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 microstructure, or its boundary conditions. As a result of this periodic structure, it has been shown that there exists band gaps for which certain frequencies of waves cannot propagate.

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. The existence of band gaps in these materials has resulted in many practical applications in subwavelength imaging, vibration, control and even acoustic cloaking.

1.2 Mechanisms for band gap formation

The formation of band gaps and effect of dispersion on waves is material dependent, but the underlying physics is the same. The two mechanisms are

1. *Bragg scattering*: At certain frequencies, a wave interacts with the structure of the material in a way that causes deconstructive interference. Here the behavior is dependent on the periodicity of the material [1].

2. *Local resonance*: When resonators are placed inside of a materials, interactions occur around the resonating frequency of the included resonators. At these frequencies, the resonators begin to absorb energy from incident waves and thus affect the propagation of the waves.

To see the effect of these phenomena on the dispersion relation itself, we refer to Figure 1 from Laude's book. When resonators are included we can predict that a band gap will form around the resonant frequency. This band gap is in addition to the band gap caused by Bragg scattering, and occasionally the two band gaps can overlap to form a larger one.

1.3 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

$$\begin{aligned} u(x) &= \tilde{u}_1(x)e^{ikx} \\ &= \tilde{u}_2(x)e^{-ikx} \end{aligned}$$

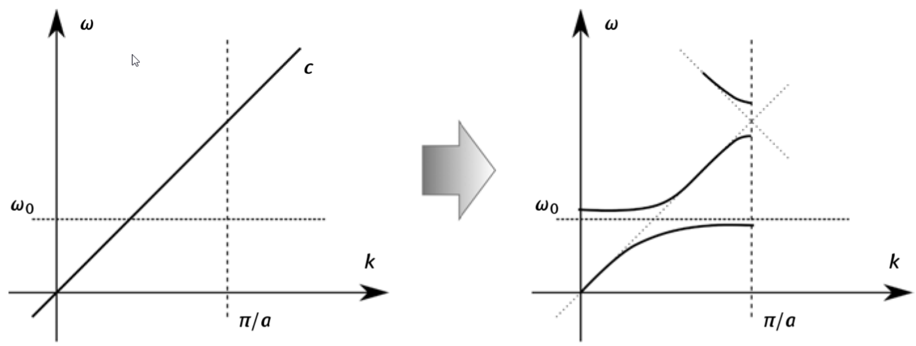

Figure 1: Given the resonant frequency of inclusions and the periodicity of the material we can get an idea of where the band gaps will form. Figure from [1]

In the above, $\tilde{f}_1$ and $\tilde{f}_2$ are also periodic in x [2].

Bloch's theorem is similar to Floquet's theorem but applies to higher dimensions [1].

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.

2 Current research in the field

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. Within the body of research on damping, studies focus on either harmonic wave propagation or free wave propagation. A study of harmonic wave propagation entails one in which the wave numbers are confined to be real while free wave propagation allows for complex wave numbers (and as a result evanescent waves). Standard computational methods as discussed in Section 4 are used in both types of studies.

In [3], dispersion relations are first obtained for a 1D diatomic lattice with linear viscous damping. The method of analysis for this example is then extended to a 1D lattice with internal resonators and also a 2D phononic crystal with square unit cells embedded with a single, denser square inclusion. The general result of including damping is the collapase of the band gap between the optical and acoustic branches of the dispersion relation. This occurs such that the optical branch lowers proportional to the amount of damping.

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.

2.3 Disordered materials

Just as sparse as nonlinear systems, the study of phononic media with disorder has not been widely researched. Incorporating even small amounts of 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 mild 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 peaks, there still exists band gaps.

An earlier paper in 2010 by, examined a 2d phononic medium with circular inclusions arranged in a lattice. 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.

2.4 Dynamic effective properties

With any heterogeneous material, it is of interest to be able to define effective properties and model the material as one homogenous material. This reduces the computational cost of modeling. Most analysis in homogenization has been done in the long wavelength limit. Trying to perform a similar type of analysis on a material with dispersive properties results in the loss of this behavior. The problem here lies in the volume averages used to calculate the effective properties. The richness in behavior of these phononic media is due to the relative motion of contituents as such the behavior is said to be nonlocal and this must be taken into affect when trying to formulate dynamic effective properties.

Michael Frazier has done some work calculating the dynamic effective viscosity in damped 1D layered structures.

