Existence of Trapped Vibration Modes in One-Dimensional Crystal Lattices

Shu-Ching Yang

Under the direction of
Rodrigo Arrieta Candia
MIT Mathematics Department

Research Science Institute
August 1, 2023

Abstract

This paper presents a rigorous proof of the existence of trapped vibration modes in a one-dimensional monatomic crystal represented as a lattice with masses and strings, subjected to perturbations. By applying the Min-max theorem, we demonstrate that modifying any number of masses, resulting in a decrease in their overall sum, leads to the emergence of at least one trapped vibration mode. We also extend our analysis to general cases where string constants can also be altered and show that as long as the net sum of elastic constants increases, trapped vibration modes still exist. These findings provide valuable insights into the dynamic behavior of perturbed lattices and hold potential applications in diverse fields.

Summary

In this paper, we provide a convincing proof that a special phenomenon called trapped vibration modes exist in one-dimensional monatomic lattices when they are subjected to perturbations, such as changes in masses or elastic constants of connecting strings. Trapped vibration modes refer to the phenomenon where nearby atoms exhibit more pronounced vibrations than those farther away. These findings provide valuable insights into the dynamic behavior of perturbed lattices with potential applications across various fields.

1 Introduction

Lattice dynamics centers on the examination of atomic vibrations within a crystalline structure. It revolves around the concept of phonons, which are collective, weakly interacting waves of atomic vibrations and their associated quasiparticles. A thorough understanding of lattice dynamics is crucial for comprehending the fundamental properties of crystalline and amorphous materials, encompassing thermodynamics and superconductivity [1].

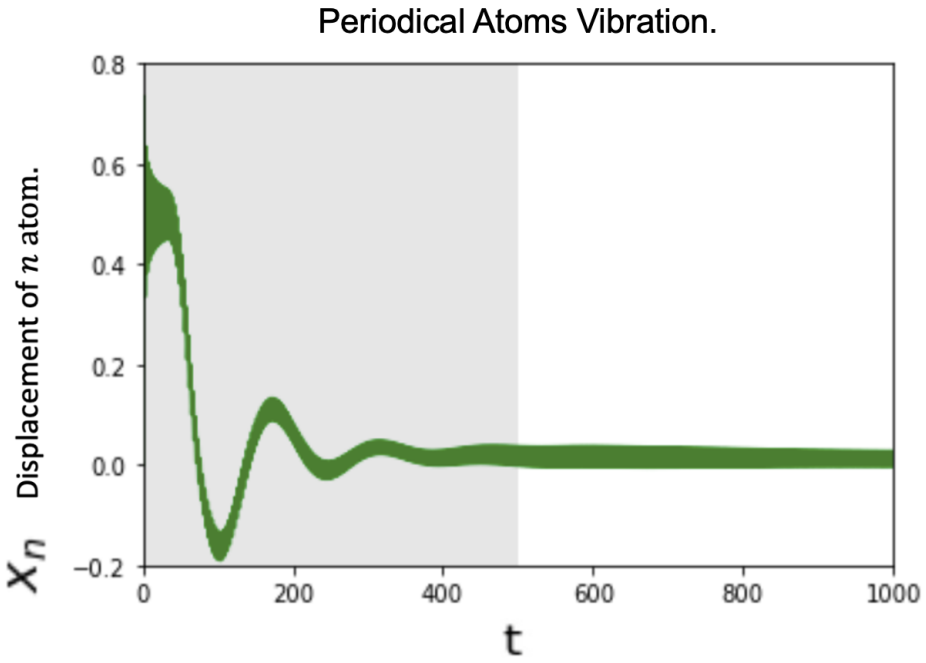

Figure 1: Atoms vibration in a periodical chain, demonstrating the horizontal displacement of the nth atom over time. Sourced from [2].

A widely adopted method for investigating atomic vibrations involves representing atoms as masses and their interactions as springs. *Harmonic approximation* is applied in this mass-spring model, assuming that the potential energy governing interactions between neighboring atoms can be approximated as a harmonic potential. This implies that interatomic forces are linear and proportional to displacements from equilibrium positions, allowing the potential energy to be expressed as a quadratic function of atomic displacements. In addition, note that only nearest neighbor interactions are considered, excluding long-range Coulomb forces and other external forces due to their minor effects compared to dominant interatomic forces. This focused approach enables efficient analysis of atomic vibrations in crystalline structures. In the mass-spring model, the force between nearby atoms is estimated using *Hooke's law*, and the equations of motion are derived from *Newton's Second Law*. In perfectly periodic crystals, we employ Bloch's theorem, so atomic displacements exhibit specific solutions known as *normal modes* $e^{i(kx-\omega t)}$ [3]. However, introducing simple point defects, such as introducing a

lighter atom or a string with higher elastic constant, disrupts the periodicity, leading to the emergence of a new *trapped vibration mode*. In this mode, oscillations become concentrated near the perturbation and decay as we move away from it. As depicted in Figure 2, the energy does not decay over time as observed in a chain of identical atoms and springs. Instead, it remains constant, allowing the activated lighter atom to vibrate indefinitely.

