

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

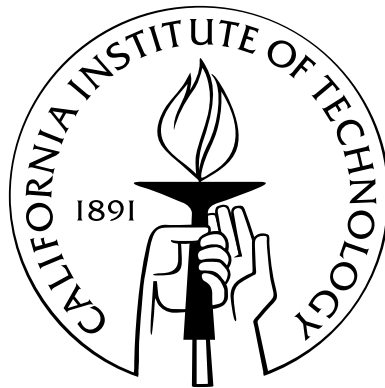
Thesis by

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)

© 2007

John K. Au

All Rights Reserved

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 acknowledgement 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 \hat{a} '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 \mathbf{E}	7
2.1.2 Wave equation for \mathbf{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

5.3	PBG and Atomic Physics	68
5.3.1	Waveguide dispersion design	69
5.3.2	Large defect region cavity design	70
6	Inverting the Helmholtz Equation	73
6.1	Introduction	73
6.2	Inverse Problem Based Design	73
6.2.1	Genetic algorithms	76
6.2.2	Topology optimization methods	77
6.2.3	Level set method	78
6.2.4	Analytical inversion of waveguide modes	78
6.2.5	Our approach	79
6.3	Inverse Helmholtz Equation	80
6.3.1	Point defects	80
6.3.2	Line defects	82
6.4	Proof of Principle	83
6.4.1	Tikhonov solution	84
6.5	Simulating Design Errors	85
6.5.1	Convex optimization regularization (COR)	88
7	From Inverse Problems to Device Design	91
7.1	3:1 Waveguide Splitter	91
7.2	Residual Norm	93
7.3	Inverse Problem Based Design Flow	97
7.3.1	Valid eigenmode landscape	99
7.4	Conclusion	102
7.4.1	Comparing Tikhonov and Convex Optimization Regularization	103
8	Results	105
8.1	Waveguide Dispersion	105
8.2	Enlarged Defect Cavity	106

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	\mathbf{E} field intensity	147
D.2.3	Mode volume	148
D.3	Inversion Errors	150

D.3.1	Correct derivation in the bulk mode basis	153
D.3.2	Compare with PRE derivation	156
D.3.3	Solving the inverse equation	157
D.4	Results Errors	158
	Bibliography	160

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

5.2	Comparing donor and acceptor modes	71
5.3	Fabrication constraints to acceptor mode	71
6.1	Dielectric function for the h_1 defect	84
6.2	Localized defect mode for the h_1 defect	85
6.3	Proof of principle solution using QR factorization	86
6.4	Proof of principle solution using Tikhonov regularization	87
6.5	Proof of principle solution using Tikhonov regularization with initial geometry	88
6.6	Designing a noisy h_1 mode using Tikhonov regularization	89
6.7	Designing a noisy h_1 mode using convex optimization regularization . .	90
7.1	Target mode for the 3:1 splitter device	92
7.2	3:1 splitter device design output	93
7.3	L-curve for 3:1 Splitter	94
7.4	3:1 splitter device design output using L-curve corner	95
7.5	3:1 splitter device final design	96
7.6	Output mode of 3:1 splitter device	97
7.7	Perturbing the dielectric	100
7.8	Perturbation to eigenmode	101
7.9	Sparsity of valid eigenmodes	101
8.1	The PCW dispersion design problem	106
8.2	Nominal h_1 defect geometry	107
8.3	Cross-section of Gaussian broadened dielectric function	108
8.4	Non-iterative result of waveguide design	110
8.5	Comparing target and result for dispersion engineering	112
8.6	Dispersion engineered waveguide design	113
8.7	Comparing the target and the result for the cavity design	115
8.8	Final enlarged defect cavity	116
8.9	Non-monotonic dependence of performance on iteration number	116

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