

Inverse design in Quantum Acoustics

Designing a Phononic Beamsplitter using Inverse Design with Adjoint
Simulation

David Hambræus

[DRAFT]

Inverse design in Quantum Acoustics:
Designing a Phononic Beamsplitter using Inverse Design with Adjoint Simulation

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Abstract

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Acknowledgements

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David Hambraeus, Gothenburg, May 2023

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Acronyms

ADAM Adaptive Moment Estimation. [v](#), [13](#), [14](#)

GD Gradient Descent. [v](#), [14](#)

PML Perfectly Matched Layer. [v](#), [15](#)

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■	General comment / question	1
■	Things that could be done now, no further simulations/consultation needed	1
■	Things that could be done now but I am not sure if I should, or how to do it	1
■	Things that can't be done yet because they depend on other things, e.g. results	1
■	Citation needed	1
■	After thesis is done, check that I've used cref and not ref	2
■	References before the dot or after? And space or no space?	2
■	Introduction to quantum acoustics...I need to read more literature I think	2
■	Restructure a little... I would like to talk about inverse design first and quantum acoustics second. Talk about how inverse design is a concept that has been applied to nanophotonics but not to quantum acoustics yet. Then talk about why we care about quantum acoustics. It feels a little bit forced to do it in that order though, talking about quantum acoustics first might be a better idea, since that would naturally lead one to introduce the problem of design.	2
■	cite something, check Ida's thesis maybe	2
■	With no external forces we get traveling modes=eigenvalues. Explain how and why periodicity means only certain modes can propagate. Good resource in Chan's thesis, or maybe solid state physics book?	5
■	Sakurai does basically the same derivation but for electronic states in a crystal lattice, but he also uses operator formalism. Can I cite that? Other option is citing Chan's PhD who do it the same way for photonic crystals and says that it can be done analogously for phononic crystals.	5
■	At some point write about phonons? I haven't really had to care about the fact that excitations are discrete so if I talk about it it'd just for applications...	7
■	Write about PML design and why we need it: Simulating infinite waveguides isn't possible because of the finite computing power. Also we don't care about stuff far away, just that there are no reflections that can interfere. Or maybe write about this in the method...	7
■	dynamic equation? Better name	9
■	Big fat box on functionals and their derivatives. I think this should be included somewhere, since very few of my peers know what a functional derivative is... Not really sure how though. I kinda like the thought of putting it in a box like this	9
■	footnote should probably be deleted...	10

■ I find the definition somewhat difficult to comprehend and really didn't understand it until I sat down and did some examples for myself. Maybe talk about analogies to vector functions.	10
■ Look over what domains all of the integrals integrate over.	10
■ This integral would be over the unit cell, or over all of space but with $\phi_i(\mathbf{x})$ being non-zero only inside the unit cell	11
■ I am mixing putting the argument in the denominator / after the functional derivative. Should I be consistent? I like after more, but it is a bit weird when putting the operant after the derivative	11
■ use the form of \hat{A} to obtain an explicit formula for this	12
■ The infamous integral. Still am not entirely sure about it, but I haven't thought more about it since I abandoned that.	12
■ more examples	13
■ Cool thing to maybe put in. If you have a linear function $f(x) = v \cdot x + k$, what is the probability that you will significantly (say more than 10% of optimal step) increase f with a random unit length step? Optimal: step in \hat{v} , $\Delta f = v \cdot \hat{v} = \ v\ $. Probability of 10% of this: $\int_{0.1}^1 (1 - x^2)^{n/2} dx / \int_{-1}^1 \dots$ use $(1 - x^2)^n \approx \exp(-nx^2)$	13
■ Pseudocode for the algorithm	14
■ Somewhere I should write about epsilon, and alpha and how I set them, but that probably needs to come later, in the method	14
■ Write about why we use the mode we use, and why I clamp the bottom. Can reference Johan and Pauls paper	15
■ Hold up. . . why do I choose an exponentially increasing imaginary component. If the two possible sources of reflections are the discontinuous jump when the pml starts and that the increase is too steep, then why not just use a straight line?	15
■ How? (Isn't it obvious?)	16
■ Create another figure that shows it in two dimensions. I'm thinking a circular boundary, and adding s in the left half and subtracting s in the right half. Alternatively adding $s \cdot x$ (unit circle centered on 0) so that it will be smooth	17
■ Write about how I use it? This feels like it should come after I've talked about computing the derivative.	17
■ Maybe I'll only mention that f is an integral of the displacement field in the theory and here give the specific formula:	18
■ Paragraph about pure part of objective function, enforcing the minimum feature size	18
■ Give the explicit formula for the gradient now that the objective function has been fully defined	18
■ Describe what optimization algorithm was used, as well as how this changed during the simulation. E.g. first 200 iterations ADAM; next ADAM but with sigmoid function application; sigmoid + feature size; and finally level-set.	18

Todonotes are organized as follows:

General comment / question

Things that could be done now, no further simulations/consultation needed

Things that could be done now but I am not sure if I should, or how to do it

Things that can't be done yet because they depend on other things, e.g. results

Citation needed

1. Introduction

After thesis is done, check that I've used cref and not ref

References before the dot or after? And space or no space?

Introduction to quantum acoustics... I need to read more literature I think

Restructure a little... I would like to talk about inverse design first and quantum acoustics second. Talk about how inverse design is a concept that has been applied to nanophotonics but not to quantum acoustics yet. Then talk about why we care about quantum acoustics. It feels a little bit forced to do it in that order though, talking about quantum acoustics first might be a better idea, since that would naturally lead one to introduce the problem of design.

