An *Ab Initio* Approach to the Inverse Problem-Based Design of Photonic Bandgap Devices

Thesis by

John K. Au

In Partial Fulfillment of the Requirements for the Degree of

Doctor of Philosophy

California Institute of Technology

Pasadena, California

2007

(Defended March 22, 2007)
Acknowledgements

Finding an advisor is arguably one of the most impactful decisions in graduate school, and I could not have chosen a better one than Hideo. If you ever talk to any of his students, you will no doubt be told about the freedom we are given to try out ideas. Rarely, though, do we follow up and explain that this freedom is not possible unless he also has enough patience to allow these ideas to bear fruit, and the tolerance for when they fail to do so. Perhaps this point is most significant to me as I may have tried his patience more than any of my other labmates during my time here! Despite my setbacks, whether they are research related or more personal in nature, he has always remained unwaveringly positive, choosing instead to focus on ways to help me move forward. I am very fortunate to have had an advisor who is as kind as he is brilliant, which is tough to accomplish when he is a certified genius. Thank you for finding ways to support me (for far longer than is perhaps deserved) so that I can graduate.

I would also like to acknowledge many of the faculty members and other mentors that have shaped how I think about science and research. In particular, I am indebted to Dr. Cohen for teaching me to ask myself the question, “wouldn’t it be nice if . . .?” It did not get me over all my hurdles, but did help tremendously in leading me to find the manageable yet still meaningful ones to climb over. I am also grateful to Dr. Kimble for adopting me and the rest of MabuchiLab into his fold during our formative years. One of the most memorable moments during my time here was the day I truly understood the difference between quantum and non-classical. I was finally able to appreciate and genuinely respect the passion and resolve he had always exhibited. Finally, Dr. Herman has been an invaluable resource during the latter half of my
time at Caltech. I have a much better appreciation for the process of research and learning, and surely would have been too stubborn to learn that lesson without his patient guidance through my most frustrating times. Outside of academics, he has also taught me a great deal about life; from operating system upgrades to effective parenting, and plenty more in between, for all of which I will always be grateful.

Many thanks to Parandeh, Marjie, Tara, Jim and Athena at the ISP for taking care of all this paperwork for us international students. I am always amazed how little I actually have to do despite nominally interacting with the government, and it is definitely to your credit.

To survive graduate school, you definitely need friends who can commiserate with you. My first couple years and all those classes would not have been the same without George Paloczi, Tobias Kippenberg, Stephan Ichiriu and Will Green. Whether it was trying to wrap up a problem set or deciding on a group to join, it was comforting knowing that I was not alone. To the members of Professor Scherer’s Nanofab lab, and especially Marko Lončar, thanks for treating me as one of your own. I only wish I could have repaid you with better performance on the basketball court.

I had the great fortune of learning from excellent postdocs during my time here. Thanks in particular to Andrew Doherty for spending a lot of time with me early on teaching me everything from quantum trajectories to stochastic calculus (and on those car rides back from ‘group meeting’ the secret to a good cup of French press coffee). Jon Williams was instrumental in getting me up to speed on the physics of photonic crystals, and I learned a great deal just generally about how to go about conducting research from working with and observing him. To Luc Bouten, who remarkably took an interest in my work, thanks for the encouraging words throughout my thesis writing process. It meant more than you might have realized.

To the most intelligent set of ‘fools’ ever assembled, my fellow students in Mabuchi-Lab: it has been an honor to have shared this part of our careers together. To the young’uns Tony, Joe, Gopal, Nicole, Nathan and Orion: thanks for revitalizing the foosball tradition. That foosball table has greatly increased both the quality and quantity of my time at Caltech, though not necessarily in that order. May it live
on and continue serving MabuchiLab at Stanford, and my best of luck to you guys in finding a regulation table. To Asa my officemate and politics liaison, thanks for the interesting conversations outside of research, and for putting up with my work area. Ramon deserves special mention for saving me in the eleventh hour by hacking the CIT thesis style file. Thanks to Tim for sharing his experiences with seeking an alternative career. Kevin ‘Employee Of The Month’ McHale deserves special acknowledgment for his contributions to chapter 4 of this thesis, which turned out to be instrumental in obtaining one of the key results of this work. I depart MabuchiLab knowing my foosball moves could not be in better hands. A huge thank you to Sheri, who keeps everything running smoothly despite having to put up with us juveniles.