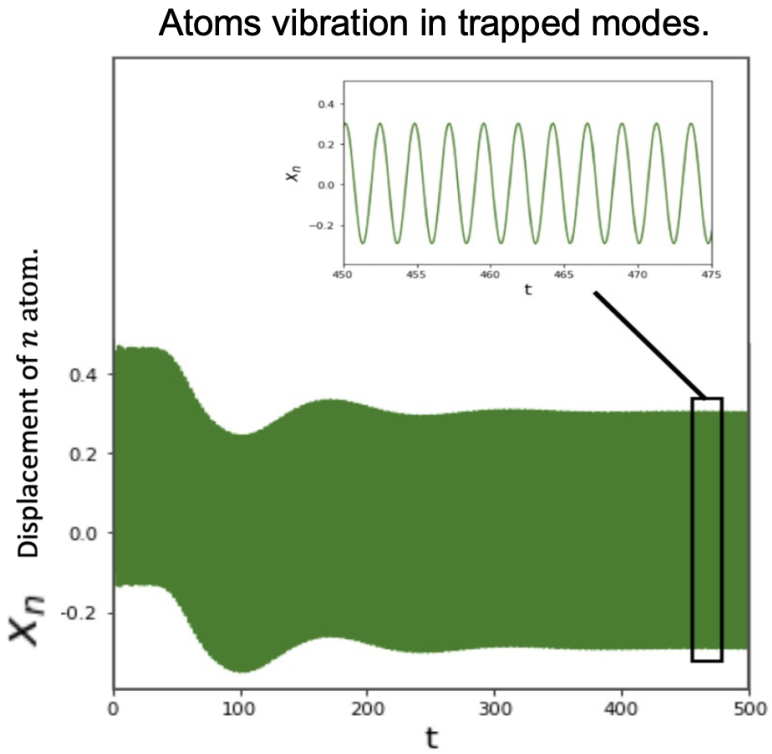

Figure 2: Atoms vibration in a perturbed case, demonstrating the horizontal displacement of the nth atom over time. Sourced from [2]

The practical uses of trapped vibration modes illuminate the captivating occurrences of localized vibration modes in various materials. Although direct experimental demonstrations of these modes in a precise manner have not yet been carried out, observations in the infrared vibration absorption spectra of alkali-halide crystals and the energy distribution of scattered neutrons in metal alloys suggest the potential existence of localized vibration modes [4]. Furthermore, measurements of the absorption spectra associated with ions in certain crystals, such as CaF_2, provide valuable insights into the behavior of light ions on fluorine sites and their interactions with lattice vibrations [5]. In the broader context of solid-state physics, the study of defects and imperfections in crystal lattices highlights their significant influence on various macroscopic properties, ranging from changes in relaxation times and transport processes to the occurrence of surface catalysis and electrical properties in semiconductors [6]. Overall, these applications underscore the relevance and significance of localized vibration modes in advancing our understanding of material behavior and potential

technological applications.

The phenomenon of *trapped vibration modes* in lattice dynamics finds analogies in other domains, notably in waveguides with guided modes and bounded states in the *Schrödinger wave equation*. While proving the existence of at least one bounded state in a 1-dimensional potential well is well-established, its extension to the 2-dimensional case presented considerable challenges. Simon's [7] 1976 proof, utilizing intricate *functional analysis tools*, resolved this issue. However, a simpler proof using the *Min-max theorem*, with a slightly more complex *trial function*, was later achieved by Yang and de Llano [8] in 1989. Yang's variational approach has demonstrated analogous results for weak periodic potentials [9] and waveguide theory [10]. In phonon theory, it has been observed from experiments that introducing simple point defects, for example, substituting an atom in a crystal with a lighter mass counterpart, results in the appearance of localized/trapped modes [5, 6]. Nonetheless, the existence of an analogous "localization theorem" in the 1-D lattice lacks rigorous proofs so far. This paper examines the following using a Min-max theorem:

Conjecture 1. *In a one-dimensional crystal modeled as a lattice of masses and springs, any finite number of masses or springs being changed will always lead to the existence of at least one trapped vibration mode, as long as the net mass is decreased or the sum of string constants is increased, even by an arbitrarily small amount.*

This paper starts by investigating the mass-string model applied to the simple harmonic oscillator and 1-D monatomic lattice in Section 2. We derive the equations of motion for both systems and the dispersion relation for the 1-D lattice. In the Section 3, we validate our s. Firstly, we proved the existence of at least one trapped vibration in the 1-D lattice when altering masses, provided the net sum of masses decreases. Subsequently, we establish the presence of trapped vibration modes in the 1-D lattice upon changing spring elastic constants, as long as the net sum of elastic spring constants increases. Additionally, we extend our findings to a generalized case where any amount of masses and spring constants in a 1-D monatomic lattice can change simultaneously. In Section 4, we present our conclusions and directions for future research.

