A study of heterogeneous materials and wave propagation in phononic media

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Contents

1 Introduction

Heterogeneous materials appear in all kinds of forms and can be found naturally and in industrial applications. Recently, interest has grown in artificially constructed phononic media which can alter the propagation of acoustic and elastic waves. A phononic medium is a heterogeneous material which possesses spatial periodicity in the arrangement of its constituents, its structure, or the boundary conditions applied to it. As a result of this periodic structure, it has been shown that there exists band gaps for which certain frequencies of waves cannot propagate. These frequency band gaps have been utilized in many engineering applications related to vibrations and the control of acoustic and elastic waves.

The goal of the independent study was to prepare for further research in phononic media. To acheive this goal there were three objectives for this independent study:

1. Study heterogeneous materials and the associated mathematical methods used to model their behavior
2. Study wave propagation in phononic media and the associated computational methods (mainly finite elements)
3. Complete a computational project related to the above studies

The study of heterogeneous materials was completed via a set of exercises from the lecture notes of Prof. Ponte-Castañeda [1]. In this report, the focus will be on the later two items. To this end, phononic media, their applications are presented, and the interesting behavior that is the presence of frequency band gaps where waves cannot propagate is presented. After introducing these concepts, the history and state of active research is outlined in the literature review section. Dispersion relations and their relation to studies in phononic media are introduced and will be central to further studies in the report and in further research. While it is favorable to have exact analytical expressions for these dispersion relations, it is not possible to calculate these by hand for more complicated materials. As such we must utilize computational methods which are presented in varying levels of detail. For future research, it is planned to use the finite element method and there is an emphasis on this method in the independent study. Finite elements is used in the 1D and 2D case in order to obtain the dispersion relation for a variety of materials. These computational tools will be integral for further research related to phononic media.

1.1 Phononic media

As mentioned before, the field of phononic media has grown tremendously in the past two decades and continues to grow today. Examples of phononic media include mass spring systems, laminates, and materials embedded with a periodic lattice of inclusions (or voids). There are several levels of classification within phononic media. In the literature a distinction, is made between phononic materials and phononic structures. Phononic materials are infinite in extent while phononic structures are finite in extent [2]. Phononic crystals refer to a heterogenous material or non-uniform material where the material phases, that may be fluid or solid, which have a periodic arrangement in space [3]. The constituents may be arranged in such a way as to have a band gap in a fixed frequency range. This band gap may even be tunable by using an outside field to modulate material properties. A further class of phononic media that is of much interest is the metamaterial. Metamaterials possess "local resonance" which is a different way for producing band gaps that is not seen in phononic crystals.

The existence of frequency band gaps in these materials has resulted in many practical applications such as:

- *Vibration control*: The simplest application would be to incorporate these phononic media in the construction of buildings or vehicles with band gaps in the range of frequencies of acoustic or elastic waves found in the operating environment in order to provide insulation.
- *Acoustic/elastic waveguides*: By simply removing inclusions in a phononic crystal it has been found that wave propagation can be localized to certain areas within the material [4].
- *Acoustic diodes*: It has been found that sonic crystals, which are phononic crystals where one or more of the material phases is a liquid, can be used in 1D acoustic diodes which allow certain waves to propagate in one direction but not in the opposite direction [5].
- *Subwavelength imaging*: Metamaterials used in acoustic imaging are able to resolve extremely small features and are not limited by the traditional diffraction limit [6].
- *Cloaking*: Using metamaterials, it is possible to direct acoustic/elastic waves around objects [7].

This, of course, is a non-exhaustive list. New studies in materials with tunable properties, damping, non-linear affects, and disorder will lead to other novel and useful applications.

1.2 Band gaps

All of the above applications rely on presence of band gaps in these phononic media. There are two mechanisms which cause band gaps to form:

1. *Bragg scattering*: At certain frequencies, waves can interact with the structure of a material in such a way that reflections off of inclusions or the structure of material itself destructively interfere with the incident wave. Here, the behavior is dependent on the periodicity in the arrangement of the material phases or structure of the material [8].
2. *Local resonance*: When resonators are placed inside of a materials, interactions occur at the resonant frequency of the resonator. At these frequencies, the resonators begin to absorb energy from incident waves and produce a band gap.

These two mechanisms have predictable effects on the frequency band structure of phononic media.

2 Literature review

Here the field of phononic media in past and present is described. Much of the work as been applied and experimental in nature. There is plenty of room for theoretical studies building off of first principles in wave propagation and mechanics. These kinds of studies are much needed in order to fully and accurately characterize phononic media. First, past studies related to phononic media are reviewed in order to examine already explored avenues of research. Afterwards, more open fields of study are presented including damping, nonlinear systems, disordered phononic media, and dynamic effective properties.

2.1 History of phononic media

Phononic crystals as a concept first appeared in the literature five years after the proposal of photonic crystals in 1987 by Yalonovitch and John [3]. The 1992 paper by Sigalas and Economou [9] proposed a 2D phononic crystal where only in-plane shear and longitudinal waves were considered and they did observe the presence of band gaps. By the next year, Sigalas and Economou were trying to find configurations that resulted in the largest band gaps [10]. They found that, for elastic waves, the matrix should be stiffer and denser than the inclusions. Also in the 90s, 3D phononic crystals, sonic crystals, free surface waves, and various symmetries in the arrangement of inclusions were the topic of much research.

In the early 2000s, applied research in phononic crystals began to grow rapidly [3]. Presence of band gaps in these materials naturally resulted in applications related to acoustic and vibrational insulation and isolation. The emergence of wave guides due to defect engineering can be traced back to 1997. There have also been applications of phononic crystals as fluid sensors to determine rheological properties, focusing of acoustic waves, acoustic/elastic logic gates, and coupling of acoustic/elastic waves with electromagnetic signals. If these previous applications are called passive wave control, the research in active wave control, where the material properties are tunable, grew right along side these efforts also beginning in the early 2000s and leading up to today.

Parallel to this thrust of phononic crystal research in the early 2000s was the discovery of band gaps much lower than expected in a 3D lattice of rubber coated lead spheres in an epoxy matrix [11]. Materials such as these are now called acoustic/elastic metamaterials, and are distinguished from phononic crystals by the presence of another band gap found below the one as characterized by the periodicity of the lattice (due to Bragg scattering). They are often times called subwavelength band gaps for this reason. These band gaps are instead due to local resonance and are the defining property of acoustic/elastic metamaterials which are sometimes referred to as locally resonant phononic crystals. Unlike, Bragg scattering band gaps the spatial arrangement of these resonators do not have an effect on the formation of local resonance band gap. These included resonators do not need to be arranged in a lattice, but often are in order to facilitate a unit cell analysis of the material.

Applications of acoustic/elastic metamaterials largely mirrors those of phononic crystals without local resonance. The presence of this subwavelength bandgap can be combined with the Bragg band gap to create an even larger range of frequencies for better acoustic/elastic wave control. The subwavelength band gap can be exploited for acoustic imaging with resolvable length scales below what is usually allowed by the diffraction limit. A radical application of these materials is acoustic cloaking where metamaterials can be used to "steer" acoustic and elastic waves around an object [7].

2.2 Active research areas and open fields

Despite the explosion of interest in phononic media, much of the literature is focused on direct applications. Many avenues of theoretical research need to be explored from a mechanics point of view. The incorporation of damping, nonlinearities, and disorder can greatly add to the predictive capability of models and may lead to more novel applications.

2.2.1 Damping

In applications, energy is often lost through damping. This will affect the propagation of waves, and thus models that consider this effect will better represent the actual behavior of a material. While there is plenty of literature pertaining to damping in periodic materials and structures, phononic media with dissipative wave propagation has not received too much attention. One method for acoustic wave propagation in sonic crystals with viscous is to give the elastic modulus an imaginary component [3]. It wasn't until recently that damping was incorporated directly into Bloch wave analysis by assuming a complex frequency [2].

Within the body of research on damping, studies focus on either harmonic wave propagation or free wave propagation. A study of harmonic or prescribed wave propagation entails one in which the frequency is confined to be real valued while free wave propagation allows for complex frequency which can result in attenuation of the wave in time. In either the case, the wavenumber is allowed to be complex which can lead to spatial attenuation. As described in Frazier's thesis, the case of harmonic wave propagation corresponds to a system that is being subject to some periodic excitation indefinitely. The case of free wave propagation corresponds to a physical system that has been subjected to an impulse loading. Each type of analysis yields unique results in the presence of damping.