3 Dispersion relations

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 waves to calculate dispersion relations, however, there is a commonality between each type of analysis. This common feature is the application of Floquet-Bloch theory.

3.1 Transfer matrix method

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. This results in the formulation of a so called transfer matrix. This type of analysis is completed by of course applying Bloch's theorem to relate the displacements and forces in one cell to another.

3.2 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 a solution of the form

$$u(x,t) = A\sin(kx - \omega t) \tag{5}$$

In fact, we can assume $u(x,t) = f(kx - \omega t)$ and the following results will still hold. 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. We call relations of this type dispersion relations. In general, dispersion relations can be written in the form

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

To get a flavor for what dispersion entails, we need to look at the phase velocities waves. The phase velocity of a wave is

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

Thus, for the scalar wave equation discussed in this introductory paragraph

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

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

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

3.3 Monatomic lattice

Take a system of n masses and springs like in Figure 2 Lets write the equations of motion for the nth mass

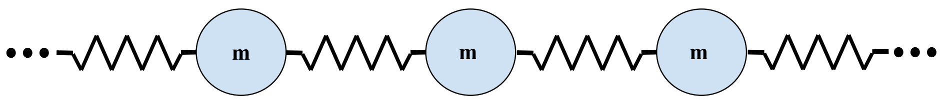

Figure 2: A system of masses connected by springs extending infinitely to the left and right.

system.

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

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 solution of the form

$$u_n = Ae^{i(kx_n - \omega t)} \tag{13}$$

A 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 3. The dispersion relation characterizes many features of the mass-

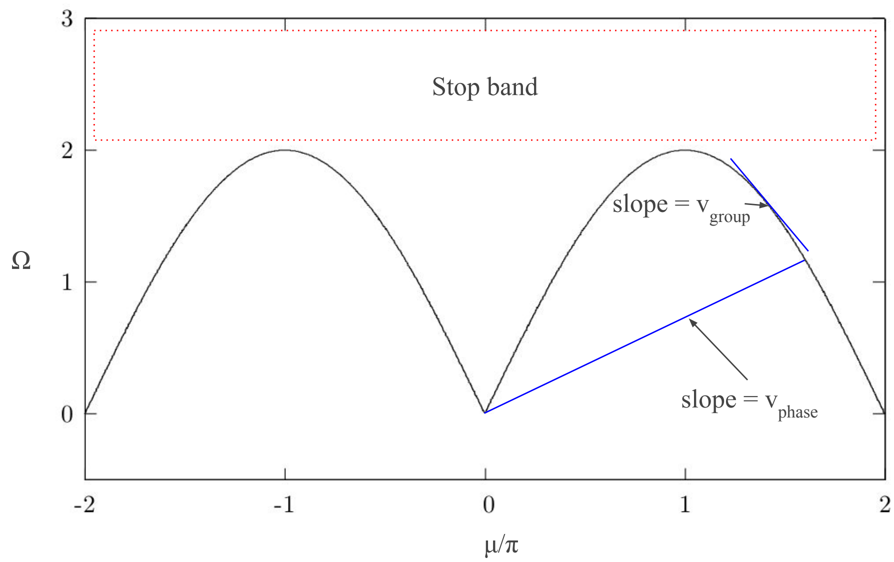

Figure 3: The non-dimensional dispersion relation for the mass spring system

spring system. In Figure 3, 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

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

3.4 Diatomic lattice

Next, we consider a diatomic lattice as shown in Figure 4.

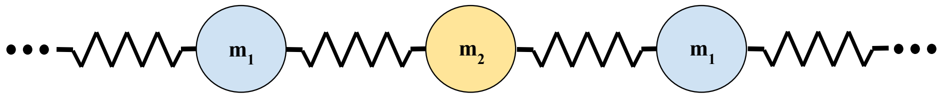

Figure 4: A system of alternating masses connected by springs extending infinitely to the left and right.