Conventionally, when designing these components, the designer comes up with a design through intuition and parametrizes it with a couple of parameters. For example they may believe that a structure with periodically placed circular holes should yield a device that performs the desired function. The parameters that are unknown might then be the distance between neighbouring holes and the radius of the holes. To find the optimal device they would then systematically test parameter values to see which give the best performance in a simulation of the device. This brute force method of design limits the possible number of parameters to a very small number. If there are 10 different values to test for each parameter, even six parameters would require 1,000,000 simulations. One can of course use smarter optimization algorithms like [bayesian optimization](#) or particle swarm optimization[1] to decrease the number of simulations needed, but it will still be of the same order.

cite something, check Ida's thesis maybe

A different approach that has been gaining some popularity is *inverse design with adjoint simulation*. [2] The idea is that if the gradient of the figure of merit with respect to the parameters can be calculated, then we can use gradient based optimization methods, which converge much faster, even if the number of parameters is very large. With these methods, one hopes to be able to search among a much more general class of designs for the optimal one. Su, Vercruysse, Skarda, Sapra, Petykiewicz, and Vuckovic has developed software that successfully uses inverse design for nanophotonic devices [3].

With this thesis, we explore the possibility of extending this paradigm to acoustic devices. In order to do so, we attempt to design a phononic beam splitter.

1.1 Thesis outline

2. Theory

2.1 Acoustic waves and waveguides

In order to efficiently model the deformation and stresses in a solid material, a linear elasticity model is often assumed. For small deformations, solid materials obey Hooke's law which in it's full form looks like

$$\sigma = C : \epsilon$$

where σ is the stress tensor, C the elasticity tensor which is a four-tensor that is a property of the material, $\epsilon := \nabla \mathbf{u} + (\nabla \mathbf{u})^T$ is the strain tensor, and $:$ denotes double scalar product. This equation is linear in \mathbf{u} , hence the name *linear* elasticity. Using this and newtons equations of motion, the equation governing the dynamics is obtained:

$$\rho \ddot{\mathbf{u}} = \nabla \cdot \sigma + \mathbf{F}.$$

where ρ is the density, \mathbf{u} is the displacement and \mathbf{F} is the externally applied force. Assuming a time harmonic solution $\mathbf{u}(\mathbf{x}, t) = \mathbf{u}(\mathbf{x})e^{i\omega t}$ with angular frequency ω this becomes

$$-\rho\omega^2 \mathbf{u} = \nabla \cdot \sigma + \mathbf{F}.$$

To combine these into one equation that can be solved for \mathbf{u} we first rewrite them in index notation to make calculations clearer:

$$\epsilon_{ij} = \frac{1}{2}(\partial_i u_j + \partial_j u_i) \tag{2.1}$$

$$\sigma_{ij} = C_{ijkl}\epsilon_{kl} \tag{2.2}$$

$$= \frac{1}{2} \left(C_{ijkl}\partial_k u_l + C_{ijlk}\partial_l u_k \right) \tag{2.3}$$

$$= C_{ijkl}\partial_k u_l \text{ because of the symmetry of } C \tag{2.4}$$

which gives

$$F_i = -\rho\omega^2 u_i - \partial_j \sigma_{ij} \tag{2.5}$$

$$= -\rho\omega^2 \delta_{ik} u_k - \partial_j \left(C_{ijkl} \partial_l u_k \right) \tag{2.6}$$

$$= - \left(\rho\omega^2 \delta_{ik} \cdot + \partial_j \left(C_{ijkl} \partial_l \cdot \right) \right) u_k \tag{2.7}$$

where the indices i, j, k, l go over the spacial dimensions x, y, z . All of the tensors in the equation above are really tensor fields, i.e. they are functions of \mathbf{x} . Defining the operator \hat{A}_{ik} as $-\left(\rho\omega^2 \delta_{ik} \cdot + \partial_j \left(C_{ijkl} \partial_l \cdot \right) \right)$ we can write

$$\hat{A}_{ik} u_k = F_i \tag{2.8}$$

With no external forces we get traveling modes=eigenvalues. Explain how and why periodicity means only certain modes can propagate. Good resource in Chan's thesis, or maybe solid state physics book?

2.1.1 Bloch States and Band Diagrams

With no external forces, i.e. $F_i = 0$, (2.8) can be written as

$$\frac{1}{\rho} \partial_j (C_{ijkl} \partial_l u_k) = \omega^2 u_i \quad (2.9)$$

which is an eigenvalue equation for the operator $\hat{O}_{ik} = \frac{1}{\rho} \partial_j (C_{ijkl} \partial_l \cdot)$ where eigenvalues are the angular frequency squared. If furthermore the structure is periodic, then the eigenstates are so called *Bloch states*.

If the structure is periodic with some periodicity \mathbf{a} , meaning that $C_{ijkl}(\mathbf{x}) = C_{ijkl}(\mathbf{x} + n\mathbf{a})$ where n is an integer, then this operator commutes with the translation operator $\hat{T}_{\mathbf{a}} \mathbf{u}(\mathbf{x}) = \mathbf{u}(\mathbf{x} + \mathbf{a})$. This means that there is a space of simultaneous eigenstates to both of them. The eigenfunctions of the translation operator are $\exp(i\mathbf{k} \cdot \mathbf{x})$ with eigenvalues $\exp(ika)$, where $a = |\mathbf{a}|$. Defining the reciprocal lattice constant $\mathbf{b} = 2\pi\mathbf{a}/a^2$, we see that the functions $\exp(i(\mathbf{k} + m\mathbf{b}) \cdot \mathbf{x})$ for integer values of m all have the same eigenvalue, which means that they form a degenerate subspace of eigenfunctions. Thus we can write the eigenfunctions of both operators as

$$\mathbf{u}_{\mathbf{k}}(\mathbf{x}) = \sum_m e^{i(\mathbf{k} + m\mathbf{b}) \cdot \mathbf{x}} \mathbf{u}_{m,\mathbf{k}}(\mathbf{x}) = e^{i\mathbf{k} \cdot \mathbf{x}} \bar{\mathbf{u}}_{\mathbf{k}}(\mathbf{x}) \quad (2.10)$$

where $\bar{\mathbf{u}}_{\mathbf{k}}$ is a periodic function with periodicity \mathbf{a} .