2 Spring-mass Models for 1-D Lattices

This section introduces the 1-D spring-mass model. We begin by simulating a harmonic oscillator with a single mass and string. Subsequently, we extend the model to monatomic and diatomic lattices, comprising an infinite chain of masses and springs.

2.1 Simple Harmonic Oscillator

To begin, we examine a basic harmonic oscillator consisting of a mass m attached to a single spring with an elastic constant J. The mass experiences a single force F, and undergoes a displacement $x(t)$ from equilibrium, as illustrated in Figure 3. The force F can be determined using two approaches. According to Newton's Second Law, $F = m\ddot{x}(t)$. On

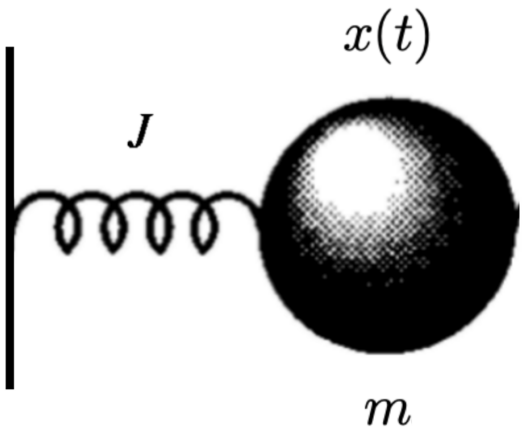

Figure 3: Simple harmonic oscillator.

the other hand, Hooke's Law states that $F = -Jx(t)$. Combining these two equations, we derive the equation of motion

$$m\ddot{x}(t) + Jx(t) = 0.$$

By solving this differential equation, we find that the motion is described by the function

$$x(t) = A\cos(\omega t + \phi), \quad \text{where } \omega = \sqrt{J/m}.$$

2.2 Unperturbed Monatomic Lattice

We can employ a spring-mass model with an infinite chain of masses and springs to simulate a 1-D crystal, where each atom is represented by a mass m and separate by the unit cell length a, the interactions between atoms with harmonic constant J are simulated using springs as illustrated in Figure 6. The displacement of the nth atom from the equilibrium position is denoted by u_n ($n \in \mathbb{Z}$). Note that we only consider the interaction between the nearest neighbour atoms in the chain. Similar to the case of a simple harmonic oscillator,

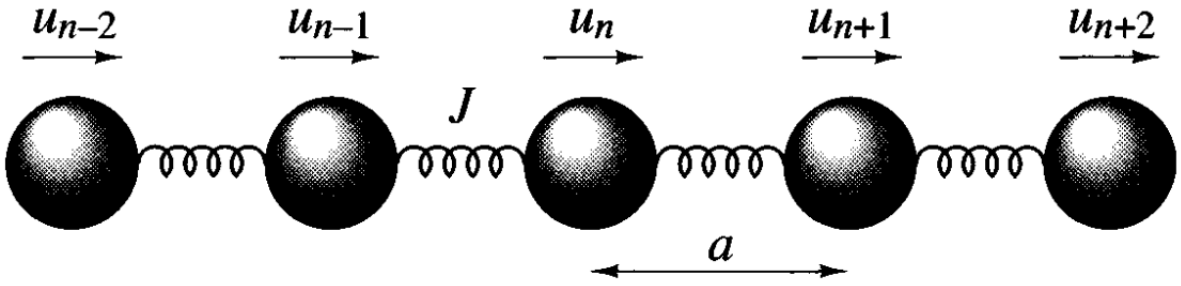

Figure 4: Linear chain model of monatomic lattice. Sourced from [1].

one approach to calculate the interactive force between two atoms is by applying Hooke's Law, which yields the result:

$$F = -J\left(u_n - u_{n+1}\right) - J\left(u_n - u_{n-1}\right) = -J\left(2u_n - u_{n+1} - u_{n-1}\right).$$

Again, another way to calculate the force is by applying Newton's Second Law. By combining both approaches, we obtain the equation of motion for the nth atom as:

$$m\frac{\partial^2 u_n}{\partial t^2} = -J\left(2u_n - u_{n+1} - u_{n-1}\right). \tag{1}$$

Based on Bloch's theorem, a commonly employed theorem in solid-state physics, the periodicity of our system implies that we can decompose an arbitrary solution as normal modes of the form

$$u_n\left(t\right) = \tilde{u}_n \exp\left(i\left(kan - \omega t\right)\right), \tag{2}$$

where k is the wave vector, ω is the angular frequency, and $\tilde{u}_n$ represents the amplitude of the wave. We next need to consider the acceleration of each atom, which is given as the second derivative of the atomic displacement:

$$\ddot{u}_n(t) = -\omega^2 \tilde{u} \exp i(kna - \omega t) = -\omega^2 u_n(t).$$

Newton's second law now links (1) and (2) together:

$$m_1\ddot{u}_n(t) = -m_1\omega^2 u_n(t) = -J\left(2u_n(t) - u_{n+1}(t) - u_{2,n-1}(t)\right). \tag{3}$$

Note that we can write

$$u_{n\pm1}(t) = u_n \exp(\pm ikna).$$

Since both side of the equation have the same constant expressions, we can divide this out of the equation to yield the dispersion relation:

$$\begin{aligned}
\omega^2 &= \frac{J}{M}(2 - e^{-ika} - e^{ika}) \\
&= \frac{2J}{M}(1 - \cos(ka)) \\
&= \frac{4J}{M}\sin^2(ka/2),
\end{aligned}$$

or

$$\omega = \sqrt{\frac{4J}{M}}|\sin(ka/2)|.$$

Plotting the graph for the dispersion relation as shown in Figure 5, we can that the maximum real value ω_k can attain is $\left(\frac{4J}{m}\right)^{1/2}$.