For a 1D layered composite with viscous damping, Frazier is able to use a transfer matrix method to derive analytical expressions for the dispersion relation [12]. Due to the nature of the viscous damping model (dependent on the strain rate), at higher frequencies the effects of damping become more apparent. First, it is found that the dispersion relations in the free wave and harmonic wave propagation cases are identical in the absence of damping. Accounting for damping, the frequency band structure tends to ascend in the prescribed wave propagation case and descend in the free wave propagation case. As the amount of damping increases, band gaps tend to close which is referred to as band gap annihilation. Additionally, the band gaps, with damping, in the free wave case much up with the natural frequencies of a finite, phononic structure with damping. The band gaps, with damping, in the prescribed wave case match up with observed attenuation in phononic media.

2.2.2 Nonlinear systems

Relative to linear studies, there have been fewer studies of nonlinear phononic materials. Due to nonlinearities, Bloch's theorem cannot not be applied in the same way to obtain an eigenvalue problem for the dispersion relation -at least not immediately. Perturbation techniques have been developed as early as 1994 in order to study weakly non-linear systems. These techniques "expand" the governing equations and produce a linear equation while instead considering the nonlinearities to be a part of forcing term.

Another way to study the dispersion properties of nonlinear systems, is to consider the real time evolution of a system -provided the system is simple enough such as a discrete lumped parameter system consisting of masses and springs. Frazier and Kochmann do just this when considering systems with bistable elements [13]. In the band gap of these phononic structures, small amplitude waves are attenuated and there is no transmission. They find that despite this conventional behavior at low driving amplitudes, there is a critical driving amplitude that will cause these bistable elements to flip to the other well of potential energy and allow for the transmission of nonlinear waves.

2.2.3 Disordered materials

Just as sparse as nonlinear systems, the study of phononic media with disorder has not been widely researched. Incorporating disorder can increase the predictablility of a model much like damping. In the manufacturing process perfect periodicity may not be able to be acheived. The difficulty in disordered phononic media is that the conventional method of Bloch wave analysis does not work. A requirement of Floquet-Bloch theory is that the material properties vary periodically with a known period. A single unit cell can no longer model the behavior of the entire system if there is even a small amount of disorder.

Recently, there has been research done on so called hyperuniform phononic crystals. Hyperuniformity is a way of categorizing point distributions. It specifically refers to distributions with the fluctuations in density completly vanish as the window of observation increases. Despite not having any periodicity, and therefore no Bragg scattering, there still exists band gaps.

In 2004, Zuo-Don and Jian-Chun used the finite difference time domain method to study a weakly disordered phononic crystal consisting of a homogeneous matrix embedded with an array of cylinders [14]. Disorder was added by perturbing the location of the cylinders. As the disorder in the system increased, it was found that the band gaps dissapeared which makes sense sense Bragg scattering occurs do to the periodicity of the inclusions. Chen and Wang used the transfer matrix method to study a 1D layered composite where the layer thickness was varied [15]. Here they look at a localization of wave propagation which is a phenomena that is expected in random materials. The localization factor that they defined is also used to study band gaps as the material becomes more disordered. An paper 2010 by, examined a 2d phononic medium with circular inclusions arranged in a lattice [16]. Disorder was added to the system by increasing or decreasing the size of the inclusions or displacing them by some small amount. Here they used the plane-wave expansion method. Of course, due to the added disorder they were no longer able to look at a single unit cell and instead define a 'supercell' for which the analysis was carried out.

3 Dispersion relations

In order to start performing research in the field of phononic media, it is of high priority to first know what dispersion relations are, how to solve for them (analytically or computationally), and when to use them. Dispersion relations provide all of the information necessary to characterize the behavior of waves propagating in a phononic medium. Mathematically, they are a relationship between the frequency of a wave and its wavenumber. From this relationship, it is possible to determine the phase velocity and group velocity. Dispersion relationships immediately indicate where the frequency band gaps of a system are. For this reason, they are also called frequency band diagrams or frequency band structures.

As will be shown, there are a variety of ways to calculate dispersion relations, however, there is a common thread between each type of analysis. This common feature is the application of Floquet-Bloch theory.

3.1 Floquet-Bloch theorem

Given the equation

$$\frac{\partial^2 u}{\partial x^2} + c(x)y = 0 \tag{1}$$

where c(x) is periodic in x, Floquet's theorem says that (1) has two solutions

$$u_1(x) = \tilde{u}_1(x)e^{ikx}$$
$$u_2(x) = \tilde{u}_2(x)e^{-ikx}$$

In the above, $\tilde{u}_1(x)$ and $\tilde{u}_2(x)$ are also periodic in x [17].

Bloch's theorem is similar to Floquet's theorem but applies to higher dimensions [8]. Given

$$-\nabla \cdot (c(\mathbf{r})\nabla u(\mathbf{r})) = \omega^2 u(\mathbf{r}) \tag{2}$$

where $c(\mathbf{r})$ is periodic in space, Bloch's theorem says equation (2) has eigensolutions

$$u(\mathbf{r}) = \tilde{u}(\mathbf{r})e^{-i\mathbf{k}\cdot\mathbf{r}} \tag{3}$$

These eigensolutions are called *Bloch waves* and equation (2) is called the periodic Helmholtz equation.

3.2 First principles and example problems

To get a flavor for what dispersion relations look like and some of the features of analytical solutions, we start by considering some simple systems. We will see that by asserting a Bloch wave solution that we can derive dispersion relations directly from a system's equations of motion.

3.2.1 Scalar wave equation

The scalar wave equation is

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} \tag{4}$$

where u is the displacement and c is the wave speed. Assume solution of the form

$$u(x,t) = \tilde{u}(x) e^{i(kx-\omega t)} \tag{5}$$

k is the wave number which describes the "spatial" frequency of the wave for a fixed time and ω is the angular frequency that describes the temporal frequency of the wave. Substituting this solution into the wave equation gives

$$\omega^2 = c^2 k^2 \tag{6}$$

Taking the square root of the above

$$\omega = \pm ck \tag{7}$$

This equation gives a relationship between the frequency of the wave and its wave number. The positive solution corresponds to a wave propagating to the right, and the negative solution corresponding to waves propagating to the left. We call relations of this type dispersion relations. It is important to note that this is a constraint on waves propagating in a system governed by (4). If a wave is a solution to (4) of the form (5) its wavenumber and frequency must satisfy the above equation.

In general, dispersion relations can be written in the form

$$\omega = \omega(k) \tag{8}$$

To understand what dispersion entails, we need to look at the phase velocities. The phase velocity is the speed at which a wave of a specific frequency propagates at in a medium. It is given by

$$v_p = \frac{\omega}{k} \tag{9}$$

Thus, for the scalar wave equation

$$v_p = c \tag{10}$$

This relation holds for all waves admissible according to (4). Here, every wave propagates at the same velocity regardless of frequency. In this case, we say that there is <u>no</u> dispersion. In systems with dispersion we expect a relation in the form (8) and also

$$v_p = v_p(\omega) = v_p(\omega(k)) \tag{11}$$

3.2.2 Monatomic lattice

Consider a system of n masses and springs like in Figure 1 The equation of motion for the nth mass in the

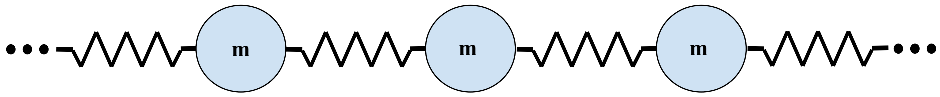

Figure 1: A system of masses connected by springs extending infinitely to the left and right.

system is

$$m\frac{\partial^2 u_n}{\partial t^2} = k(u_{n-1} - u_n) - k(u_n - u_{n+1}) = ku_{n-1} - 2ku_n + ku_{n+1} \tag{12}$$

where u_n gives the displacement of the nth node and k is the spring constant of each spring. To acquire the dispersion relation for this system we assume a Bloch wave solution of the form

$$u_n(x,t) = \tilde{u}(x_n)e^{i(kx_n - \omega t)} \tag{13}$$

$\tilde{u}(x)$ is the amplitude of the wave and $x_n = nl$ where l is the distance between the masses. Substituting the above into the equation of motion

$$\begin{aligned}
-m\omega^2 u_n &= ke^{i(k(n-1)l-\omega t)} - 2ku_n + ke^{i(k(n+1)l-\omega t)} \\
&= ke^{-ikl}u_n + ke^{ikl}u_n - 2ku_n \\
&= k\cos(kl)u_n - 2ku_n
\end{aligned}$$

Thus,

$$\left[2\omega_0^2(1-\cos(kl)) - \omega^2\right]u_n = 0 \tag{14}$$

where $\omega_0 = \sqrt{k/m}$ The above has a trivial solution when $u_n = 0$. Not so trivial solutions exist when

$$2\omega_0^2(1-\cos(kl)) - \omega^2 = 0 \tag{15}$$

We can write the dispersion relation for waves propagating through our mass spring system as

$$\omega = \pm\sqrt{2\omega_0^2(1-\cos(kl))} \tag{16}$$

It is now becoming apparent that in a system of n masses and springs that there is dispersion. To see this explicitly, write the phase velocity

$$v_p = \frac{w(k)}{k} = \frac{\pm\sqrt{2\omega_0^2(1-\cos(kl))}}{k} \tag{17}$$

Clearly, the phase velocity is a function of wave number/frequency which indicates dispersivity of the system.