Sakurai does basically the same derivation but for electronic states in a crystal lattice, but he also uses operator formalism. Can I cite that? Other option is citing Chan's PhD who do it the same way for photonic crystals and says that it can be done analogously for phononic crystals.

The solutions to these eigenvalue equations are often called modes, and each mode has both a frequency and a wave vector. This gives rise to a band diagram, where the frequency is plotted as a function of the wave vector.

2.1.1.1 Concrete example of phononic crystal

In this work, a rectangular waveguide patterned with ellipses is used. The structure is clamped at the bottom (meaning that we use a fixed boundary condition there) while the other sides are free. A top down schematic of the unit cell can be seen in [figure 2.1](#).

Enforcing a wave vector $\mathbf{k} = k\hat{\mathbf{y}}$ and running COMSOL to find the eigenmodes with their corresponding frequencies for this structure yields the band diagram in

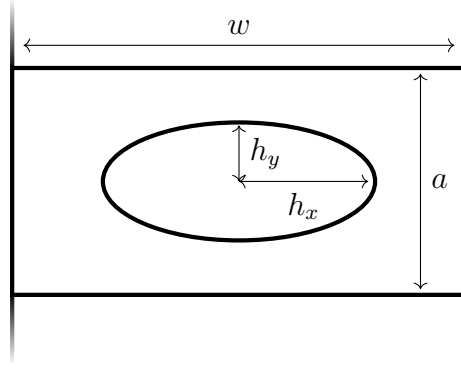


Figure 2.1: Top down view of unit cell of a phononic crystal.

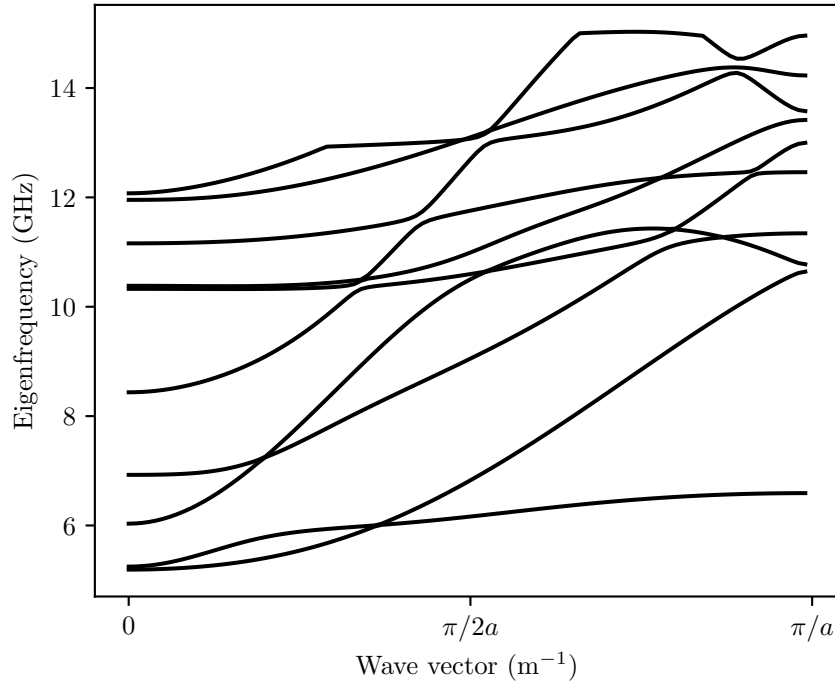


Figure 2.2: Band diagram of phononic crystal defined in [figure 2.1](#).

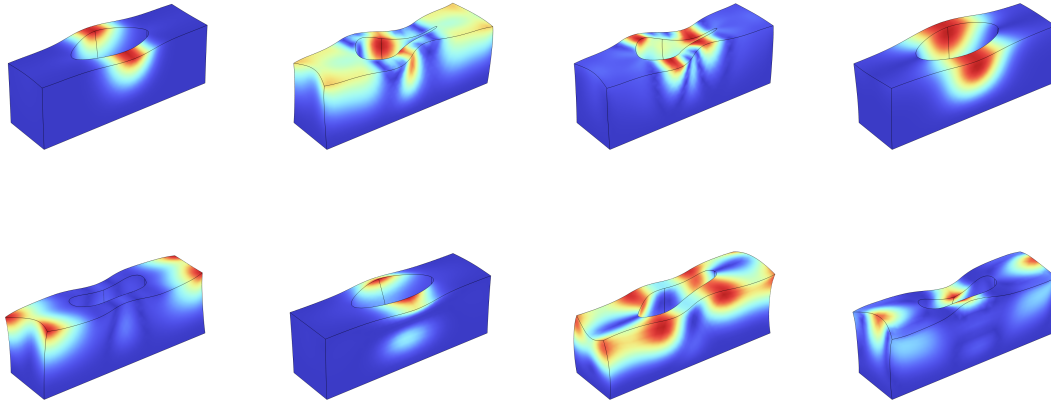


Figure 2.3: Mode shapes for the lowest eight modes at $k = 0.9\pi/a$. The color denotes the absolute value of the displacement.

figure 2.2. Figure 2.3 shows the shapes of the eight lowest lying eigenmodes at $k = 0.9\pi/a$.