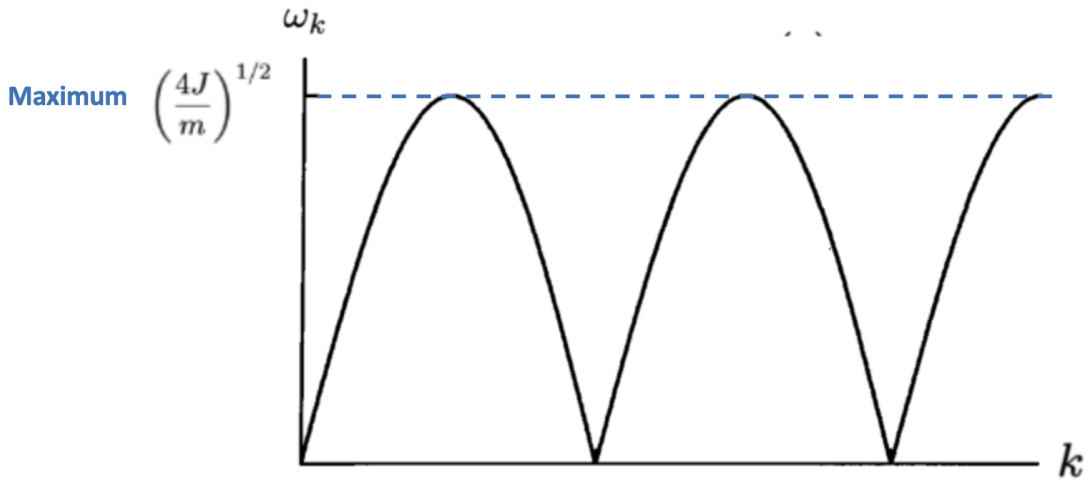

Figure 5: Dispersion relation of 1-D monatomic crystal lattice. Sourced from [1] and the notations have been modified.

3 Trapped Modes in Perturbed 1-D Lattice

In this section, we prove our in a one-dimensional crystal modeled as a lattice of masses and springs. Any changes in masses or springs will always lead to the existence of at least one trapped vibration mode, provided that the net mass is decreased and the net sum of spring constants is increased, even by an arbitrarily small amount. An explicit solution is not required to establish this, instead, we employ the Min-max theorem, which has been previously utilized to demonstrate the existence of bound modes in the context of the Schrödinger equation or guided modes in waveguides. Initially, we establish the existence of trapped vibration modes in one-dimensional monatomic lattices by considering changing masses. Subsequently, we extend our research to encompass scenarios where any number of spring constants can be modified simultaneously.

3.1 Perturbed Lattice with Changing Masses

We start with a monatomic lattice comprising masses M and elastic constant J, as shown in Figure 6. In this case, we explore a scenario where any number of masses in the infinite linear chain of atoms have been altered, and their mass is denoted by M_n. We define

$$\frac{1}{r_0} = \frac{J}{M}, \quad \frac{1}{r_n} = \frac{J}{M_n}, \quad \text{and} \quad \frac{1}{r_n} = \frac{1}{r_0} + \Delta_n,$$

In line with the approach used in Section 2, we derive the equation of motion for each atom in the chain based on Newton's Second Law and Hooke's Law: $M_n\ddot{u}_n = J\left(2u_n - u_{n-1} - u_{n+1}\right)$, where u_n represents the displacement of the nth atom from its equilibrium position. Due to the broken periodicity caused by altered masses, we cannot apply Bloch's theorem as in (2).

Nevertheless, we still search for time-harmonic solutions of the form $u_n(t) = \tilde{u}_n e^{-i\omega t}$. As a result, we obtain an equation similar to (3), given by:

$$\frac{M_n}{J}(2\tilde{u}_n - \tilde{u}_{n-1} - \tilde{u}_{n+1}) = \omega^2 \tilde{u}_n, \quad n \in \mathbb{Z}, \tag{4}$$

