Inverse design of quantum acoustic devices

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April 17, 2023

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

List of Todos

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cite something, check Ida's thesis maybe 5

cite the thing the danish guys cited 5

maybe cite *inverse design in nanophotonics* 5

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Show our mode as example of this, and include band diagram 6

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1 Introduction

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

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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, the even 6 parameters would require 1,000,000 simulations. One can of course use smarter optimization algorithms like bayesian optimization or particle swarm optimization 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*. 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 et al. has developed software that successfully uses inverse design for nanophotonic devices [1].

cite the thing the danish guys cited

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.

maybe cite *inverse design in nanophotonics*

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

$$\sigma_{ij} = C_{ijkl}\epsilon_{jl}$$

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

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

where ρ is the density, $\boldsymbol{u}$ is the displacement and $\boldsymbol{F}$ is the externally applied force.

Proper derivation for equation below? It is relatively straightforward but requires some effort

Assuming a time harmonic solution $\boldsymbol{u}(\boldsymbol{x}, t) = \boldsymbol{u}(x)e^{i\omega t}$ and plugging this into the governing equations yields

$$-\rho\omega^2 u_i = \partial_j C_{ijkl}\partial_k u_l + F_i \tag{1}$$

written in index notation for clarity.

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?

At some point write about phonons? I haven't really had to care about phonons so if I talk about it it's just for applications...

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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 function[1], 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 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.

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

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

adjoint simulation is to find $\frac{\mathrm{d}f_{\text{obj}}}{\mathrm{d}p}$. This can be expanded through the chain rule as

$$\frac{\mathrm{d}f_{\text{obj}}}{\mathrm{d}p} = \frac{\mathrm{d}f_{\text{obj}}}{\mathrm{d}v}\frac{\mathrm{d}v}{\mathrm{d}p}.$$

To find the latter factor we do

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

which gives

$$\frac{\mathrm{d}f_{\text{obj}}}{\mathrm{d}p} = -\frac{\mathrm{d}f_{\text{obj}}}{\mathrm{d}v}A^{-1}\frac{\mathrm{d}A}{\mathrm{d}p}v \tag{2}$$

$$= -\left(A^{-T}\frac{\mathrm{d}f_{\text{obj}}}{\mathrm{d}v}^{T}\right)^{T}\frac{\mathrm{d}A}{\mathrm{d}p}v \tag{3}$$

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

$$A^{T}\tilde{v} = \frac{\mathrm{d}f_{\text{obj}}}{\mathrm{d}v}^{T}, \tag{4}$$

hence the name adjoint simulation. As it turns out, A is often symmetric which means that this is simply a normal simulation but with $\frac{\mathrm{d}f_{\text{obj}}}{\mathrm{d}v}^{T}$ 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 $\frac{\mathrm{d}A}{\mathrm{d}p}$ is a three-tensor with dimension $m \times l \times n$. Thus calculating $A^{-1}\frac{\mathrm{d}A}{\mathrm{d}p}$ directly involves solving $Ax = w$ for a three-tensor, and calculating $A^{-1}\left(\frac{\mathrm{d}A}{\mathrm{d}p}v\right)$ involves solving for a matrix, both of which are orders of magnitude more computationally expensive than solving for a vector.

Specific derivation with acoustics

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2.2.2 Optimization Algorithms

General paragraph on the benefits of gradient based optimization algorithms vs other algorithms? And general overview of the optimization process: simulate – compute gradient – step

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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 1

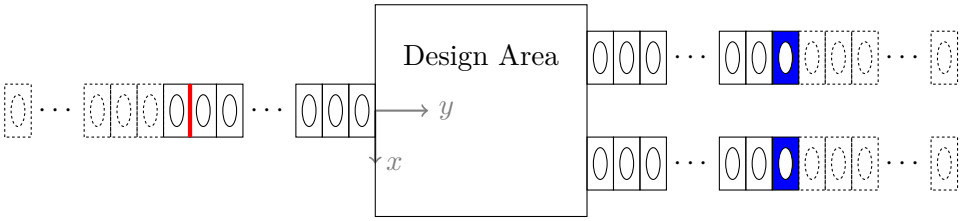

Figure 1: *Device design to be optimized. At the red line, a wave traveling right is excited. On the blue unit cells is where the output is measured. The dashed unit cells are Perfectly Matched Layer (PML)*

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

3.1.1 Level-set

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Description of it's advantages: Easily evolved (level-set equation), no connectivity issues, see level-set book

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3.1.2 Objective function

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$$f_{\text{obj}} = \int_{\Omega_1} \boldsymbol{m_1^*}(\boldsymbol{x})\boldsymbol{u}(\boldsymbol{x})\,\mathrm{d}x + \int_{\Omega_2} \boldsymbol{m_2^*}(\boldsymbol{x})\boldsymbol{u}(\boldsymbol{x}) \tag{5}$$

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

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References

[1] Logan Su et al. “Nanophotonic Inverse Design with SPINS: Software Architecture and Practical Considerations”. In: (2019). arXiv: 1910.04829 [physics.app-ph].