At some point write about phonons? I haven't really had to care about the fact that excitations are discrete so if I talk about it it'd just for applications...

Write about PML design and why we need it: Simulating infinite waveguides isn't possible because of the finite computing power. Also we don't care about stuff far away, just that there are no reflections that can interfere. Or maybe write about this in the method...

2.2 Inverse Design

Inverse design is a design paradigm where the design of a device is guided fully by the desired characteristics. These desired characteristics are quantified through what is called an objective function¹, which I will denote f_{obj} , that should be maximized. When coupled with *adjoint simulation*, which is a clever way to compute gradients, and gradient based optimization algorithms, this is a very powerful methodology.

An overview of the design process is as follows:

1. Initialize a random device design.
2. Calculate the gradient of the design through the adjoint method.
3. Update the device design using the gradient according to the optimization

¹Also called *figure of merit (FoM)* by some.

algorithm.

4. If the device performance is good enough, terminate optimization, else return to step 2.

2.2.1 Adjoint Simulation

Adjoint simulation is a way to compute the gradient of f_{obj} with respect to the design, which in our case means with respect to the material parameters. I will in this section first give a general derivation, followed by the case of inverse design in acoustics.

2.2.1.1 General Derivation

Let f_{obj} be a function which depends on some (large) vector v . The vector v can be calculated by solving the linear equation $Av = b$, where b is a fixed vector and A is a matrix that depends on a vector of design parameters p . The overall goal is to find the parameters p that maximize the objective function f_{obj} . The goal of adjoint simulation is to find $\frac{df_{\text{obj}}}{dp}$. This can be expanded through the chain rule as

$$\frac{df_{\text{obj}}}{dp} = \frac{df_{\text{obj}}}{dv} \frac{dv}{dp}.$$

To find the latter factor we do

$$\begin{aligned} \frac{d}{dp}[Av = b] &\implies \frac{dA}{dp}v + A\frac{dv}{dp} = 0 \\ &\implies \frac{dv}{dp} = -A^{-1}\frac{dA}{dp}v \end{aligned}$$

which gives

$$\frac{df_{\text{obj}}}{dp} = -\frac{df_{\text{obj}}}{dv}A^{-1}\frac{dA}{dp}v \quad (2.11)$$

$$= -\left(A^{-T}\frac{df_{\text{obj}}}{dv}^T\right)^T \frac{dA}{dp}v \quad (2.12)$$

The first factor of this product is the solution to the *adjoint problem*

$$A^T\tilde{v} = \frac{df_{\text{obj}}}{dv}^T, \quad (2.13)$$

hence the name adjoint simulation. As it turns out, A is often symmetric (or self-adjoint) which means that this is simply a normal simulation but with df_{obj}/dv^T (or $df_{\text{obj}}/dv^\dagger$) as the source. Thus, to obtain the derivative we just need to run an additional simulation with a different input.

Now you might be wondering: what have we gained by this? Let n be the dimension of v , m the dimension of p and l the dimension of b . This means that A is a matrix

with dimension $l \times n$ and dA/dp is a three-tensor with dimension $m \times l \times n$. Thus calculating $A^{-1}dA/dp$ directly involves solving $Ax = w$ for a three-tensor, and calculating $A^{-1}(dA/dp)v$ involves solving for a matrix, both of which are orders of magnitude more computationally expensive than solving for a vector.

2.2.1.2 Specific derivation with acoustics

Now we turn to the specific case of acoustic devices. Here $Av = b$ is replaced by the dynamic equation of linear elasticity:

$$\hat{A}_{ik}u_k = F_i \quad (2.14)$$

dynamic
equation?
Better
name

Instead of vectors, like we saw in [section 2.2.1.1](#), these quantities are now functions² of \mathbf{x} . Analogously to the vector of design parameters we now have a *design field* $p(\mathbf{x})$.

On functionals and their derivatives

Big fat box on functionals and their derivatives. I think this should be included somewhere, since very few of my peers know what a functional derivative is... Not really sure how though. I kinda like the thought of putting it in a box like this

Our f_{obj} is no longer a function, but rather a *functional*, and thus we need to use the functional derivative instead of the ordinary derivative. One can think of a functional as a function of a function, i.e. something that maps an element of a function space to a scalar number. There are also functionals which depend on both a function and a real number, or on multiple functions. Below I will give an overview of the notational conventions I use, and then give the definition of the functional derivative as well as some useful properties of it.

Let \mathcal{Y} be a function space of functions $\mathbb{R} \rightarrow \mathbb{R}$. A functional $F : \mathcal{Y} \rightarrow \mathbb{R}$ evaluated at the function $f \in \mathcal{Y}$ is notated with the function in square brackets: $F[f]$. If the functional additionally depends on a real number, $G : \mathcal{Y} \times \mathbb{R} \rightarrow \mathbb{R}$, that is put in round brackets: $G[f](x)$. Note that in principle, F is the functional while $F[f]$ is just a number, analogously to how f is a function while $f(x)$ is a real number.

The functional derivative of F with respect to it's function argument is a functional $\mathcal{Y} \times \mathbb{R} \rightarrow \mathbb{R}$ denoted $\delta F[f]/\delta f$. In this expression, f is technically a dummy function, writing $\delta F[g]/\delta g$ is exactly the same functional. Almost always the functional derivative will be evaluated at some function h . In the

²Vector-valued functionals, but that is not the important part here.

stringent notation this is written

$$\frac{\delta F[g]}{\delta g}[h] \quad (2.15)$$

and is simply an ordinary function $\mathbb{R} \rightarrow \mathbb{R}$. However, I will use the notation $\delta F/\delta h$ for this, to make the equations clearer.^a

footnote should probably be deleted...