After assuming a harmonic motion

$$u_n = \tilde{u}(x_n)e^{i\omega t} \tag{20}$$

The equations of motion for a diatomic lattice can be written

$$(-\omega^2 m_2 + 2k)u_{2n} - k(u_{2n-1} + u_{2n+1}) = 0 \tag{21}$$

$$(-\omega^2 m_1 + 2k)u_{2n+1} - k(u_{2n} + u_{2n+2}) = 0 \tag{22}$$

We can write this in a matrix for

$$(\mathbf{K}_n - \omega^2\mathbf{M})\mathbf{u}_n + \mathbf{K}_{n-1}\mathbf{u}_{n-1} + \mathbf{K}_{n+1}\mathbf{u}_{n+1} = 0 \tag{23}$$

where

$$\mathbf{u}_n = \begin{bmatrix} u_{2n} \\ u_{2n+1} \end{bmatrix} \tag{24}$$

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

$$\mathbf{u_n} = \hat{\mathbf{u}}(\mu)e^{in\mu} \tag{25}$$

Finally, we can write

$$\left[\mathbf{K}_n + \mathbf{K}_{n-1}e^{-i\mu} + \mathbf{K}_{n+1}e^{i\mu} - \omega^2\mathbf{M}\right]\hat{\mathbf{u}}(\mu)e^{in\mu} = 0 \tag{26}$$

$$\left[\bar{\mathbf{K}}(\mu) - \omega^2\mathbf{M}\right]\hat{\mathbf{u}}(\mu)e^{in\mu} = 0 \tag{27}$$

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

$$\omega = \pm\sqrt{k\frac{m_1+m_2}{m_1m_2} \pm k\sqrt{\left(\frac{m_1+m_2}{m_1m_2}\right) - \frac{4(\sin ka)^2}{m_1m_2}}} \tag{28}$$

4 Computational methods for phononic media

4.1 Plane-wave expansion method

According to [4], the plane-wave method is widely used because of its convenience. Apparently, the drawback of the method is slow convergence.

1. To start expand the displacements and material properties in the wave equation in terms of a Fourier series (assert solutions in the form of Bloch waves)

2. Substitute these expansions back into the wave equation

3. After forming some kind of inner products, an eigenvalue problem can be found

4. In order to actually find the dispersion relations, one must solve the eigenvalue problem for a range of wave numbers

4.2 Finite difference method

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

1. Instead of expanding the solution on material properties, the differential operators of the wave equation are expanded using standard finite differences

2. The equations of motion can be written as a matrix equation

3. An eigenvalue problem appears after asserting a Bloch wave type solution

4. Once again the eigenvalue problem must be solved for a range of wave numbers

4.3 Finite element method

The finite element method is useful for complex material geometries. When applied to periodic systems, the domain of computation is greatly reduced via application of Bloch's theorem. The standard outline for the finite element method is as follows

1. Formulate the weak form of the wave function by multiplying by a trial function and integrating

2. Write the equation in matrix form by allowing the solution to be expressed as a combination of weight functions

3. Apply the Bloch's theorem

4. Solve the resulting eigenvalue problem for a range of wave numbers

4.4 Multiple scattering method

Compared to the above methods, the multiple scattering method has an advantage when the material under consideration contains scattering elements (resonators?). 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

5.1 Monatomic lattice

Here we verify the results of Section 3.3. The system is modeled using the equations of motion (12) and the Verlet integration method. Figure 5 displays the dispersion relation for the mass spring system which has been calculated from the real time evolution of the system. The system is excited in a range of frequencies between $\Omega = 0$ and $\Omega = 2$. For each of the frequencies, the system is allowed to evolve and the Fourier transform of the resulting wave is computed. In the reciprocal space, there is an obvious peak at one wave number. This wave number is then plotted with its corresponding frequency.