Take our dispersion relation (16) and nondimensionalize by letting $\Omega = \frac{\omega}{\omega_0}$ and $\mu = kl$. Then,

$$\Omega = \pm\sqrt{2(1-cos(\mu))} \tag{18}$$

The positive part is plotted in Figure 2. Notice that it is periodic in μ. The section of the dispersion relation from $-\pi$ to π is called the first Brillouin zone. Due to symmetry, we also define the irreducible Brillouin zone

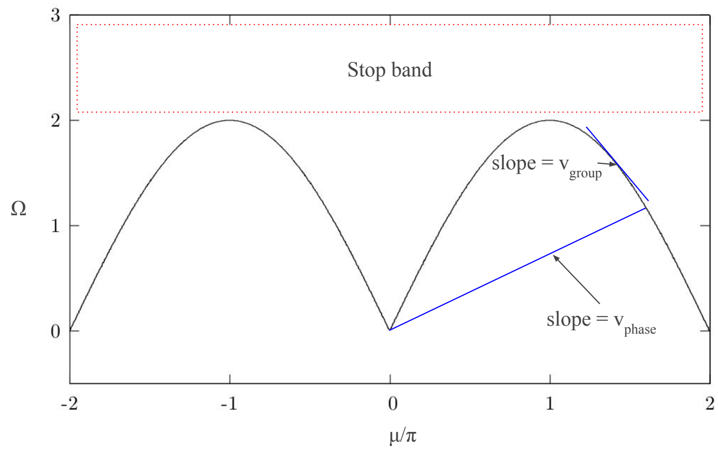

Figure 2: The non-dimensional dispersion relation for the mass spring system

(IBZ) as the section from 0 to $\frac{\pi}{2}$. The dispersion relation characterizes many features of the mass-spring system. In Figure 2, it is easy to identify the phase and group velocities along the curve for different waves propagating through the system.

At first glance, it appears that there are no frequencies above $\Omega = 2$. In this region (called the stop band), waves experience attenuation and exponentially die off. Wave numbers in the stop band are imaginary. Looking at (13), it becomes obvious where the attenuation comes from. Waves whose wave numbers are imaginary are called *evanescent* waves.

Solving for wavenumber in terms of a given frequency

$$\mu = \arccos\left(1 - \frac{\Omega^2}{2}\right) \tag{19}$$

We see that when $\Omega > 2$ the wave number becomes complex valued. The expression for (19) when we extend the values of μ into the complex plane is

$$\mu = -i \log\left[\xi + i(1 - \xi^2)^{\frac{1}{2}}\right] \tag{20}$$

where

$$\xi = 1 - \frac{\Omega^2}{2} \tag{21}$$

The implication here is that when the wave number becomes imaginary the i in the wavenumber will multiply with i in (13) resulting in a exponential decay of the solution in space. This means there is no wave propagation.

3.2.3 Diatomic lattice

Next, we consider a diatomic lattice as shown in Figure 3 with alternating masses, but springs of the same spring constants. There are two ways to solve this problem. The first is called the inverse method which imposes a wave number and gives frequencies. The second is the direct method which imposes a frequency and gives wave numbers. We will use the inverse method for the diatomic lattice and later for a laminate use the transfer matrix method. After assuming a harmonic motion

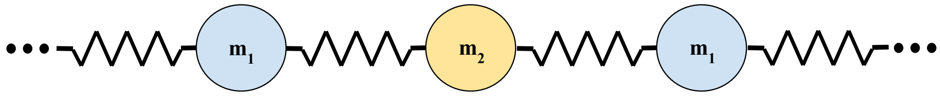

Figure 3: A system of alternating masses connected by springs extending infinitely to the left and right.

$$u_n = \tilde{u}(x_n)e^{i\omega t} \tag{22}$$

The equations of motion for a diatomic lattice can be written

$$(-\omega^2 m_2 + 2k)u_{2n} - k(u_{2n-1} + u_{2n+1}) = 0 \tag{23}$$

$$(-\omega^2 m_1 + 2k)u_{2n+1} - k(u_{2n} + u_{2n+2}) = 0 \tag{24}$$

We can write this in a matrix form

$$(\mathbf{K}_n - \omega^2\mathbf{M})\mathbf{u}_n + \mathbf{K}_{n-1}\mathbf{u}_{n-1} + \mathbf{K}_{n+1}\mathbf{u}_{n+1} = 0 \tag{25}$$

where

$$\mathbf{u}_n = \begin{bmatrix} u_{2n} \\ u_{2n+1} \end{bmatrix} \tag{26}$$

We will use the inverse method to solve for the dispersion relation. We use Bloch's theorem to write

$$\mathbf{u_n} = \hat{\mathbf{u}}(\mu)e^{in\mu} \tag{27}$$

Finally, we can write

$$\left[\mathbf{K}_n + \mathbf{K}_{n-1}e^{-i\mu} + \mathbf{K}_{n+1}e^{i\mu} - \omega^2\mathbf{M}\right]\hat{\mathbf{u}}(\mu)e^{in\mu} = 0 \tag{28}$$

and condensing all of the stiffness matrices

$$\left[\tilde{\mathbf{K}}(\mu) - \omega^2\mathbf{M}\right]\hat{\mathbf{u}}(\mu)e^{in\mu} = 0 \tag{29}$$

Calculating the determinant of the matrix on the left we get the relation

$$\omega = \pm\sqrt{k\frac{m_1+m_2}{m_1 m_2} \pm k\sqrt{\left(\frac{m_1+m_2}{m_1 m_2}\right) - \frac{4(\sin\mu)^2}{m_1 m_2}}} \tag{30}$$

The dispersion relation for the diatomic lattice is shown in Figure 4. Notice that there are now two curves unlike in the monatomic case. Each curve corresponds to a mode of vibration where in this case the bottom one is called the acoustic mode and the top is called the optical mode. Another notable feature is the formation of a band gap in between the two modes. Like the monatomic case the wavenumbers become imaginary in this region. Additionally, there is still a stop band, but in this case the cutoff frequency is lower -about $\Omega = 1.75$.

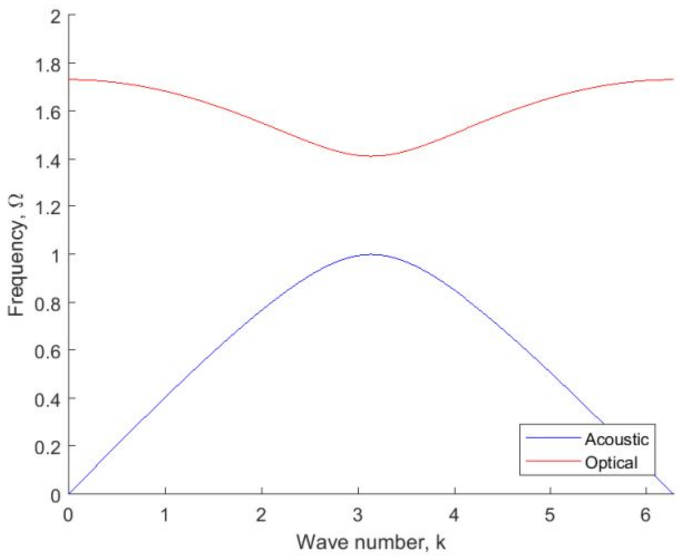

Figure 4: Dispersion relation for the diatomic lattice system with $m_1 = 1$, $m_2 = 2$, and $k = 1$.