^aThis is consistent with how many other authors use the notation, though whether that is an *intentional* notational simplification or not I will leave unsaid...

In addition, when evaluating the functional derivative at a point, the argument can be put either after it, or in the denominator:

$$\frac{\delta F[g]}{\delta g}[h](x) = \frac{\delta F}{\delta h}(x) = \frac{\delta F}{\delta h(x)}. \quad (2.16)$$

The functional derivative is defined by

$$\int \frac{\delta F}{\delta f}(x) \varphi(x) dx = \frac{d}{d\varepsilon} F[f + \varepsilon \varphi] \quad (2.17)$$

where F is a functional of f and φ is an arbitrary test function.

I find the definition somewhat difficult to comprehend and really didn't understand it until I sat down and did some examples for myself. Maybe talk about analogies to vector functions...

I will use two properties of the functional derivative:

- If F is the functional $F[f](y) = f(y)$, then $\delta F(y)/\delta f(x) = \delta(y - x)$.
- The chain rule: if F is a functional with one function argument, G is a functional with one function and one real argument, and H is the functional defined as $H[f] = F[G[f](y)]$, then

$$\frac{\delta H}{\delta f}(x) = \int \frac{\delta F}{\delta G[f]}(y) \frac{dG(y)}{df}(x) dy \quad (2.18)$$

Look over what domains all of the integrals integrate over.

For simplicity I will limit myself to the case where the objective function is an overlap

integral of the displacement field $u_k(\mathbf{x})$ with some function $\varphi_k^*(\mathbf{x})$:

$$f_{\text{obj}}[\mathbf{u}] = \int u_i(\mathbf{x}) \varphi_i^*(\mathbf{x}) d\mathbf{x}. \quad (2.19)$$

Such an integral is a scalar product in the space where $\mathbf{u}(\mathbf{x})$ resides.

Analogously to the general derivation, we will use the chain rule to expand $\delta f_{\text{obj}}/\delta p(\mathbf{x})$. However, because \mathbf{u} is in general complex, I will split it into its real and imaginary components: $u_i = v_i + iw_i$.

$$\frac{\delta f_{\text{obj}}}{\delta p}(\mathbf{x}) = \int_{\Omega} d\mathbf{y} \frac{\delta f_{\text{obj}}}{\delta v_i}(\mathbf{y}) \frac{\delta v_i(\mathbf{y})}{\delta p}(\mathbf{x}) + \frac{\delta f_{\text{obj}}}{\delta w_i}(\mathbf{y}) \frac{\delta w_i(\mathbf{y})}{\delta p}(\mathbf{x}) \quad (2.20)$$

The first factor of each of the two terms is easy enough to calculate:

$$\frac{\delta f_{\text{obj}}}{\delta v_i}(\mathbf{y}) = \frac{\delta}{\delta v_i(\mathbf{y})} \int_{\Omega} u_j(\mathbf{x}) \varphi_j^*(\mathbf{x}) d\mathbf{x} \quad (2.21)$$

$$= \int_{\Omega} \frac{\delta}{\delta v_i(\mathbf{y})} u_j(\mathbf{x}) \varphi_j^*(\mathbf{x}) d\mathbf{x} \quad (2.22)$$

$$= \int_{\Omega} \delta(\mathbf{x} - \mathbf{y}) \delta_{ij} \varphi_j^*(\mathbf{x}) d\mathbf{x} \quad (2.23)$$

$$= \varphi_i^*(\mathbf{y}) \quad (2.24)$$

and

$$\frac{\delta f_{\text{obj}}}{\delta w_i}(\mathbf{y}) = \frac{\delta}{\delta w_i(\mathbf{y})} \int_{\Omega} u_j(\mathbf{x}) \varphi_j^*(\mathbf{x}) d\mathbf{x} \quad (2.25)$$

$$= \int_{\Omega} \frac{\delta}{\delta w_i(\mathbf{y})} u_j(\mathbf{x}) \varphi_j^*(\mathbf{x}) d\mathbf{x} \quad (2.26)$$

$$= \int_{\Omega} i \delta(\mathbf{x} - \mathbf{y}) \delta_{ij} \varphi_j^*(\mathbf{x}) d\mathbf{x} \quad (2.27)$$

$$= i \varphi_i^*(\mathbf{y}) \quad (2.28)$$

which gives us

$$\frac{\delta f_{\text{obj}}}{\delta p}(\mathbf{x}) = \int_{\Omega} d\mathbf{y} \varphi_i^*(\mathbf{y}) \frac{\delta v_i(\mathbf{y})}{\delta p}(\mathbf{x}) + i \varphi_i^*(\mathbf{y}) \frac{\delta w_i(\mathbf{y})}{\delta p}(\mathbf{x}) \quad (2.29)$$

$$= \int_{\Omega} d\mathbf{y} \varphi_i^*(\mathbf{y}) \text{Re} \left(\frac{\delta u_i(\mathbf{y})}{\delta p}(\mathbf{x}) \right) + i \varphi_i^*(\mathbf{y}) \text{Im} \left(\frac{\delta u_i(\mathbf{y})}{\delta p}(\mathbf{x}) \right) \quad (2.30)$$

$$= \int_{\Omega} d\mathbf{y} \varphi_i^*(\mathbf{y}) \frac{\delta u_i(\mathbf{y})}{\delta p}(\mathbf{x}) \quad (2.31)$$