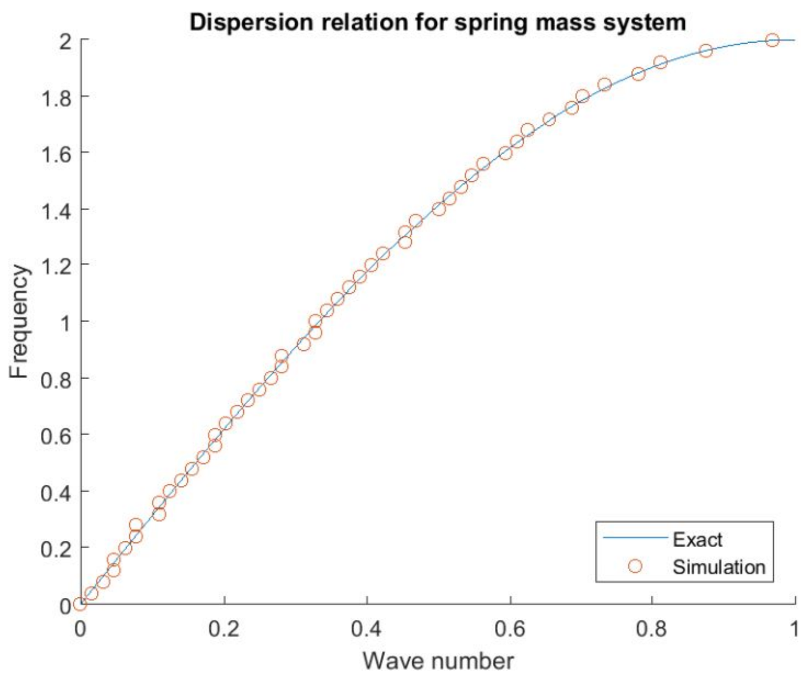

Figure 5: Using a Fourier transform in space, wave lengths for different excitation frequencies are identified and plotted

Applying a sinusoidal, forcing term to the first mass it is easy to explore the attenuation effect at the stop band as seen in Figure 3. Figures 6 and 7 display snapshots of the system at excitation frequencies above and below $\Omega = 2$. There is an obvious drop in amplitude inside and outside of the stop band.

5.2 Diatomic lattice

Here the results for a diatomic lattice are presented from a similar simulation to the above.