Equation (4) can be reformulated by defining the space of infinite sequences $\mathbb{C}^{\mathbb{Z}}$. For any $u \in \mathbb{C}^{\mathbb{Z}}$, we can express $\tilde{u}$ as an infinite complex vector:

$$\tilde{u}^{\mathsf{T}} = (\dots, \tilde{u}_{-2}, \tilde{u}_{-1}, \tilde{u}_0, \tilde{u}_1, \tilde{u}_2, \dots),$$

representing the displacement from equilibrium of all infinite atoms. Next, we introduce the operator $T : \mathbb{C}^{\mathbb{Z}} \to \mathbb{C}^{\mathbb{Z}}$ as

$$(Tu)_n = \frac{M_n}{J}(2u_n - u_{n-1} - u_{n+1}),$$

for $n \in \mathbb{Z}$ and $u \in \mathbb{C}^{\mathbb{Z}}$. With this, we can rewrite (4) as:

$$T\tilde{u} = \omega^2 \tilde{u}. \tag{5}$$

Consequently, the solution to our perturbed problem correspond to eigenvectors of the operator T with an eigenvalue of ω^2. The dispersion relation can be categorized into two parts: the allowed frequencies and the forbidden frequencies, as depicted in Figure 5. Values of ω falling within the forbidden region would result in an imaginary k, leading to a trapped vibration mode where the corresponding waves decay as they move away from the perturbed atom. This phenomenon is a characteristic feature of trapped vibration modes. Therefore, to establish the existence of a trapped vibration mode in a 1-D lattice, it suffices to demonstrate the presence of ω values within the forbidden region.

3.2 Min-max theorem Proof for the Existence of Trapped Modes in Perturbed 1-D Lattice with Changing Masses

The masses M_n can vary in weight, either being heavier or lighter than the original mass M. However, there are two specific conditions that need to be satisfied:

- The net mass is decreased:
$$\sum_{n=-\infty}^{\infty} \Delta_n > 0, \tag{6}$$
- The sum of absolute mass differences is finite:
$$\sum_{n=-\infty}^{\infty} |\Delta_n| < \infty.$$

Theorem 2. *In a one-dimensional crystal modeled as a lattice of masses and springs, any number of masses being changed will always lead to the existence of at least one trapped vibration mode, as long as the net mass is decreased, even by an arbitrarily small amount.*

Proof. Min-max Theorem, also known as *Variational Principle*, stated that for any self-adjoint operator $\hat{A}$, the largest eigenvalue $\omega_{\max}$ maximizes the Rayleigh quotient $R\{u\}$ for all u, and the smallest eigenvalue $\omega_{\min}$ minimizes $R\{u\}$ for all u.

Definition 3.

$$\langle u, v\rangle = \sum_{n=-\infty}^{\infty} \overline{u_n} v_n \frac{M_n}{J}, \quad u, v \in l_r^2, \quad l^2 = \left\{u \in \mathbb{C}^{\mathbb{Z}} : \langle u, u\rangle < \infty\right\}.$$

Rayleigh Quotient The Rayleigh quotient of the self-adjoint operator $\hat{A}$, for any $u \in V$, is

$$R_{\hat{A}}\{u\} = \frac{\langle u, \hat{A}u\rangle}{\langle u, u\rangle}.$$

It's worth mentioning that R is a functional, mapping the function u to a number.

To establish the existence of trapped modes, it is not necessary to find a specific value of ω within the forbidden region. Instead, we can use the Min-max Theorem to demonstrate that the upper range of all ω values falls within the forbidden area, represented as $\omega^2 > \frac{4J}{M}$. As depicted in equation (5), ω^2 represents the eigenvalue of the given eigenproblem. Our objective is to determine a specific function v^* that leads to a Rayleigh quotient$R_T\{v^*\}$ greater than $\frac{4J}{M}$. To achieve this, we employ the trial solution $v_n^* = \alpha^{|n|}$, where α is a free parameter, and $|\alpha| < 1$. We take $\alpha \to -1$.

Proposition 4. *$\langle v^*, v^*\rangle < \infty$ and $\langle Tv^*, Tv^*\rangle < \infty$, therefore u, $Tu \in l_r^2$*

Proof.

$$\begin{aligned}\langle v^*, v^*\rangle &= \sum_{n=-\infty}^{\infty} \overline{v_n} v_n \frac{Mn}{J}, \\ &= \sum_{n=-\infty}^{\infty} \alpha^{2|n|} \frac{Mn}{J}.\end{aligned}$$

Theorem 5 (Tannery's Theorem)**.** *Let $S_n = \sum_{k=0}^{\infty} a_k(n)$ and suppose that $\lim_{n\to\infty} a_k(n) = b_k$. If $|a_k(n)| \le M_k$ and $\sum_{k=0}^{\infty} M_k < \infty$, then $\lim_{n\to\infty} S_n = \sum_{k=0}^{\infty} b_k$. [11]*

We take $\alpha \to -1$. Because of Condition 1 3.2, we can apply the Tannery's Theorem 5 which allow us to move the limitation $\alpha \to -1$ inside. Thus

$$\begin{aligned}\langle v^*, v^*\rangle &= \sum_{n=-\infty}^{\infty} r_n, \\ &< \infty.\end{aligned}$$

$$\begin{aligned}\langle v^*, Tv^*\rangle &= \sum_{n=-\infty}^{\infty} \overline{(2v_n - v_{n-1} - v_{n+1})}\,(2v_n - v_{n-1} - v_{n+1}) \cdot \left|\frac{M_n}{J}\right|^2, \\ &= \sum_{n=-\infty}^{\infty} \left|2\alpha^{|n|} - \alpha^{|n-1|} - \alpha^{|n+1|}\right|^2 \cdot \left|\frac{M_n}{J}\right|^2.\end{aligned}$$