3.2.4 Laminate

The transfer matrix method enforces continuity between layers of a system. At the interface between two unit cells the displacements must be equal and the forces or tractions must be as well. First, a relationship between these variables must be derived from one end of the unit cell to the other end. The relationship can be written in a matrix called the transfer matrix. This type of analysis is completed by applying Bloch's theorem to relate the displacements and forces in one cell to another. Here we outline the anlaysis of Shmuel [18]

Consider a two phase laminate, with layer thicknesses $h^{(p)}$ and lamination direction n. A plane wave in layer i that is propagating in the direction of n has the general form

$$u^{(p)} = m^{(p)} e^{ik^{(p)}(n\cdot x - c^{(p)}t)} \tag{31}$$

where $m^{(p)}$ is the polarization and $c^{(p)}$ is the wave speed. From the above and the constitutive equations for linear elasticity, a relationship for the displacements at each end of a single layer can be written

$$\begin{bmatrix} u^{(p)}(x + h^{(p)}n, t) \\ t^{(p)}(x + h^{(p)}n, t) \end{bmatrix} = \begin{bmatrix} \cos k^{(p)}h^{(p)} & \frac{\sin k^{(p)}h^{(p)}}{\tilde{\mu}^{(p)}k^{(p)}} \\ -\tilde{\mu}^{(p)}k^{(p)}\sin k^{(p)}h^{(p)} & \cos k^{(p)}h^{(p)} \end{bmatrix} \begin{bmatrix} u^{(p)}(x, t) \\ t^{(p)}(x, t) \end{bmatrix} \tag{32}$$

$\tilde{\mu}$ is a combination of Lamé constants which is different for transverse and longitudinal waves. The matrix $T^{(p)}$ is the transfer matrix for one layer.

In order to relate, the displacements at the opposite ends of the unit cell of this two phase laminate we need two transfer matrices.

$$\begin{bmatrix} u^{(1)}(x + h^{(1)}n + h^{(2)}n, t) \\ t^{(1)}(x + h^{(1)}n + h^{(2)}n, t) \end{bmatrix} = T^{(2)}T^{(1)} \begin{bmatrix} u^{(1)}(x, t) \\ t^{(1)}(x, t) \end{bmatrix} \tag{33}$$

At this point, we use Bloch's theorem to enforce that the displacements at the boundary of the unit cell must be equal up to a phase constant. The end result is an equation of the form

$$\left(T^{(2)}T^{(1)} - \lambda I\right) \begin{bmatrix} u^{(1)}(x,t) \\ t^{(1)}(x,t) \end{bmatrix} = 0 \tag{34}$$

where $\lambda = e^{ik_b h}$ (h is the width of the unit cell) and k_b is the Bloch wavenumber. The determinant of the matrix must be equal to zero which generates a dispersion relation. Given a frequency ω , the dispersion relation gives a set of corresponding k_b (where $\omega = c^{(p)}k^{(p)}$ in the above equations).

4 Computational methods for phononic media

While we were able to derive explicit dispersion relations in the examples given in the previous section, it is quickly becomes unfeasible even for some 2D and most 3D cases. We must turn to computational analysis in these cases in order to compute the dispersion relations for these phononic media. Here the four most prominent methods in the literature are the plane-wave expansion method, finite difference method, finite element method, and the multiple scattering method. Each is explained briefly in this section, however, for the independent study we choose to specialize in the finite element method which will also be used in further research.

According to [19], the plane-wave method is widely used because of its convenience. Apparently, the drawback of this method is slow convergence. In general, the displacements and material properties are first expanded in a series related to the lattice vectors and a Bloch wave solution is asserted. These expansion are substituted back into the wave equation which after some manipulation leads to an eigenvalue problem [3].

Finite difference methods are similar to the plane wave expansion method with the advantage that the solution convergence is faster for materials with multiple phases. Instead of expanding the solution and material properties, the differential operators of the wave equation are approximated using standard finite difference formulas. At this point, it is possible to solve the equations at various time steps to obtain the real time evolution of the system. From the real time evolution, it is possible to take the Fourier transform of the data in order to obtain the wave number of a wave for which the excitation frequency is known and thus form a dispersion relation. Alternatively, asserting a Bloch wave solution after using the finite difference approximation results in an eigenvalue value problem that yields eigenfrequencies given an imposed wave number.

The finite element method is useful for complex material geometries. A weak from of the governing equations is still formulated by multiplying by a trial function, but the integration is performed only over a unit cell which represents the phononic medium of interest. After approximating the solution and trial function with appropriate weight functions, we can proceed in two ways much like in the finite difference method. It is possible to use a central difference approximation for the time derivative and calculate the real time evolution (for more detail see Appendix A.2). This, however, is computationally inefficient. Instead, we apply Bloch's theorem. In this case, Bloch's theorem can be used to impose a Bloch condition on the boundary which reduces the degrees of freedoms of the system by relating the displacements at one boundary to the opposite boundary plus a phase multiplier. This process results in an eigenvalue problem similar to the above two cases. As this method will be used in future studies, it will be elaborated on in detail in upcoming sections.

Compared to the above methods, the multiple scattering method has an advantage when the material under consideration contains scattering elements. The method relies on separating the solution into fields associated with the incident wave and then waves scattered from each scattering element in the system. Once the solution, at a single scattering element a system of equations can be solved for the rest of the scattered fields. The dispersion relations are then found by application of Bloch's theorem.

5 Analysis of lattice structures via real time evolution

Here, the monatomic and diatomic lattice systems are computationally realized using the finite difference time domain method. A Bloch wave solution is not imposed which will allow us to directly visualize the behavior of the system inside and outside of the band gaps and stop bands. Additionally, the (discrete) Fourier transform of the real time evolution data is taken in order to find the dispersion relations in each case.

5.1 Monatomic lattice

A monatomic lattice with 100 masses is modeled using the equations of motion (12) and the Verlet integration method. The Verlet integration method is involves a central difference approximation for the time derivative in Newton's equations. See Appendix A.1 for more details on the Verlet integration method. One end of the system is subject to a harmonic excitation with a prescribed frequency, and the other end is allowed to freely move. For the material parameters, we choose $m = 1$ and $k = 1$.

In order to compute the dispersion relation of the system, a range of frequencies is prescribed from $\Omega = 0$ to $\Omega = 2$. At each frequency and after allowing the system to evolve in time, a Fourier transform of the system is taken in the space domain. From the Fourier transform of the displacements, which is now in the wavenumber domain (recall that the wave number can be thought of as the spatial frequency of the wave), the location of the peak of the spectrum is taken as the wavenumber for the corresponding excitation frequency. The result is Figure 5. The results are in good agreement with the derived dispersion relation, but there is noticeable error due to reflections at the free end of the chain. If the chain of masses was longer, this would not be less of a problem.

Increasing the frequency of the harmonic excitation above the cutoff frequency of the system it is easy to explore the attenuation effect at the stop band as seen in Figure 2. Figures 6 and 7 display snapshots of

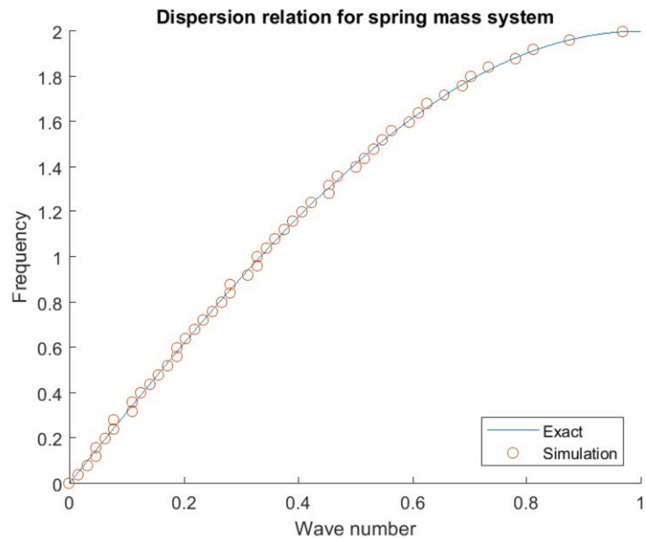

Figure 5: Using a Fourier transform in space, wave lengths for different excitation frequencies are identified and plotted

the system at excitation frequencies above and below $\Omega = 2$. There is an obvious drop in amplitude inside and outside of the stop band.

