Inverse design of quantum acoustic devices

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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

Contents

1 Introduction

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

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

maybe cite *inverse design in nanophotonics*

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

Maybe some mechanics theory? Linear elastic material etc. Maybe also mode shape and what the waveguides / mode that we are designing for is? should that be here? It doesn't really fit in the method section I think... And more generally how waveguides work?

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

Minus sign here? Inconsistent with 3.21 in Chan's PhD thesis, but that is not consistent with itself... (3.19). Comsol has the minus sign, so probably Chan's equation has a typo.

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

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?

2.2 Adjoint Simulation

Introduce the point of inverse design, that there is an objective function / figure of merit and that we want to find the derivative of it w.r.t the material parameters.

Derive the general case: governing eq $Au = b$

Derive specific case (with functional analysis): borrowing heavily from the mathy notes is possible. Derivation is theoretically possible without specifying that the objective function is an overlap integral, only using equation (1), but the equations would be *a lot* longer and more abstruse, so I don't think that it is a good idea.

2.3 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

Paragraph describing regular gradient descent

Paragraph describing the ADAM algorithm

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

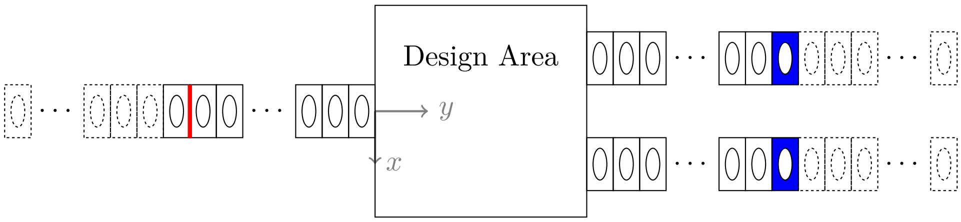

Figure 1: *Device design to be optimized. At the red line, a wave traveling right is excited. On the blue unit cells is where the output is measured. The dashed unit cells are Perfectly Matched Layer (PML)*

3.1.1 Level-set

Description of what level-set is: A way of storing a boundary between two regions; and how it works: Signed distance function

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

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

3.1.2 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:

$$f_{\text{obj}} = \int_{\Omega_1} \boldsymbol{m}_{\boldsymbol{1}}^*(\boldsymbol{x})\boldsymbol{u}(\boldsymbol{x})\,\mathrm{d}x + \int_{\Omega_2} \boldsymbol{m}_{\boldsymbol{2}}^*(\boldsymbol{x})\boldsymbol{u}(\boldsymbol{x}) \tag{2}$$

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 Discussion

6 Conclusions

References

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