Life definitely would not have been the same without the original crew, going way back to in an era when group meeting had an Alias, and the ˆa’s annihilated rather than get annihilated. Good times . . . Ben, thanks for opening my eyes to what intense passion for science is all about. Mike, my true Laker brother, how will I ever forget chasing that factor of two with you? To Andy, for the numerous athletic activities that helped keep me sane, and last but not least, Stockton, thanks especially for helping me keep it real during the home stretch. I have many fond memories of our years together. Thanks for being such an integral part of my grad school experience.

To the rest of my thesis defense committee Oskar Painter, Chiara Daraio and Axel Scherer: Thanks for agreeing to be on my committee, and for the positive feedback and insightful questions you had during the defense. To you, the reader. Even if you are just reading the acknowledgements, I hope it has not been a waste of time.

My two little angels Charis and Akirin: you have brought such joy to me and kept me balanced. Thanks for reminding me of the importance of wonderment and curiosity.

And finally, my dearest wife Yuki, to properly thank you would more than double the length of this thesis. I still cannot fathom how blessed I am to have you in my life. Thanks for persevering with me, and just being with me throughout this journey. This is our victory.
Abstract

We present an *ab initio* treatment of the inverse photonic bandgap (or photonic crystal) device design problem. Using first principles, we derive the two-dimensional inverse Helmholtz equation that solves for the dielectric function that supports a given electromagnetic field with the desired properties. We show that the problem is ill-posed, meaning a solution often does not exist for the design problem. Our work elucidates fundamental limits to any inverse problem based design approach for arbitrary and optimal design of photonic devices. Despite these severe limitations, we achieve remarkable success in two design problems of particular importance to atomic physics applications, but also of general importance to the rest of the photonic community. As the first demonstration of our technique, we *arbitrarily* design the full dispersion curve of a photonic crystal waveguide. Dispersion control is important for maintaining the shape of pulses as they propagate along the waveguide. For our second demonstration, we take a point defect photonic crystal cavity in the nominal acceptor configuration (where the central defect has a lower index of refraction than the bulk material) and force it into the donor configuration (where the defect has a higher index of refraction than the bulk material), while requiring that the electromagnetic field maintain the properties of the acceptor mode. We were able to cross over this threshold while retaining a 93.6% overlap with the original mode.
Contents

Acknowledgements iii

Abstract vi

Contents vii

List of Figures xiv

List of Tables xv

1 Introduction 1

1.1 Overview ........................................ 1

1.2 Organization of the Thesis ...................... 2

I Mathematical Formalism 4

2 The Helmholtz Equation 5

2.1 Bulk Photonic Crystal .............................. 6

2.1.1 Wave equation for \( E \) .......................... 7

2.1.2 Wave equation for \( H \) .......................... 8

2.2 2D Plane Wave Expansion (PWE) Method .......... 8

2.2.1 Boundary conditions ............................ 10

2.3 Supercell Treatment ................................. 14

2.3.1 Point defect: cavity .............................. 14

2.3.2 Line defect: waveguide ......................... 17
2.4 Convergence Issues of the PWE Method ........................................ 17

3 Inverse Problems ................................................................. 20
    3.1 Introduction ........................................................................ 21
        3.1.1 Examples .................................................................. 22
        3.1.2 Well-posedness ....................................................... 24
    3.2 Matrices as Linear Operators ................................................ 25
        3.2.1 A numerical example ............................................... 25
        3.2.2 Singular value decomposition ...................................... 29
    3.3 Regularization and the L-curve ............................................. 32
        3.3.1 An alternate interpretation ......................................... 34
    3.4 Conclusion ......................................................................... 35
        3.4.1 Parameter estimation vs. design .................................. 37