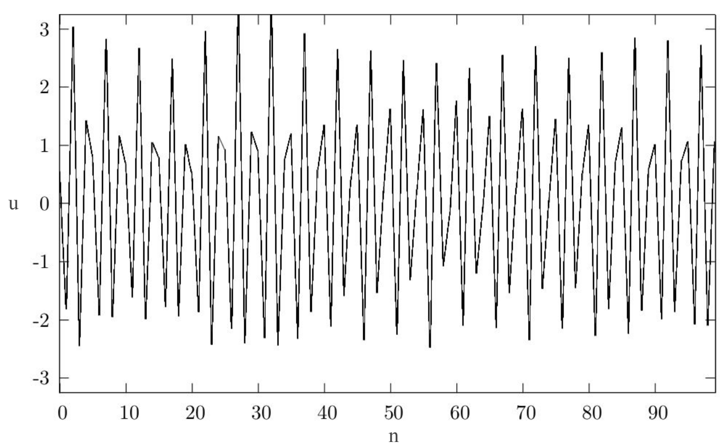

Figure 6: Snapshot of mass spring system with $\Omega = 1.9$

From the finite difference time domain method, it is also possible to calculate the values of the imaginary wavenumbers that occur for frequencies above cutoff frequencies. This is done by fitting a complex exponential to the evanescent waves and finding the power of the exponential term. Figure 8 has the results of the fitting process overlaid on top of the exact plot of the evanescent wavenumbers. Closer to the cutoff frequency, the results are not in good agreement. This is due to the reflections of the wave at the boundary of the system.

Another way to identify band gaps in a system without calculating the Fourier transform is by comparing

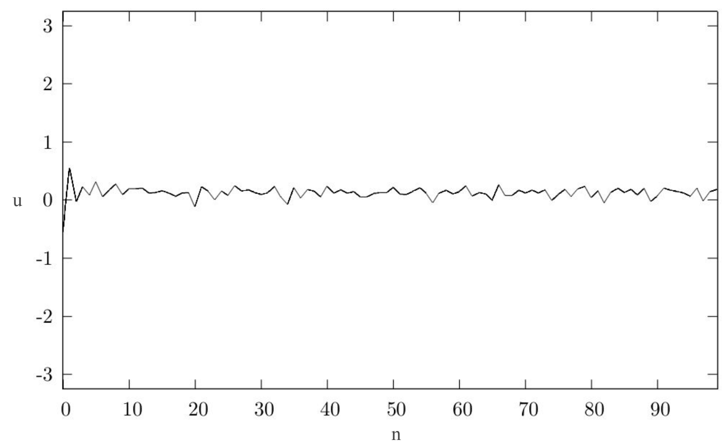

Figure 7: Snapshot of mass spring system with $\Omega = 2.1$

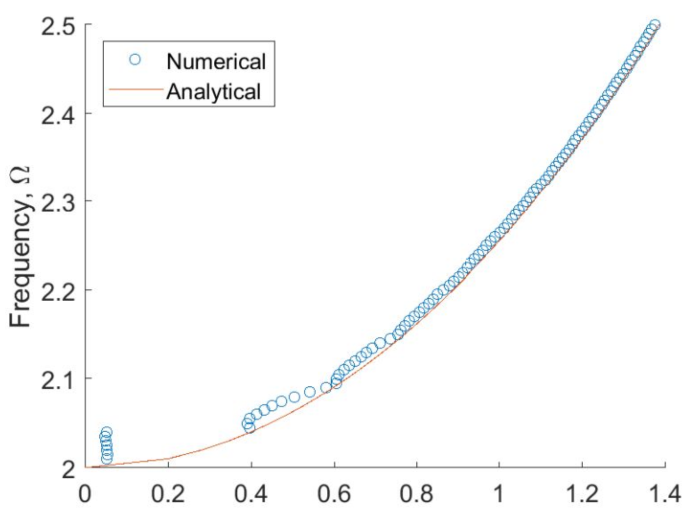

Figure 8: Here, the results of the exponential fitting process of the evanescent waves are plotted.

the amplitude of harmonic excitation to the maximum displacement at the free end. Sweeping over frequencies and plotting the ratio of displacements at each end results in a transmission loss diagram as in Figure 9. It is apparent from Figure 9 that there is a cutoff frequency at $\Omega = 2$. This may be inferred even before

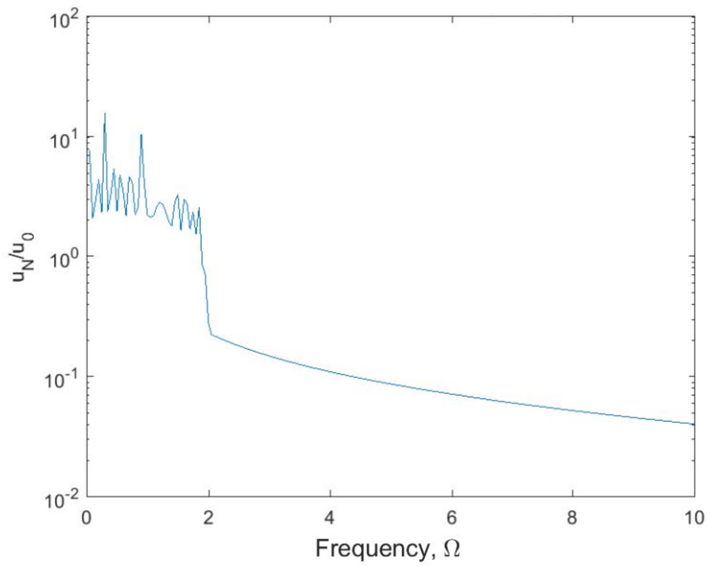

Figure 9: The displacement of the excited mass and the free mass are compared to construct this transmission-loss diagram.

seeing the dispersion relation of the monatomic lattice beforehand.

5.2 Diatomic lattice

We also perform a finite difference time domain analysis for the diatomic lattice with $m_1 = 1$, $m_2 = 2$, and $k = 1$. The results from taken the Fourier transform of the data and also the previously derived analytical expressions are plotted in Figure 10. From the real time evolution we are able to recover the band gap between the two modes of vibration and also the stop band. Additionally, the transmission-loss diagram is also plotted in Figure 11 to illustrate the attenuation that the system undergoes. It does appear that there is attenuation in the band gap and above the stop band.

6 Analysis of 1D continuum materials via finite element method

6.1 Uniform bar

As a first exercise in using finite elements to find the dispersion properties of materials, we will consider a uniform bar in one dimension. For the one dimensional problem, the elasticity equations we want to solve

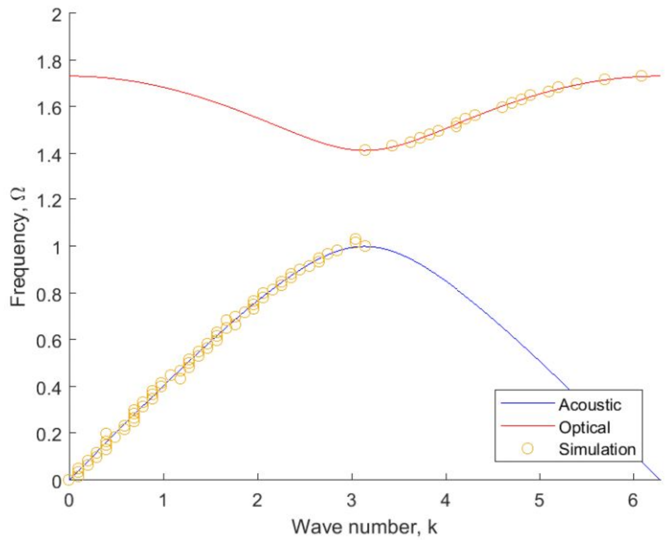

Figure 10: The results for the finite difference time domain method are plotted along side the exact dispersion relation derived using the inverse method.

