”, which is a variable with 7 entries, starting from 0. Next, these loaded in parameters must be assigned to their respective constants defined in the header. Note, the RK4 method requires each parameter to be multiplied by the time step “dt”. The purpose of the initialize call of the plugin is to specify the value of
all parameters for each vector component \( x, y, \) and \( z \) (hence the for-loop), in their correct units. The initialize scheme of our plugin class can be seen in Figure C.2.

Next the storage fields of our plugin need to be initialized. Our plugin has 3 storage fields \( \rho_{01}^{\text{Re}}, \rho_{01}^{\text{Im}}, \) and \( \rho_{11} \), of which only \( \rho_{11} \) needs to be initialized. The reason being numerical efficiency. Our simulations reach steady state much more quickly when an external source excites the individual QDs instead of giving them an initial polarization. In addition, each QDs inversion level is set near the steady state value determined by equation 2.64, which helps speed up the numerics as well. Unless specified, each storage field is initialized to
Figure C.2: Main Script (1).

```cpp
#include "BlochEquations.h"
#include <cmath>
#include <fstream>

const double BlochEquationPlugin::hbar = 6.582119288e-16; // units of [eV/s]
const double BlochEquationPlugin::pi = 3.1415926535897931;
const double BlochEquationPlugin::eps0 = 8.854187817e-12;
const double BlochEquationPlugin::c = 2.997924588e8;

cost char* BlochEquationPlugin::names[9] = {"w0", "Gamma", "gamma", "Pump", "Initial Inversion [rho22]", "Dipole Moment [Debye]", "N Density", 0};

void BlochEquationPlugin::initialize(const double** parameters, double dt)
{
    for(int l=0; l<3; l++)
    {
        double w00 = parameters[0][l];
        double Gamma = parameters[1][l];
        double gamma_p = parameters[2][l];
        double P_incoh = parameters[3][l];
        double Initial_inv = parameters[4][l];
        double d_in = parameters[5][l];
        double N_in = parameters[6][l];
        // in units of Debye.

        // give properties in all three dimensions
        Initial_inv[l] = Initial_inv[l];

        // calculate update quantities
        P_fact[l] = d_in*N_in*7.5346827e-19; /* Now in units [V/m = electric field] -
            using Debye = 1/c*10^-21 [C/m], N units of [m^-3], and Eps0 units [C/(V*m)] */
        chi[l] = d_in*0.20819434e-10/hbar; // Units [m/(Vs)]

        // Prepare Input Parameters
        A[l] = (Gamma + gamma_p + P_incoh)/2.*dt;
        Gamma[l] = Gamma_in*dt;
        w0[l] = w00*dt;
        P_incoh[l] = P_incoh_in*dt;
        chi[l] = chi[l]*dt;
    }
}
```

zero, which is why Figure C.3 only specifies $\rho_{11}(t = 0)$.

Figure C.3: Main Script (2).

```cpp
void BlochEquationPlugin::initializeStorage(int axis, float* storage)
{
    // initialize the electron level populations, which are the only non-zero storage
    storage[2] = float(Initial_inv[axis]);
}
```

Now that all parameters are specified and initialized, we define our plugin calculation in Figure C.4, and calls in Figure C.5. The plugin calculation is simply RK4 applied to our OBEs, while updating the respective storage fields, and returning the polarization
modulation defined by equation 5.11.

```c
float BlochEquationPlugin::calculate(int axes, float U, float V, float E, float* storage) {
    double CohReal = storage[0];
    double CohImag = storage[1];
    double UpperL = storage[2];
    double K1 = -A[axes]*CohReal - w0[axes]*CohImag;
    double L1 = w0[axes]*CohReal - A[axes]*CohImag + chi[axes]*E*(2.*UpperL - 1.);
    double M1 = -2.*chi[axes]*E*CohImag + P_incoh[axes]*(1. - UpperL) - Gamma[axes]*UpperL;
    double K2 = -A[axes]*(CohReal + K1/2.) - w0[axes]*(CohImag + L1/2.);
    double L2 = w0[axes]*(CohReal + K1/2.) - A[axes]*(CohImag + L1/2.) +
                 chi[axes]*E*(2.*(UpperL + M1) - 1.);
    double M2 = -2.*chi[axes]*E*(CohImag + L1/2.) + P_incoh[axes]*(1. - (UpperL + M1/2.)) +
                 Gamma[axes]*(UpperL + M1/2.);
    double K3 = -A[axes]*(CohReal + K2/2.) - w0[axes]*(CohImag + L2/2.);
    double L3 = w0[axes]*(CohReal + K2/2.) - A[axes]*(CohImag + L2/2.) +
                 chi[axes]*E*(2.*(UpperL + M2) - 1.);
    double M3 = -2.*chi[axes]*E*(CohImag + L2/2.) + P_incoh[axes]*(1. - (UpperL + M2/2.)) +
                 Gamma[axes]*(UpperL + M2/2.);
    double K4 = -A[axes]*(CohReal + K3) - w0[axes]*(CohImag + L3);
    double L4 = w0[axes]*(CohReal + K3) - A[axes]*(CohImag + L3) +
                 chi[axes]*E*(2.*(UpperL + M3) - 1.);
    double M4 = -2.*chi[axes]*E*(CohImag + L3) + P_incoh[axes]*(1. - (UpperL + M3)) +
                 Gamma[axes]*(UpperL + M3);
    CohReal = CohReal + (K1 + 2.*K2 + 2.*K3 + K4)/6.;
    CohImag = CohImag + (L1 + 2.*L2 + 2.*L3 + L4)/6.;
    UpperL = UpperL + (M1 + 2.*M2 + 2.*M3 + M4)/6.;
    double Pnpl = P_fact[axes]*CohReal;
    storage[0] = float(CohReal);
    storage[1] = float(CohImag);
    storage[2] = float(UpperL);
    return float((V-Pnpl)/U);
}
```