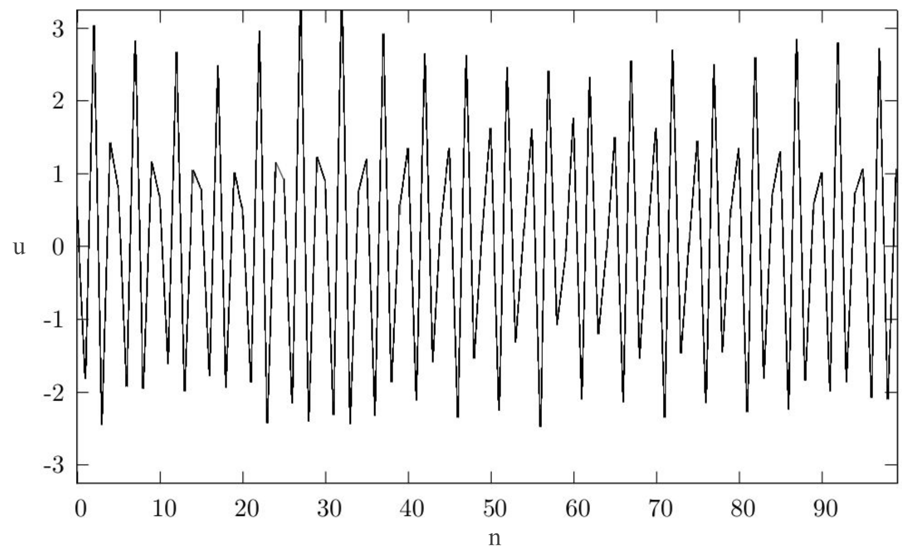

Figure 6: Snapshot of mass spring system with $\Omega = 1.9$

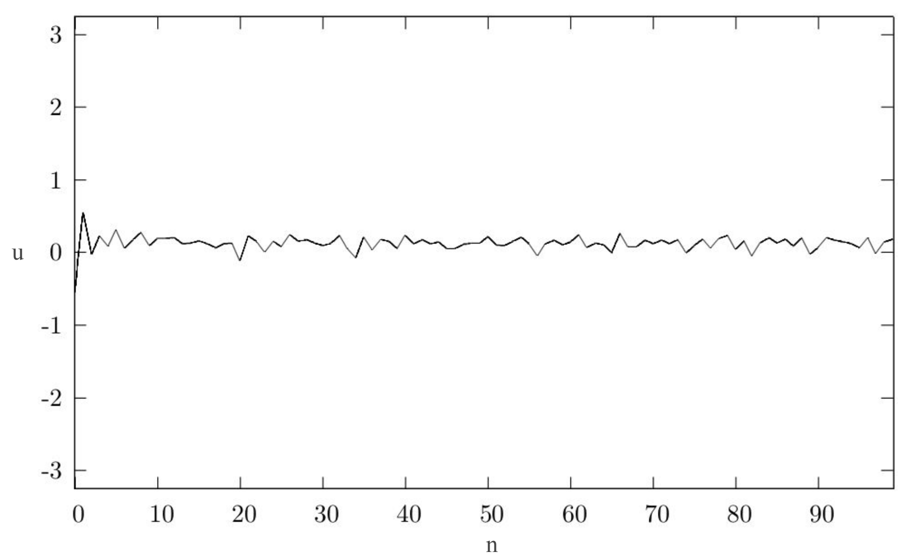

Figure 7: Snapshot of mass spring system with $\Omega = 2.1$

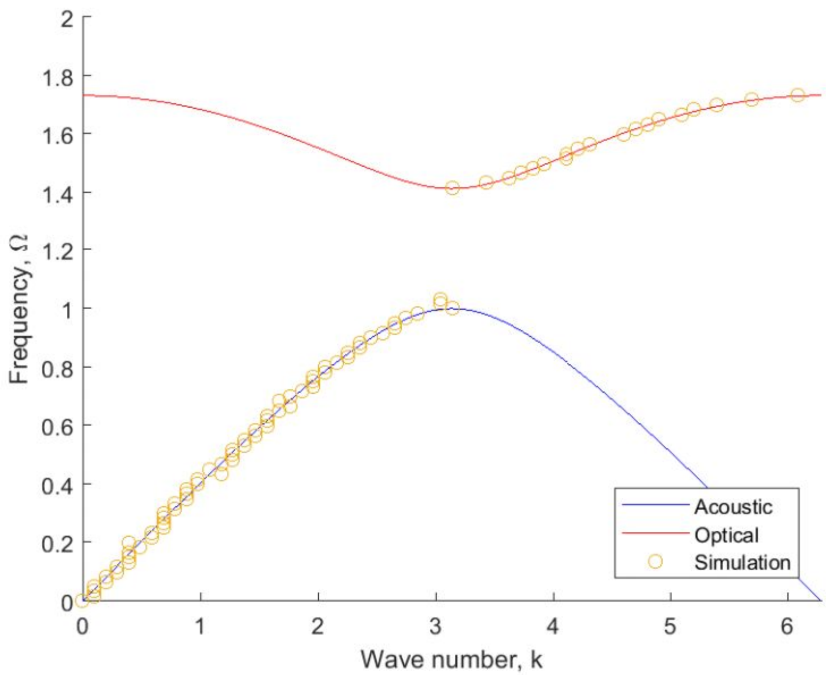

Figure 8: Dispersion relation for the diatomic lattice

6 Analysis of 1D continuum materials via finite element method

6.1 1D uniform bar

As a first exercise in using finite elements to find the dispersion properties of materials, we will solve for the real time evolution of a waves in a bar and find the dispersion relation in a similar manner as in the mass-spring system (using the Fourier transform in space). For the one dimensional problem, the elasticity equations we want to solve are.

$$\frac{\partial \sigma_x}{\partial x} + b_i = \rho \frac{\partial^2 u_x}{\partial t^2}, \quad x \in [0, L] \quad \text{(Equilibrium)} \tag{29}$$

$$\sigma_x = E\varepsilon_x \quad \text{(Constitutive relation)} \tag{30}$$

$$\varepsilon_x = \frac{\partial u_x}{\partial x} \quad \text{(Strain-displacement)} \tag{31}$$

$$u_x(x = 0, t) = A_0 sin(\omega t) \tag{32}$$

$$\sigma_x(x = L, t) = 0 \tag{33}$$

Note that the finite element solution with n nodes is analogous to the mass spring system with n masses. Here, we can relate the material properties via $\rho = \frac{M}{AL}$ and $E = \frac{kL}{A}$. Thus, for a system of n masses, the analogous system in finite elements has material properties

$$\rho = \frac{n}{d(n-1)} \tag{34}$$

and

$$E = \frac{k_{eff} \times d(n-1)}{1} = (1/k + \cdots)^{-1} \times d(n-1) = \frac{d(n-1)}{n} \tag{35}$$

where $L = d(n-1)$ and we require that the nodes have the spacing with respect to each other as the springs to with each other.