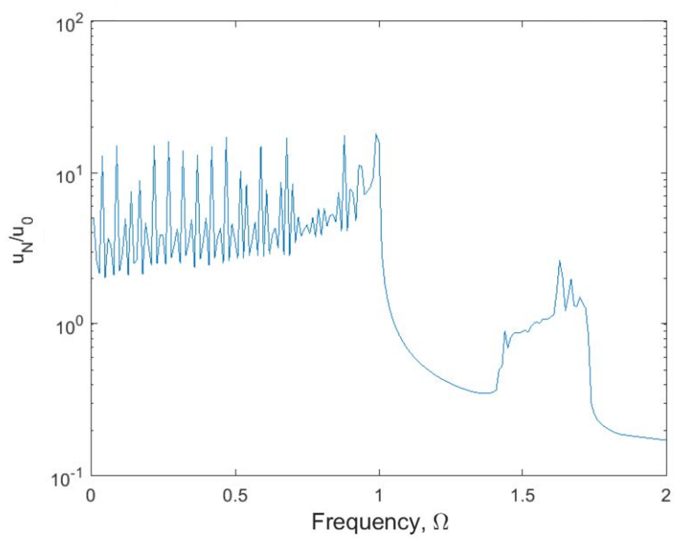

Figure 11: The displacement of the excited mass and the free mass in the diatomic lattice are compared to construct this transmission-loss diagram.

are.

$$\frac{\partial \sigma_x}{\partial x} + b_i = \rho \frac{\partial^2 u_x}{\partial t^2}, \quad x \in [0, L] \quad \text{(Equilibrium)} \tag{35}$$

$$\sigma_x = E\varepsilon_x \quad \text{(Constitutive relation)} \tag{36}$$

$$\varepsilon_x = \frac{\partial u_x}{\partial x} \quad \text{(Strain-displacement)} \tag{37}$$

$$u_x(x = 0, t) = A_0 sin(\omega t) \tag{38}$$

$$\sigma_x(x = L, t) = 0 \tag{39}$$

In the absence of body forces, we can find the weak form of the equilibrium equation by multiplying by a test function φ and integrating of the domain.

$$\int_0^L \varphi \frac{\partial \sigma_x}{\partial x} dx = \int_0^L \varphi \rho \frac{\partial^2 u_x}{\partial t^2} dx \tag{40}$$

Using integration by parts on the LHS of the above we find that

$$\varphi(L)\sigma_x(L) - \varphi(0)\sigma_x(0) - \int_0^1 \frac{\partial \varphi}{\partial x} \sigma_x dx = \int_0^L \varphi \rho \frac{\partial^2 u_x}{\partial t^2} dx \tag{41}$$

Applying boundary conditions, constitutive relation, and the strain-displacement equation we arrive at the weak form of the equation

$$\int_0^1 \frac{\partial \varphi}{\partial x} E \frac{\partial u_x}{\partial x} dx + \int_0^L \varphi \rho \frac{\partial^2 u_x}{\partial t^2} dx = 0 \tag{42}$$

Now, we approximate our test function and solution using linear shape functions

$$\varphi = N_i(x) \tag{43}$$

$$u_x = \sum_j a_j(t) N_j(x) \tag{44}$$

Then,

$$\int_0^1 \frac{\partial N_i(x)}{\partial x} E \sum_j \frac{\partial N_j(x)}{\partial x} a_j dx + \int_0^L N_i \rho \sum_j N_j \frac{\partial^2 a_j(t)}{\partial t^2} dx = 0 \tag{45}$$

Rearranging,

$$\int_0^1 E \sum_j \frac{\partial N_i(x)}{\partial x} \frac{\partial N_j(x)}{\partial x} a_j dx + \int_0^L \rho \sum_j N_i N_j \frac{\partial^2 a_j(t)}{\partial t^2} dx = 0 \tag{46}$$

Finally, we write the above equation in matrix form

$$Ka + M\ddot{a} = 0 \tag{47}$$

where K is called the stiffness matrix, and M is called the mass matrix.

We now assume a harmonic solution of the form

$$a = \tilde{a} e^{i\omega t} \tag{48}$$

such that the second order differential equation (47) becomes a complex eigenvalue problem:

$$Ka - \omega^2 Ma = (K - \omega^2 M)a = 0 \tag{49}$$

Note that as of now K and M are not functions of the wave number and solving the eigenvalue problem as is does not yield any information about the dispersion properties of the system. To obtain this dependence the Bloch condition must be enforced.

The Bloch condition is similar to the periodic boundary condition and is a manifestation of Bloch's theorem much like the Bloch wave solution that was asserted when analytically solving for the dispersion relation

$$a(x+h) = a(x) \quad \text{(Periodic boundary condition)} \tag{50}$$

where h is the size of the unit cell. The difference between the two conditions is a single multiplicative factor:

$$a(x+h) = e^{ik_x h} a(x) \quad \text{(Bloch condition)} \tag{51}$$

The multiplicative factor in the boundary condition shifts is such that when the wave reaches a boundary it is phase shifted to match the wave at the opposite boundary such that there is no interference.

Enforcing the condition is done via a linear transformation which in one dimension is

$$T = \begin{bmatrix} 1 & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \\ e^{ik_x h} & \mathbf{0} \end{bmatrix} \tag{52}$$

where $\mathbf{I}$ is an identity matrix with dimensions equal to the number of interior nodes (in the one dimensional case this is the total number of nodes minus two). Using this transformation matrix we reduce the number of degrees of freedoms in our system and write

$$a = \begin{bmatrix} a_{left} \\ a_{int} \\ a_{right} \end{bmatrix} = \begin{bmatrix} 1 & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \\ e^{ik_x h} & \mathbf{0} \end{bmatrix} \begin{bmatrix} a_{left} \\ a_{int} \end{bmatrix} = T\hat{a} \tag{53}$$

Our eigenvalue problem is now

$$(K - \omega^2 M)T\hat{a} = 0 \tag{54}$$

To make it so our matrix is square, and therefore invertible, we premultiply the equation by $\bar{T}^T$

$$(\hat{K} - \omega^2 \hat{M})\hat{a} = 0 \tag{55}$$

where

$$\hat{K}(k_x) = \bar{T}^T K T \tag{56}$$

and

$$\hat{M}(k_x) = \bar{T}^T M T \tag{57}$$

We are now in position to extract the dispersion properties of the uniform bar. The eigenvalue problem is solved several times for values of k_x, and we obtain several corresponding values for ω. The dispersion relation for the uniform bar is plotted in Figure 12. The dispersion relation has only has straight lines indicating

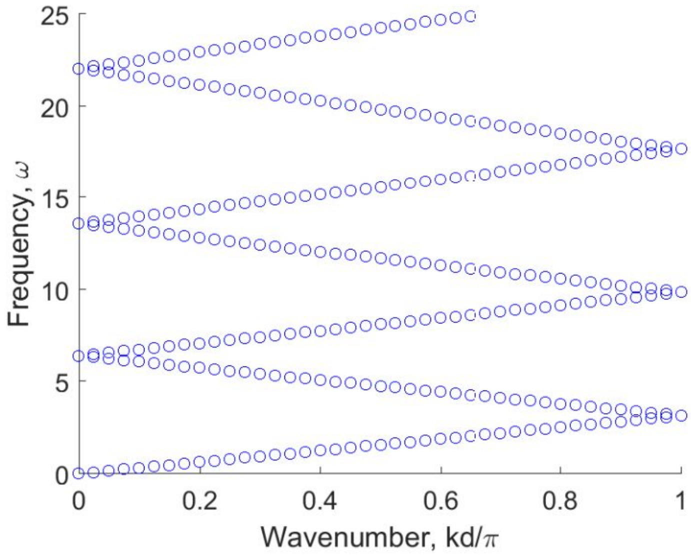

Figure 12: Dispersion relation for a uniform bar with $E = 1$ and $\rho = 1$.

there is no dispersion which is what we expect for a uniform material. No band gaps form because there are no periodic inclusions or structure to produce Bragg scattering. There are several modes corresponding to forward and backward propagating waves and it is verified that the wave speed is equal to one since when $k = \pm\omega$ for all wavenumbers.

6.2 Layered composite

For the layered composite, a bimaterial unit cell is consider as shown in Figure 13 with a stiffer and denser material in the center with length equal to that of a half the length of the unit cell. The same finite element

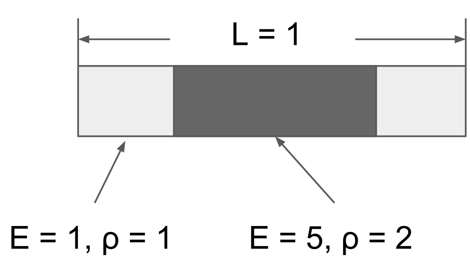

Figure 13: Unit cell of the layered composite with each phase occupying an equal volume fraction.

analysis as performed on this layered composite resulting in the dispersion relation shown in Figure 14. Due to the periodicity of the material, we see the formation of band gaps and the presence of dispersion.