Figure C.4: Main Script (3).

Finally, once both the .cpp and .h files are finished, they must be compiled and the resulting shared object file moved to the correct Lumerical material plugin folder. To correctly compile the shared object file first requires the .cpp file to be compiled as an object file, ending in “.o”. This is can be accomplished using the gcc command in the terminal, and then the “.o” file is compiled as a “.so” file, where a prefix “lib” is usually added as common practice. This “libABC.so” file then moved to the plugins/materials folder, which is located in the lumerical/fdtd/bin folder. This directory is under opt in Unix machines; however, for running westgrid simulations with a created plugin, one must also compile the
.cpp file to “libABC.so” on the westgrid server, as the shared object file requires knowledge of all files compile prior to its inception. Thus, a WestGrid (www.westgrid.ca) user must know where the Lumerical directory that they use is kept, so they can add the “libABC.so” file to the plugins/materials folder.

Once the shared object file is added to Lumerical’s plugins/materials directory, it will appear in the GUI material database, when a user looks to add a new material.
Appendix D

Additional Manuscript Fitting

To match quality factors, we start by assuming the M1 $Q$-factor is the most important, and only focus on optimizing it over all cavity lengths. Recall from Chapter 5 that 2D $Q$-factor is varied by the length of PC membrane on either side of the PC cavity. Measuring this distance in lattice constants $a$, Figure D.1a compares PC membrane length to passive $Q$ measurements, demonstrating an optimal distance of $8a$ before terminating the PC membrane, measured for cavity lengths L5-L15. A direct comparison between 2D and 3D $Q$-factors can be seen in Figure 5.4a, in Chapter 5.

![Figure D.1: (a) Comparison of 2D Q factors of various simulation set-ups to the 3D full numerical solution, which itself was determined rigorously. (b) Epsilon matching to get both M1 and M2 as close to their 3D simulation as possible.](image-url)
To match the real eigenvalue $f$ properties of the 2D simulations with passive 3D simulations $f_0$, we observe both M1 and M2 peak frequencies, since optimizing their relationship together is more important than single mode optimizing. This is done because the physics of mode competition is sensitive to the positions of each modes frequency, which can be present in lasing structures [Liu et al. [2014a]]. In Figure D.1b, we vary the bulk refractive index $n$ for passive simulations, and compare the difference to both M1 and M2’s difference with their 3D counterpart. A refractive index of 2.54 is chosen using this figure, since the overall frequency difference is best optimized for both modes.

The simulations run time before reaching SS is sensitive to initial parameters. This was first discovered by simulations using a plane wave pulse with unity amplitude (which is defined by a continuous wave normalize described on Lumerical’s webpage [Lumerical]), compared to simulations with an increased pulse amplitude given to be the same order of magnitude as the SS lasing E-field. Looking at Figure D.2, the time required to reach SS is drastically reduced when the initial pulse amplitude is set larger than the SS value.

![Figure D.2](image-url)

Figure D.2: Comparison between a large and small initial pulse amplitudes used to initially excite a lasing L5 cavity (pump rate $P = 8$ ns). The smaller pump amplitude takes longer to reach SS, as the radiation builds up in the cavity. The units for the electric field amplitude are in CW normalization units, which is described in detail on Lumerical’s webpage [Lumerical]. The result shown here is consistent for larger cavity lengths.