4 Convex Optimization .............................................................. 39
    4.1 Introduction ........................................................................ 40
        4.1.1 Organization ............................................................. 41
    4.2 Derivatives ........................................................................ 42
        4.2.1 Complex variables ..................................................... 44
    4.3 Convex Sets and Functions .................................................. 47
        4.3.1 Convexity conditions ................................................ 49
    4.4 Gradient and Newton Methods ............................................. 50
        4.4.1 Unconstrained optimization ...................................... 51
        4.4.2 Incorporating constraints: barrier method .................. 58
    4.5 Conclusion ......................................................................... 61

II Device Design ........................................................................ 63

5 Photonic Bandgap Devices: An Overview ................................. 64
    5.1 Introduction ...................................................................... 64
    5.2 Building Blocks .............................................................. 66
8.2.1 The direct solution ........................................... 109
8.3 Iterative Approach ............................................. 110
  8.3.1 Dispersion design .......................................... 111
  8.3.2 Cavity design ................................................ 113
8.4 Concluding Remarks ........................................... 117

Appendices ......................................................... 118

A Sample Matlab Code to Illustrate Ill-Conditioning .......... 119
B Barrier Functions of Complex Variables ..................... 121
C Fourier Transforms .............................................. 123
  C.1 Boundary Conditions and Fourier Space ................... 124
  C.2 Numerical Implementation ................................... 127
  C.3 The Symmetry Problem ....................................... 130
    C.3.1 The underlying real-space function .................... 131
    C.3.2 Even vs. odd ............................................. 132
  C.4 Fourier Factorization ........................................ 134
  C.5 Conclusion .................................................... 137
D Detailed Errata for Geremia 2002 .............................. 138
  D.1 Introduction .................................................. 138
    D.1.1 Relevant abstract of Geremia 2002 .................... 138
    D.1.2 Typographical errors .................................... 139
    D.1.3 Proposed typographical errata ......................... 144
  D.2 Mode Optimization Errors ................................... 146
    D.2.1 Q factor .................................................. 146
    D.2.2 E field intensity ....................................... 147
    D.2.3 Mode volume ............................................. 148
  D.3 Inversion Errors .............................................. 150
List of Figures

2.1 Geometry of 2D hexagonal lattice ........................................ 10
2.2 Geometry of reciprocal lattice of a 2D hexagonal lattice .............. 11
2.3 Point defect cavity in supercell approximation ............................ 15
2.4 Line defect waveguide in supercell approximation ....................... 16

3.1 Stability of Hilbert matrix .................................................. 27
3.2 Stability of Hilbert matrix .................................................. 29
3.3 Linear transformation under the SVD ...................................... 30
3.4 L-curve for the Hilbert operator inverse problem ....................... 34
3.5 Spectrum of singular values for the Hilbert operator ................... 36
3.6 Spectrum of singular values for the inverse photonic problem .......... 37

4.1 Graphical representation of test for convex function ..................... 48
4.2 Convex sets ........................................................................ 49
4.3 Global underestimator of a convex function ................................ 50
4.4 Backtracking line search ..................................................... 53
4.5 Gradient method convergence comparison .................................. 54
4.6 Problems with the gradient method ....................................... 55
4.7 Second-order approximation of objective function ..................... 56
4.8 Newton method convergence comparison .................................. 57
4.9 The log barrier function ..................................................... 59
4.10 Modified objective function ............................................... 60
4.11 Poor quadratic fit with log barrier ....................................... 62

5.1 Photonic crystal waveguide .................................................. 66
C.1 Fourier transform of a square pulse .................................... 126
C.2 Domain convention for the FFT ......................................... 129
C.3 Shifting the origin in a 2D FFT .......................................... 130
C.4 Underlying continuous functions corresponding to $N$ FFT coefficients . 132
C.5 Even vs. Odd numbered FFTs .......................................... 134
C.6 An arbitrary discontinuous real-space function in 2D ............... 135
C.7 Comparing FFT coefficients in an even vs. odd grid ............. 136
C.8 Laurent’s Rule vs. Inverse Rule ....................................... 137

D.1 Incorrect orthogonality condition .................................... 152
List of Tables

4.1 Performance of gradient method ........................................... 54
4.2 Performance of Newton’s method ........................................... 57