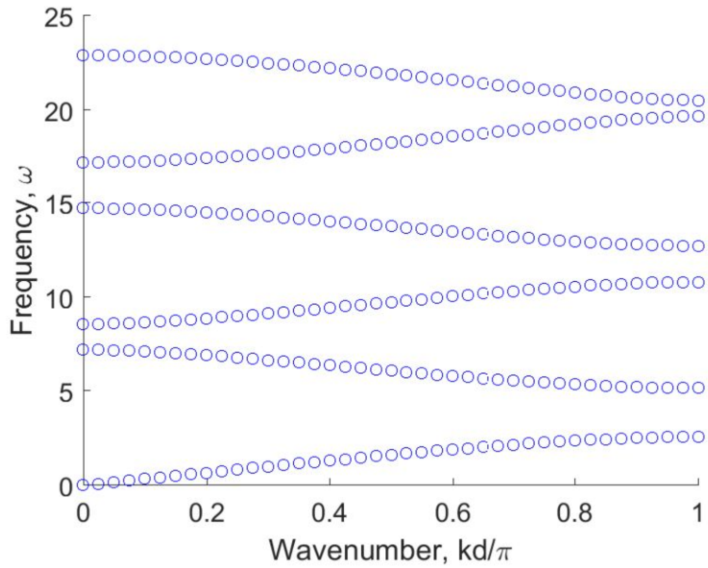

Figure 14: Dispersion relation from the finite element analysis of a unit cell of the layered composite

7 Analysis of 2D continuum materials via finite element method

Extending finite elements to 2D, we find that after considering the principle of virtual work and approximating our solution using linear shape functions that

$$\left[\int_{\Omega}(BN)^T CBNdV\right]a - \left[\int_{\Omega}N^T\rho NdV\right]\ddot{a} = 0 \tag{58}$$

where

$$N = \begin{bmatrix} N_1 & 0 & N_2 & 0 & ... & N_n & 0 \\ 0 & N_1 & 0 & N_2 & ... & 0 & N_n \end{bmatrix} \tag{59}$$

and

$$B = \begin{bmatrix} \frac{\partial}{\partial x} & 0 \\ 0 & \frac{\partial}{\partial y} \\ \frac{\partial}{\partial y} & \frac{\partial}{\partial x} \end{bmatrix} \tag{60}$$

For our constitutive relation we consider an isotropic material with

$$\sigma_{ij} = 2\mu\varepsilon_{ij} + \lambda\varepsilon_{kk}\delta_{ij} \tag{61}$$

such that

$$C = \begin{bmatrix} 2\mu+\lambda & \lambda & 0 \\ \lambda & 2\mu+\lambda & 0 \\ 0 & 0 & 2\mu \end{bmatrix} \tag{62}$$

Note that this corresponds to a 2D material and not a 3D material in plane strain or plane stress.

We can write our matrix form in the same form as in the 1D case and also assume a harmonic solution.

$$Ka - M\ddot{a} = \left(K - \omega^2 M\right) a = 0 \tag{63}$$

Furthermore, we will apply the Bloch condition again. The linear transformation matrix is more complicated due to the added dimension. In order to impose the Bloch condition in 2D, the degrees of freedom of the unit cell must be divided into interior nodes and boundary nodes according to Figure 15. Based on the

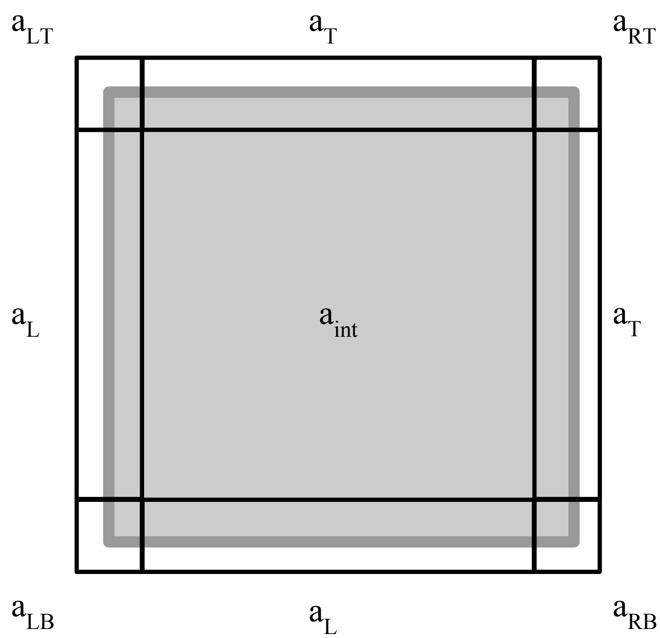

Figure 15: The degrees of freedom are partitioned into nodes at the left-top (LT), right-top (RT), left-bottom (LB), right-bottom (RB) corners. Non-corner nodes are further divided into right (R), left (L), top (T), bottom (B) sides and also interior (int)

aforementioned partitioning scheme, the degrees of freedom are reduced according to the following

$$a = \begin{bmatrix} a_B \\ a_L \\ a_{LB} \\ a_{int} \\ a_T \\ a_R \\ a_{RB} \\ a_{LT} \\ a_{RT} \end{bmatrix} = \begin{bmatrix} \mathbf{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{I} \\ e^{ik_y h_y} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & e^{ik_x h_x} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & e^{ik_x h_x} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & e^{ik_y h_y} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & e^{ik_x h_x} e^{ik_y h_y} & \mathbf{0} \end{bmatrix} \begin{bmatrix} a_B \\ a_L \\ a_{LB} \\ a_{int} \end{bmatrix} = T\hat{a} \tag{64}$$

Now we post- and pre- multiply 63 by T and its complex conjugate $\bar{T}$ and obtain a complex eigenvalue problem similar to the 1D case. We then follow the same process of prescribing wavenumbers and solving the eigenvalue problem to obtain the corresponding frequencies.

7.1 Uniform material

Here we consider a uniform material with Lamé constants $\lambda = 1$ and $\mu = 1$. In order to fully characterize the wave propagation features of the 2D material, we only need to solve the eigenvalue equation for wave vectors in the irreducible Brillouin zone (IBZ) depicted in Figure 13.

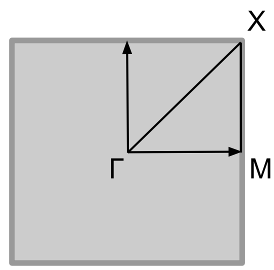

Figure 16: Unit cell for the homogeneous material

The result of solving the eigenvalue equation along the (IBZ) is shown in Figure 17. The dispersion relation is considerably more complex and it appears that for a given frequency there are sometime two possible wavenumbers along each side of the IBZ. These degeneracies are due to the fact that the 2D material supports longitudinal and transverse waves. Most of the dispersion curves are straight which is expected for a uniform material. The curved lines can be attributed to Bloch harmonics [20].

7.2 Laminate

A similar analysis is performed for a laminate with one material phase with $\lambda_1 = 160$, $\mu_1 = 1$, and $\rho_1 = 8$ surrounded by a second material phase with $\lambda_2 = \mu_2 = \rho_2 = 1$ on the outside of the unit cell.

7.3 Material with inclusions

8 Future work

In the near future it would be interesting to examine the effect of disorder on the diatomic mass spring system. Additionally, it would be of interest to develop a finite element method for analysis of disordered materials. Perhaps a modification of the Bloch condition or the consideration of "supercell" may be what is needed.

Additionally, it is of future research interest to explore dynamic homogenization of these phononic media. This is going to require a more thorough knowledge of static homogenization theory such that a generalization

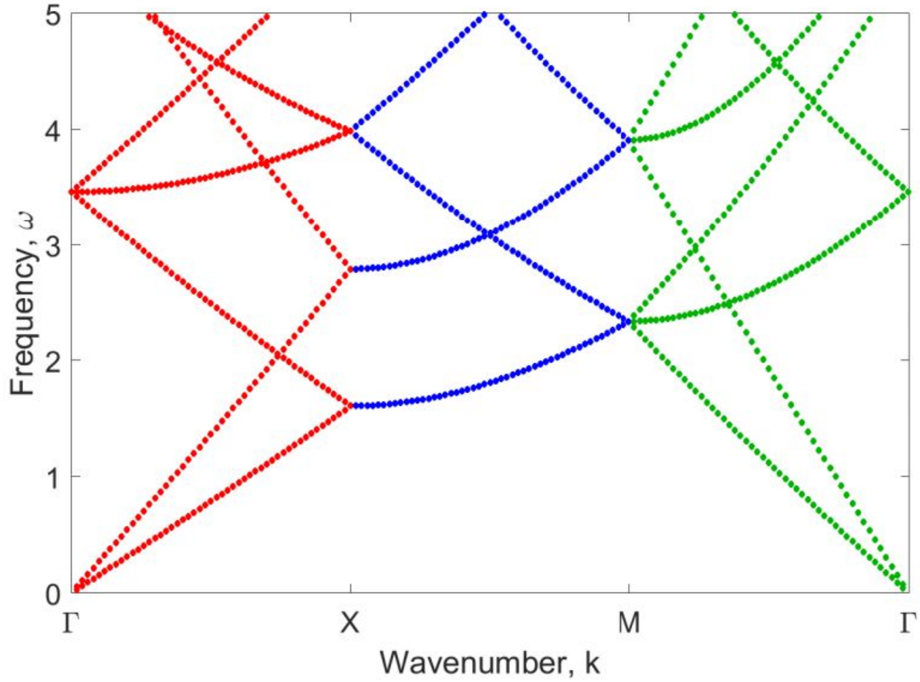

Figure 17: Dispersion relation for the 2D homogeneous material plotted along the IBZ