Again, we take $\alpha \to -1$ and apply the Tannery's Theorem 5. Thus,

$$\begin{aligned}\langle v^*, Tv^* \rangle &= 16 \sum_{n=-\infty}^{\infty} \left| \frac{M_n}{J} \right|^2, \\ &< \infty.\end{aligned}$$

□

Proposition 6. *T is self-adjoint.*

Proof. As illustrated in Section 3.1,

$$(Tu)_n = \frac{M_n}{J}(2u_n - u_{n-1} - u_{n+1}).$$

Suppose now we have other operators D, D^T and $W : \mathbb{C}^{\mathbb{Z}} \to \mathbb{C}^{\mathbb{Z}}$, where

$$(Du)_n \equiv u_{n+1} - u_n, \quad (D^\top u)_n \equiv u_{n-1} - u_n, \quad \text{and} \quad (Wu)_n \equiv \frac{M_n}{J}.$$

Therefore, we have

$$\left(D^\top (Du)\right)_n \equiv (Du)_n + (Du)_{n-1} \equiv (u_{n+1} - u_n) + (u_n - u_{n-1}) = 2u_n - u_{n-1} - u_{n+1},$$

and

$$\left(W\left(D^\top (Du)\right)\right) n \equiv \frac{M_n}{J}\left(2u_n - u_{n-1} - u_{n+1}\right) \equiv (Tu)_n.$$

In this case,

$$\langle u, Tv \rangle = \left\langle u, WD^\top Dv \right\rangle = \left\langle D^\top Du, wv \right\rangle = \langle Tu, v \rangle.$$

□

Proposition 7. $R_T\{v^*\} > \frac{4J}{M}$.

Proof. Multiplying both sides of $R_T\{v^*\} > \frac{4J}{M}$ by $\langle v, v^* \rangle$, we obtain the following equations for the left and right-hand sides. Note that we take $\alpha \to -1$ and apply the Tannery's Theorem 5 when computing.

$$LHS = \langle Dv^*, (WD)v^* \rangle = \sum_{n=-\infty}^{\infty} \left(v_n^2 + v_{n+1}^2\right) - 2\sum_{n=-\infty}^{\infty} v_n v_{n+1} = \frac{2\alpha^2 - 4\alpha + 2}{1 - \alpha^2}.$$

$$\begin{aligned}RHS &= \frac{4J}{M} \sum_{n=-\infty}^{\infty} |v_n|^2 \left(\frac{1}{r_0} - \Delta_n\right), \\ &= 4\left(1 + 2\sum_{n=1}^{\infty} |v_n|^2\right) - \frac{4J}{M} \sum_{n=-\infty}^{\infty} |v_n|^2 \cdot \Delta_n, \\ &= 4 + \frac{8\alpha^2}{1 - \alpha^2} - \frac{4J}{M} \sum_{n=-\infty}^{\infty} |v_n|^2 \cdot \Delta_n.\end{aligned}$$

If $LHS > RHS$, then $R_T\{v^*\} > \frac{4J}{M}$.

$$\begin{aligned} LHS - RHS &= \frac{2\alpha^2 - 4\alpha + 2}{1-\alpha^2} - \frac{8\alpha^2}{1-\alpha^2} - 4 + \frac{4J}{M}\sum_{n=-\infty}^{\infty} |V_n^*|^2 \cdot \Delta_n, \\ &= \frac{4-4\alpha^2}{1-\alpha^2} + \frac{2(1+\alpha)^2}{(1-\alpha)(1+\alpha)} - 4 + \frac{4J}{M}\sum_{n=-\infty}^{\infty} |V_n^*|^2 \cdot \Delta_n, \\ &= \sum_{n=-\infty}^{\infty} \alpha^{2|n|} \cdot \Delta_n. \end{aligned}$$

Based on the Tannery's Theorem 5, we define $F_\alpha(n) = \alpha^{|2n|}$, and $F[n] = \Delta_n$, let $G(n) = |\Delta_n|$.

$$\begin{aligned} F_\alpha(n) &= \alpha^{|2n|} \cdot \Delta_n, \quad \text{where} \quad |\alpha| < 1, \\ &< \Delta_n, \\ &= G(n). \end{aligned}$$

Therefore,

$$\sum_{n=-\infty}^{\infty} \alpha^{2|n|} \cdot \Delta_n > 0, \quad \text{and} \quad LHS > RHS.$$

□

□

3.3 Perturbed Lattice with Changing Masses and Modified Spring Elastic Constants

Building upon the previously discussed scenario of altered masses in Section 3.1, we now extend our investigation to cases where any number of spring constants are modified. As illustrated in Figure 5, the mass is denoted by M_n while the spring constants are denoted by J_n, with $n \in \mathbb{Z}$.