This integral would be over the unit cell, or over all of space but with $\phi_i(\mathbf{x})$ being non-zero only inside the unit cell

I am mixing putting the argument in the denominator / after the functional derivative. Should I be consistent? I like after more, but it is a bit weird when putting the operand after the derivative

To find $\delta u_i(\mathbf{y})/\delta p(\mathbf{x})$ we apply $\delta/\delta p(\mathbf{x})$ to equation (2.14), which gives us

$$0 = \frac{\delta \hat{A}_{ik}}{\delta p}(\mathbf{x}) u_k(\mathbf{y}) + \hat{A}_{ik} \frac{\delta u_k(\mathbf{y})}{\delta p(\mathbf{x})} \quad (2.32)$$

The point of inverse design is that we now want to find an adjoint field $\tilde{u}_i(\mathbf{y})$ such that the integral in equation (2.31) is

$$\int_{\Omega} d\mathbf{y} \varphi_i^*(\mathbf{y}) \frac{\delta u_i(\mathbf{y})}{\delta p}(\mathbf{x}) = \int_{\Omega} d\mathbf{y} \tilde{u}_i(\mathbf{y}) \hat{A}_{ik} \frac{\delta u_k(\mathbf{y})}{\delta p}(\mathbf{x}) \quad (2.33)$$

which by equation (2.32) is equal to

$$\int_{\Omega} d\mathbf{y} \tilde{u}_i(\mathbf{y}) \frac{\delta \hat{A}_{ik}}{\delta p}(\mathbf{x}) u_k(\mathbf{y}). \quad (2.34)$$

use the form of \hat{A} to obtain an explicit formula for this

The way to find this \tilde{u}_i is through an adjoint simulation.

When discretizing space (2.33) becomes

$$\varphi_a^* \eta_{ab} = \tilde{u}_c A_{ca} \eta_{ab} \quad (2.35)$$

Meaning that to find \tilde{u} we solve

$$\varphi_a^* = \tilde{u}_c A_{ca} \quad (2.36)$$

or, taking the hermitian adjoint of both sides

$$A_{ac}^\dagger \tilde{u}_c^* = \varphi_a \quad (2.37)$$

which in normal matrix notation is

$$A^\dagger \tilde{u}^* = \varphi \quad (2.38)$$

The infamous integral. Still am not entirely sure about it, but I haven't thought more about it since I abandoned that.

2.2.2 Optimization Algorithms

In the last section I painstakingly derived how one can obtain the gradient, and in this section I will attempt to justify that by describing how one can use the gradient. I will begin by describing the advantages of gradient based optimization algorithms over those that don't use the gradient. Following that I describe the algorithm that I used, as well as some of its predecessors.

An optimization algorithm is an algorithm for finding the optimum of a function. The function is often called the *objective function* or the *cost function*. A very naive optimization method would be to simply try some number of inputs and then choose the one with the highest function value. This would require a large number of points before a good value is found, which means that it would take a long time. An improvement to this method is to use the information gained from the points already tried to decide which points to try next. If some point has a bad value, then try somewhere else; if some point has a good value, try another close by. Examples of algorithms that do this are bayesian optimization, particle swarm optimization, However, if the input to your function is very high-dimensional, choosing a random direction step in for your next try is very unlikely to yield a much better value. For such functions, it is essential that you know in which direction the function increases the fastest, so that you can choose your next point in that direction. That is why we want to use gradient based optimization algorithms; they enable us to quickly find the right direction to go in for best improvement.

more examples

Cool thing to maybe put in. If you have a linear function $f(x) = v \cdot x + k$, what is the probability that you will significantly (say more than 10% of optimal step) increase f with a random unit length step? Optimal: step in \hat{v} , $\Delta f = v \cdot \hat{v} = \|v\|$. Probability of 10% of this: $\int_{0.1}^1 (1 - x^2)^{n/2} dx / \int_{-1}^1 \dots$ use $(1 - x^2)^n \approx \exp(-nx^2)$.

2.2.2.1 Gradient Descent

The simplest gradient based optimization algorithm is called *gradient descent*. Like all of the algorithms I will describe it is an iterative algorithm, meaning that it generates a sequence of points that converges to an optimum, and the next point in the sequence is derived from the previous ones. In the case of gradient descent, the next point is gotten by

$$p_n = p_{n-1} + \eta g_{n-1} \quad (2.39)$$

where η is the so called *learning rate* and g_{n-1} is the gradient of the objective function at p_{n-1} . For ordinary gradient descent the learning rate would be fixed, and choosing an appropriate value for this parameter is one of the problems of this method. If a too high value is chosen, then the steps taken will be too large and the optimum might be missed entirely. A too low value results in too small steps which will yield a slow convergence. Almost all gradient descent implementations use a so called learning schedule, which means that η is not constant during the learning. This introduces the additional problem of how to choose how fast and between which values it should change.

2.2.2.2 Adaptive Moment Estimation (ADAM)

The [ADAM](#) algorithm is an improved version of gradient descent. It has three main differences:

1. Each dimension has a separate learning rate.

2. The learning rate is automatically set from the previously seen gradients.
3. The evolution carries some momentum.

Figure 2.4 shows the difference in performance between ADAM and GD. With a slightly too large learning rate, the GD algorithm gets stuck in an oscillation and makes very little progress towards the minimum. If the learning rate is decreased, the oscillations disappear but the stepsize is now too small to make it all the way to the true minimum. Since the ADAM algorithm has some momentum, the motion along the valley gets compounded while the motion perpendicular gets dampened which means that the oscillations are not as much of a problem. The adaptive learning rate also means that the algorithm doesn't get stuck prematurely due to the small gradient at the bottom of the valley.