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.

$$\int_0^L \varphi \frac{\partial \sigma_x}{\partial x} dx = \int_0^L \varphi \rho \frac{\partial^2 u_x}{\partial t^2} dx \tag{36}$$

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

$$\varphi(L)\sigma_x(L) - \varphi(0)\sigma_x(0) - \int_0^1 \frac{\partial \varphi}{\partial x} \sigma_x dx = \int_0^L \varphi \rho \frac{\partial^2 u_x}{\partial t^2} dx \tag{37}$$

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

$$\int_0^1 \frac{\partial \varphi}{\partial x} E \frac{\partial u_x}{\partial x} dx + \int_0^L \varphi \rho \frac{\partial^2 u_x}{\partial t^2} dx = 0 \tag{38}$$

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

$$\varphi = N_i(x) \tag{39}$$

$$u_x = \sum_j a_j(t) N_j(x) \tag{40}$$

Then,

$$\int_0^1 \frac{\partial N_i(x)}{\partial x} E \sum_j \frac{\partial N_j(x)}{\partial x} a_j dx + \int_0^L N_i \rho \sum_j N_j \frac{\partial^2 a_j(t)}{\partial t^2} dx = 0 \tag{41}$$

Rearranging,

$$\int_0^1 E \sum_j \frac{\partial N_i(x)}{\partial x} \frac{\partial N_j(x)}{\partial x} a_j dx + \int_0^L \rho \sum_j N_i N_j \frac{\partial^2 a_j(t)}{\partial t^2} dx = 0 \tag{42}$$

Finally, we write the above equation in matrix form

$$Ka + M\ddot{a} = 0 \tag{43}$$

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

We now assume a solution of the form

$$a = ae^{i(kx - \omega t)} \tag{44}$$

such that the second order differential equation (43) becomes a complex eigenvalue problem:

$$Ka - \omega^2 Ma = (K - \omega^2 M)a = 0 \tag{45}$$

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

$$a(x+h) = a(x) \quad \text{(Periodic boundary condition)} \tag{46}$$

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

$$a(x+h) = e^{ik_x h} a(x) \quad \text{(Bloch condition)} \tag{47}$$

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

$$T = \begin{bmatrix} 1 & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \\ e^{ik_x h} & \mathbf{0} \end{bmatrix} \tag{48}$$

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

$$a = \begin{bmatrix} a_{left} \\ a_{int} \\ a_{right} \end{bmatrix} = \begin{bmatrix} 1 & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \\ e^{ik_x h} & \mathbf{0} \end{bmatrix} \begin{bmatrix} a_{left} \\ a_{int} \end{bmatrix} = T\hat{a} \tag{49}$$

Our eigenvalue problem is now

$$(K - \omega^2 M)T\hat{a} = 0 \tag{50}$$

To make it so our matrix is square, and therefore invertible, we premultiply the equation by T^T

$$(\hat{K} - \omega^2 \hat{M})\hat{a} = 0 \tag{51}$$

where

$$\hat{K}(k_x) = T^T K T \tag{52}$$

and

$$\hat{M}(k_x) = T^T M T \tag{53}$$

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.

7 Analysis of 2D continuum materials via finite element method

8 Conclusion

9 Future work

10 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

$$x_n^{t+1} = 2x_n^t - x_n^{t-1} + a(x_n^t)\Delta t^2 \tag{54}$$

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 (43), 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 (43). We partition the matrices

$$\begin{bmatrix} K_{11} & K_{1a} \\ K_{a1} & K_{aa} \end{bmatrix} \begin{bmatrix} a_1 \\ a \end{bmatrix} + \begin{bmatrix} M_{11} & M_{1a} \\ M_{a1} & M_{aa} \end{bmatrix} \begin{bmatrix} \ddot{a_1} \\ \ddot{a} \end{bmatrix} = 0 \tag{55}$$

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 (55).

$$K_{aa}a + M_{aa}\ddot{a} = -a_1 K_{a1} - \ddot{a_1} M_{a1} \tag{56}$$

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

$$K_{aa}a^t + M_{aa}\frac{a^{t+1} - 2a^t + a^{t-1}}{\Delta t^2} = -a_1^{t+1}K_{a1} - \ddot{a_1}^{t+1}M_{a1} \tag{57}$$

Solving for a^{t+1}

$$a^{t+1} = M_{aa}^{-1}(-a_1^{t+1}K_{a1} - \ddot{a_1}^{t+1}M_{a1} - K_{aa}a^t)\Delta t^2 + 2a^t - a^{t-1} \tag{58}$$

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