Similar with Section 3.1, we derive the equation of motion for each atom in the chain based on Newton's Second Law and Hooke's Law: $M_n\ddot{u}_n = J_n(u_n - u_{n-1}) + J_{n+1}(u_n - u_{n+1})$, where u_n represents the displacement of the nth atom from its equilibrium position. Due to the broken periodicity, we cannot apply Bloch's theorem as in (2). Nevertheless, we still search for time-harmonic solutions of the form $u_n(t) = \tilde{u}_n e^{-i\omega t}$. As a result, we obtain an equation similar to (3), given by

$$\frac{M_n}{J_n}(\tilde{u}_n - \tilde{u}_{n-1}) + \frac{M_n}{J_{n+1}}(\tilde{u}_n - \tilde{u}_{n+1}) = \omega^2 \tilde{u}_n, \quad n \in \mathbb{Z}. \tag{7}$$

Equation (7) can be reformulated by defining the space of infinite sequences $\mathbb{C}^{\mathbb{Z}}$. For any $u \in \mathbb{C}^{\mathbb{Z}}$, we can express $\tilde{u}$ as an infinite complex vector

$$\tilde{u}^{\mathsf{T}} = (\ldots, \tilde{u}_{-2}, \tilde{u}_{-1}, \tilde{u}_0, \tilde{u}_1, \tilde{u}_2, \ldots),$$

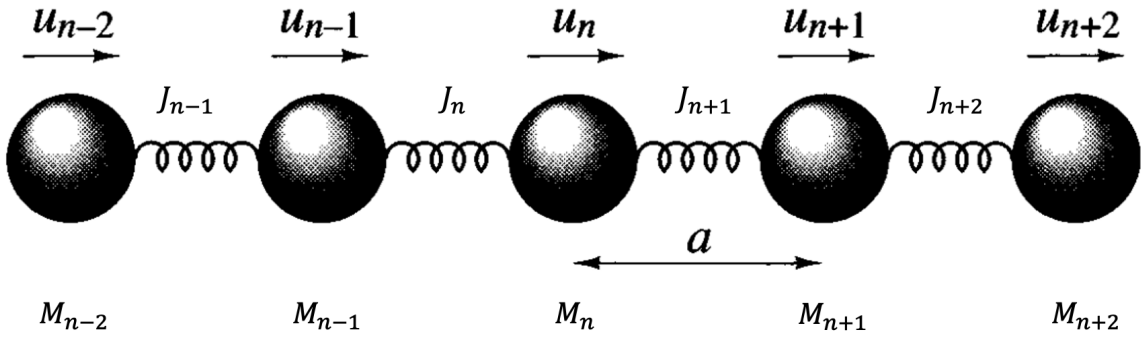

Figure 6: Linear chain model of monatomic lattice with changing masses and spring elastic constants. Sourced from [1] and the notations have been modified.

representing the displacement from equilibrium of all infinite atoms. Next, we introduce the operator P and $\Delta t : \mathbb{C}^{\mathbb{Z}} \to \mathbb{C}^{\mathbb{Z}}$ as

$$(Pu)_n = \frac{M_n}{J_n}(u_n - u_{n-1}) + \frac{M_n}{J_{n+1}}(u_n - u_{n+1}). \tag{8}$$

Note that

$$(Tu)_n = \frac{M_n}{J}(2u_n - u_{n-1} - u_{n+1}).$$

Therefore, we can write (8) into

$$(Pu)_n = (Tu)_n + (\Delta t)_n.$$

For $n \in \mathbb{Z}$ and $u \in \mathbb{C}^{\mathbb{Z}}$. With this, we rewrite (4) as:

$$P\tilde{u} = \omega^2 \tilde{u}.$$

Consequently, the solution to our perturbed problem correspond to eigenvectors of the operator P with an eigenvalue of ω^2.

3.4 Min-max theorem Proof for the Existence of Trapped Modes in Generalized Case

The elastic constant J_n can vary, either being heavier or lighter than the original mass J. However, there are two specific conditions that need to be satisfied:

- The net sum of elastic constants is increased,

$$\sum_{n=-\infty}^{\infty} \Delta J_n > 0. \tag{9}$$

- The net sum of elastic constants is finite,

$$\sum_{n=-\infty}^{\infty} |\Delta J_n| < \infty. \tag{10}$$

Theorem 8. *In a one-dimensional crystal modeled as a lattice of masses and springs, any number of springs being changed will always lead to the existence of at least one trapped vibration mode, as long as the net sum of spring constants is increased, even by an arbitrarily small amount.*

Proof. Similar with the proof mentioned in Section 3.2, by applying Min-max theorem, we only need to find a v^* that allow the Rayleigh quotient$R_P\{v^*\}$ greater than $\frac{4J}{M}$.