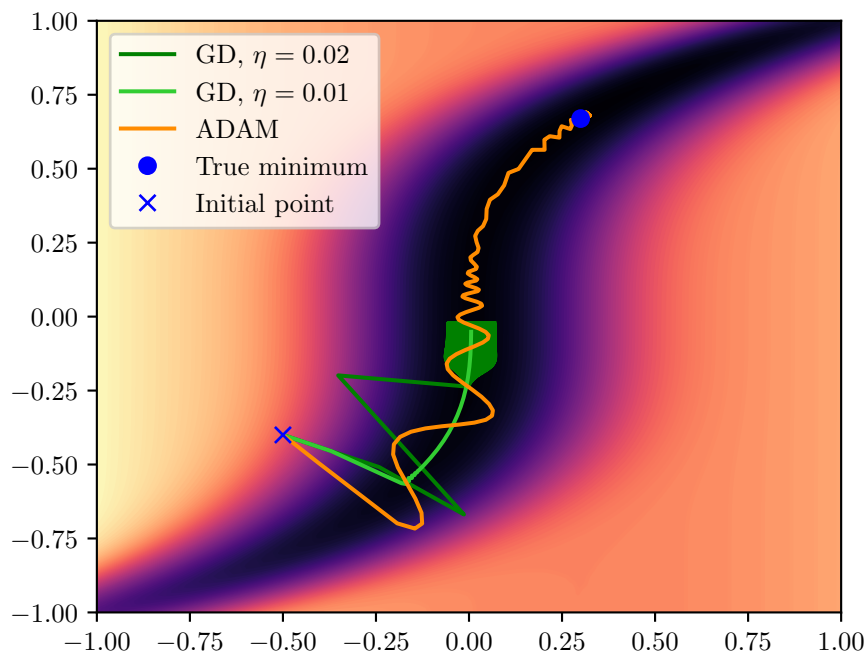


Figure 2.4: A comparison between ADAM and GD in an optimization landscape with a narrow canyon. The two different GD algorithms are shown with 1000 steps, while 200 steps with the ADAM algorithm are shown.

Pseudocode for the algorithm

Somewhere I should write about epsilon, and alpha and how I set them, but that probably needs to come later, in the method

3. Methods

The aim of this thesis is to use inverse design to find a phononic beamsplitter, a task that can be divided into three parts: First, some definitions of what should be designed and what constitutes a “good” design needs to be made. Second, we need a way to calculate the gradient of the “goodness” with respect to the design. And lastly, we need a gradient based optimization algorithm to find the optimal design. All of this will be described in this chapter.

3.1 Design

The device design to be optimized can be seen in figure 3.1

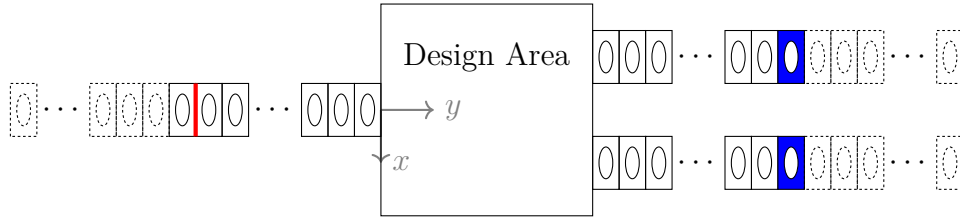


Figure 3.1: Device design to be optimized. At the red line, a wave traveling right is excited. On the blue unit cells is where the output is measured. The dashed unit cells are *PML*

Write about why we use the mode we use, and why I clamp the bottom. Can reference Johan and Pauls paper

3.1.1 Perfectly Matched Layers (PMLs)

Ideally, we would like to have infinite waveguides but that cannot be done in practice. Instead, *PMLs* are placed at the caps of the input and output waveguides. The purpose of the *PML* is to absorb any incoming waves without reflection, which would make it act as if there was an infinite waveguide on the other side into which the waves propagate indefinitely. The way to accomplish this is to add an imaginary component to the density of the material. If there is an abrupt transition from a real density to a significant imaginary part, reflections will be created at that transition instead. Therefore, the imaginary part is taken to be exponentially increasing:

$$\rho_{\text{im}} = \rho_{\text{si}} \cdot s \cdot e^{-|y-y_0|/d} \quad (3.1)$$

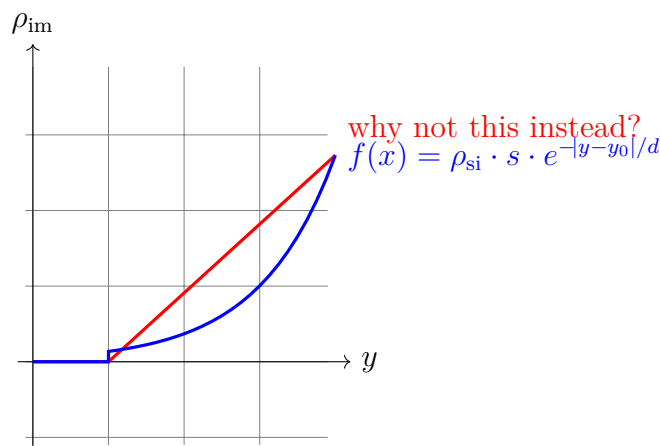


Figure 3.2: Profile of the imaginary component of the waveguides

Hold up. . . why do I choose an exponentially increasing imaginary component. If the two possible sources of reflections are the discontinuous jump when the pml starts and that the increase is too steep, then why not just use a straight line?