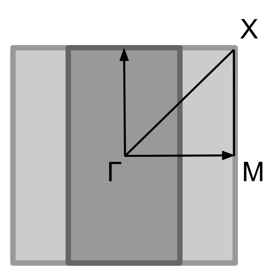

Figure 18: Unit cell for the laminate

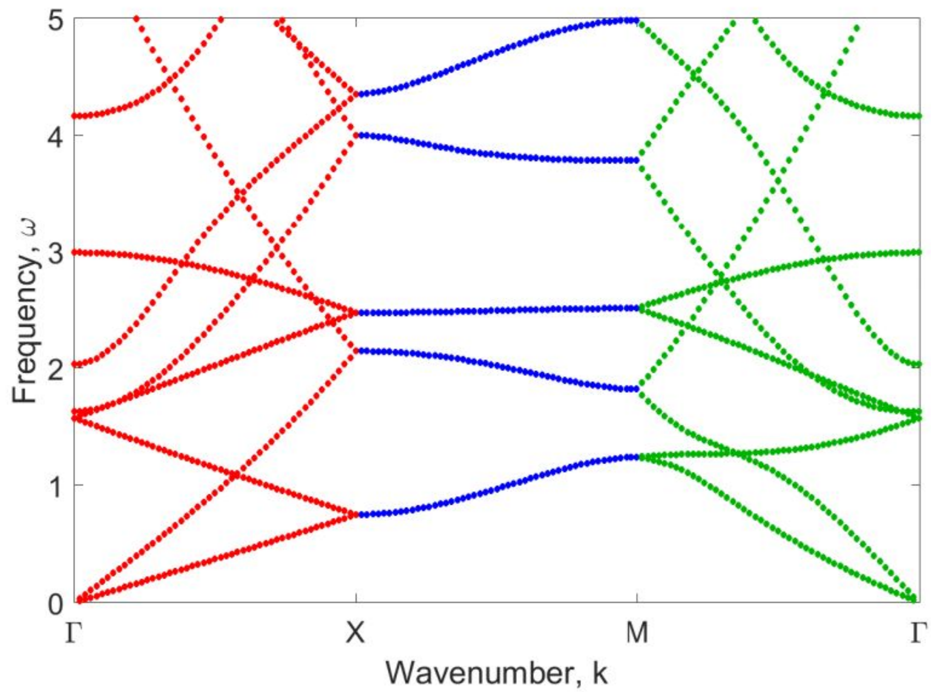

Figure 19: Dispersion relation for the laminate plotted along the IBZ

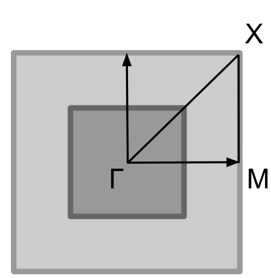

Figure 20: Unit cell for the 2D material with square inclusions

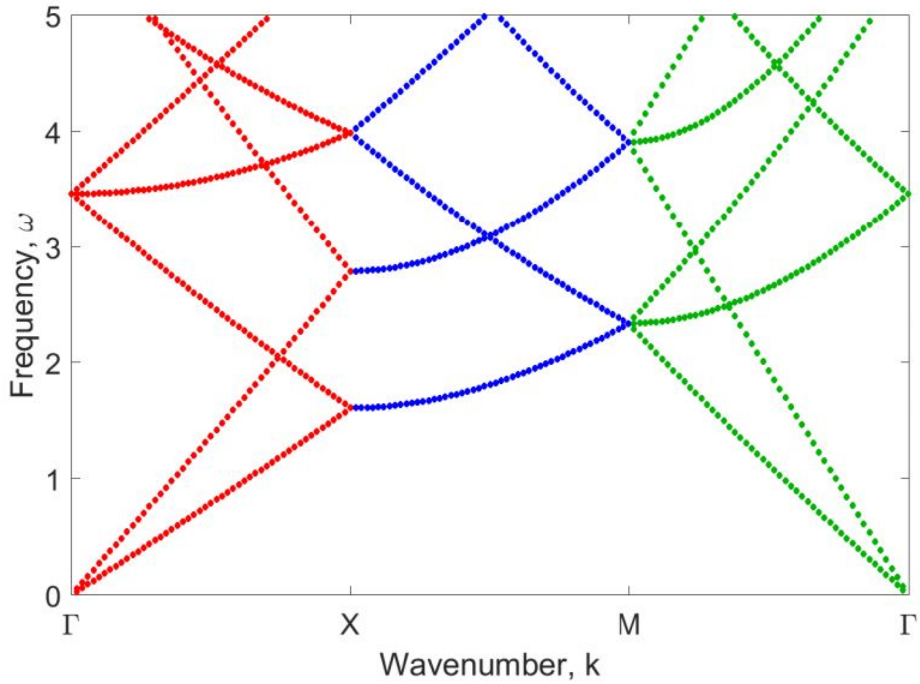

Figure 21: Dispersion relation for the 2D material with square inclusions plotted along the IBZ

may be made.

9 Conclusion

At the heart of research in phononic media, dispersion relations encapsulate a majority of the information needed to characterize the wave propagation in materials. In this independent study, a large amount of effort was put into developing the analytical and computational skills needed to calculate dispersion relations. As such, we are well poised to thrust ourselves into one of the active research areas of damping, nonlinear systems, or disordered systems and soon enough should be able to study dynamic homogenization of these phononic media.

10 Additional studies of heterogeneous materials

In addition to this study of phononic media, much time and effort was put into the notes of Prof. Ponte-Castañeda. Attached to this document, are solutions to various problems in the lecture notes.

11 Acknowledgements

I would like to thank my advisors Prof. Ponte-Castañeda and Prof. Reina for guidance this semester. Additionally, I would like to thank Chenchen Liu of Prof. Reina's group for helping me get a grip of using finite elements and Bloch analysis for this phononic media.

A Appendix

A.1 Verlet integration

For a single particle, the Verlet integration method is used to calculate its trajectory given that the forces (and therefore the acceleration) are known. The algorithm is

$$x_n^{t+1} = 2x_n^t - x_n^{t-1} + a(x_n^t)\Delta t^2 \tag{65}$$

where t denotes the current time step, x is the particle position, $a(x_n)$ is the acceleration, and Δt is suitably small time step. b

A.2 Finite difference in time for real time evolution FEM

For equation (47), it is possible to apply a finite difference method in time in order to get the real time evolution of the uniform bar. First, in order to apply the displacement boundary conditions at the left boundary, we need to modify (47). We partition the matrices

$$\begin{bmatrix} K_{11} & K_{1a} \\ K_{a1} & K_{aa} \end{bmatrix} \begin{bmatrix} a_1 \\ a \end{bmatrix} + \begin{bmatrix} M_{11} & M_{1a} \\ M_{a1} & M_{aa} \end{bmatrix} \begin{bmatrix} \ddot{a_1} \\ \ddot{a} \end{bmatrix} = 0 \tag{66}$$

Here, K_{11} and M_{11} denote the entry in the first row and first column. K_{1a} and M_{1a} are row vectors of the rest of the entries in the first row and K_{a1} and M_{a1} are column vectors of the remaining elements of the first column. K_{aa} and M_{aa} are then matrices of the remaining elements of the matrices K and M. Since we know a_1 and $\ddot{a_1}$ (these are the displacement and acceleration at the first node), we only wish to solve the bottom row of (66).

$$K_{aa}a + M_{aa}\ddot{a} = -a_1 K_{a1} - \ddot{a_1} M_{a1} \tag{67}$$

To solve the above we discretize $\ddot{a}$ in time using an explicit finite difference scheme.

$$K_{aa}a^t + M_{aa}\frac{a^{t+1} - 2a^t + a^{t-1}}{\Delta t^2} = -a_1^{t+1}K_{a1} - \ddot{a_1}^{t+1}M_{a1} \tag{68}$$

Solving for a^{t+1}

$$a^{t+1} = M_{aa}^{-1}(-a_1^{t+1}K_{a1} - \ddot{a_1}^{t+1}M_{a1} - K_{aa}a^t)\Delta t^2 + 2a^t - a^{t-1} \tag{69}$$

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