3.1.2 Level-set

Ultimately, we want our device to consist of regions of material and regions of no material. There are basically two ways of doing this. The first, and perhaps most intuitive, is to simply store the coordinates of the boundary between the filled and empty regions. In addition to storing the coordinates, one must also store which points neighbour which. The second method, which is the one used in this report, is called the *level-set method*. In this method, the boundary is not directly stored, but rather is stored via an *implicit function*, $\phi(x)$, defined such that the boundary is the 0-isocontour of ϕ .

There are two main advantages of using the level-set method rather than directly storing the boundary points. Firstly, when moving the boundary we would like to do so in the normal direction, as moving it along itself has no effect. Computing the normal direction of a directly stored boundary is slightly cumbersome, though certainly achievable. With level-set, moving the boundary in the normal direction is as easy as adding a constant to the implicit function. Secondly, while the boundary is changing the resolution in one part might need to be increased while the resolution in another needs to be decreased. Deciding where and when to add new points is non-trivial when directly storing the boundary. Furthermore, if two boundaries merge, or if one splits in two, points need to be removed and the connectivities changed, which is quite complex. Figure 3.3 illustrates these problems with direct storage concretely. Both of these issues are automatically handled with the level-set method.

How? (Isn't it obvious?)

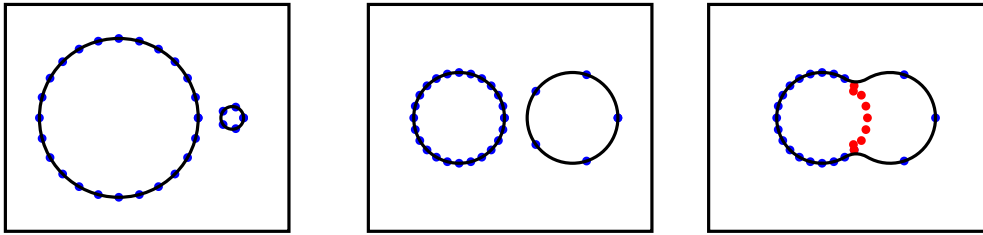


Figure 3.3: Possible evolution of boundary. In the leftmost figure, the boundary is defined by pretty much evenly spaced points. In the center figure the boundaries have moved and the spacing is no longer even, and the right circle is very poorly resolved. The rightmost figure shows the boundary after the two circles moved closer together. Now there are multiple points that need to be removed, marked in red, and the connectivity of the points that remain must be changed such that the two boundaries are merged.

There are of course a lot of possible functions $\phi(x)$ that have a given boundary as it's 0-isocontour. There is one choice that simplifies a lot of calculations though: the signed distance function. This function is defined as the distance from the closest point on the boundary, with a plus sign if it is inside and a minus sign if it is outside the boundary. It has the advantage that if one wishes to locally shift the boundary some length s in the normal direction, then simply add s to the function there. Figure 3.4 shows this effect in one dimension.

Create another figure that shows it in two dimensions. I'm thinking a circular boundary, and adding s in the left half and subtracting s in the right half. Alternatively adding $s \cdot x$ (unit circle centered on 0) so that it will be smooth

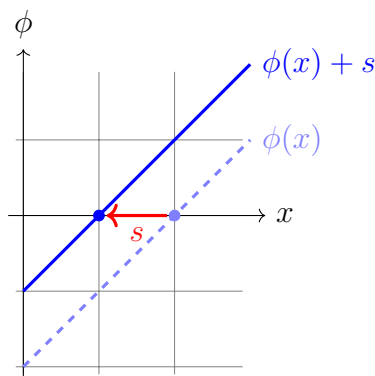


Figure 3.4: Adding s to the signed distance function shifts boundary by s .

Write about how I use it? This feels like it should come after I've talked about computing the derivative.

3.1.3 Objective function

Maybe I'll only mention that f is an integral of the displacement field in the theory and here give the specific formula:

$$f_{\text{obj}} = \int_{\Omega_1} \mathbf{m}_1^*(\mathbf{x}) \mathbf{u}(\mathbf{x}) \, d\mathbf{x} + \int_{\Omega_2} \mathbf{m}_2^*(\mathbf{x}) \mathbf{u}(\mathbf{x}) \, d\mathbf{x} \quad (3.2)$$

Paragraph about pure part of objective function, enforcing the minimum feature size

3.2 Adjoint Simulation

Give the explicit formula for the gradient now that the objective function has been fully defined

3.3 Optimization

Describe what optimization algorithm was used, as well as how this changed during the simulation. E.g. first 200 iterations ADAM; next ADAM but with sigmoid function application; sigmoid + feature size; and finally level-set.

4. Results

5. Conclusion

References

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- [2] S. Molesky, Z. Lin, A. Y. Piggott, W. Jin, J. Vucković, and A. W. Rodriguez, “Inverse design in nanophotonics,” *Nature Photonics*, vol. 12, no. 11, pp. 659–670, Nov. 2018, Number: 11 Publisher: Nature Publishing Group. DOI: [10.1038/s41566-018-0246-9](https://doi.org/10.1038/s41566-018-0246-9). [Online]. Available: <https://www.nature.com/articles/s41566-018-0246-9> (visited on 2023-04-14).
- [3] L. Su, D. Vercruysse, J. Skarda, N. V. Sapra, J. A. Petykiewicz, and J. Vuckovic, “Nanophotonic inverse design with spins: Software architecture and practical considerations,” 2019. arXiv: [1910.04829](https://arxiv.org/abs/1910.04829) [[physics.app-ph](#)].

A. First appendix

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B. Second appendix

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