Proposition 9. *P is a self-adjoint operator.*

Proof. Since $(Pu)_n = (Tu)_n + (\Delta t)_n$, and the self-adjointness of T has been previously established 6, our focus remains on demonstrating that Δt is also self-adjoint, which, in turn, confirms the self-adjointness of P.
By definition

$$\langle u, \Delta t v\rangle = \sum_{n=-\infty}^{\infty} \left[\Delta J_{n+1}\left(v_n - v_{n+1}\right)\overline{u_n} + \Delta J_n\left(v_n - v_{n-1}\right)\overline{u_n}\right],$$

$$\langle \Delta t u, v\rangle = \sum_{n=-\infty}^{\infty} \left[\Delta J_{n+1}\overline{(u_n - u_{n+1})}v_n + \Delta J_n\overline{(u_n - u_{n-1})}v_n\right].$$

Since n range from $-\infty$ to ∞, we can replace $n \to n-1$. Therefore,

$$\langle u, \Delta t v\rangle = \sum_{n=-\infty}^{\infty} \left[v_{n-1}\overline{u_{n-1}} - v_n\overline{u_{n-1}} + v_n\overline{u_n} - v_{n-1}\overline{u_n}\right]\Delta J_n,$$

$$\langle \Delta t u, v\rangle = \sum_{n=-\infty}^{\infty} \left[u_{n-1}\overline{v_{n-1}} - u_n\overline{v_{n-1}} + u_n\overline{v_n} - u_{n-1}\overline{v_n}\right]\Delta J_n.$$

This implies that $\langle u, \Delta t v\rangle = \langle \Delta t u, v\rangle$, thus Δt is self-adjoint. □

Proposition 10. *$R_P\{v^*\} > \frac{4J}{M}$.*

Proof. We take $\alpha \to -1$. Because of Condition 1 9, we can apply the Tannery's Theorem 5 which allow us to move the limitation $\alpha \to -1$ inside. Multiplying both sides of $R_P\{v^*\} > \frac{4J}{M}$

by $\langle v^*, v^* \rangle$, we obtain the following equations:

$$\begin{aligned} LHS - RHS &= \langle v^*, Tv^* \rangle + \langle v^*, \Delta t v^* \rangle - \frac{4J}{M} \langle v^*, v^* \rangle, \\ &= \sum_{n=-\infty}^{\infty} \alpha^{2|n|} \cdot \Delta n + \sum_{n=-\infty}^{\infty} \left[\Delta J_{n+1} \left(v_n - v_{n+1} \right) \overline{v_n} + \Delta J_n \left(v_n - v_{n-1} \right) v_n \right], \\ &= \sum_{n=-\infty}^{\infty} \Delta J_n \left[v_{n-1} - v_n \right]^2, \\ &= 4 \sum \Delta J_n, \\ &> 0. \end{aligned}$$

Note that we take $\alpha \to -1$ and apply the Tannery's Theorem 5. □

□

4 Conclusion

This paper presents a rigorous proof establishing the existence of trapped vibration modes in a 1-D monatomic lattice under perturbations. By utilizing the powerful Min-max theorem, we demonstrate that when a certain number of masses are altered, while ensuring a decrease in the net sum of masses, at least one trapped vibration mode emerges. Subsequently, we extend this investigation to changes in spring elastic constants, revealing that under the condition of an increased net sum of spring constants, trapped vibration modes persist in the lattice. Notably, we generalize our approach to encompass scenarios where both masses and spring constants are simultaneously modified. Our findings provide deeper insights into the dynamic behavior of perturbed lattices, with potential applications in various fields.

The phenomenon of trapped vibration modes in crystal lattices and guided modes in waveguides captivates researchers due to its widespread relevance across scientific domains. Notably, both of these phenomena have been successfully demonstrated through algebraic proofs in their 1-D manifestations. However, extending these proofs to the more intricate 2-D cases has remained a significant challenge. A notable breakthrough in addressing 2-D waveguide modes came with Yang and de Llano's pioneering work, where they successfully employed the Min-max theorem for their algebraic proof. Despite this progress, the quest for an analogous algebraic proof for trapped modes in 2-D crystal lattices remains ongoing.

In this paper, we contribute a proof for the existence of trapped vibration modes in a generalized 1-D monatomic crystal lattice, utilizing the Min-max theorem. Our successful demonstration in the 1-D case encourages us to explore more complex scenarios, such as 1-D diatomic crystal lattices, while also driving us towards resolving the challenges presented by 2-D lattice cases.

5 Acknowledgments

I extend my heartfelt gratitude to my mentor, Rodrigo Arrieta Candia, for his invaluable guidance and mentorship throughout this summer. I am also thankful to Dr. Tanya Khovanova for her helpful suggestions on the paper. Additionally, I express my gratitude to Professor Johnson for proposing my project and providing valuable insights. Special thanks go to my tutor, Peter Gaydarov, and my teaching assistant, Allen Lin, and Max Bee-Lindgren for their useful advice on my presentation and paper. Lastly, I would like to thank RSI, CEE, MIT and the sponsers of RSI for providing me with this wonderful opportunity to conduct research this summer.

References

[1] M. T. Dove. *Introduction to lattice dynamics*. Number 4. Cambridge university press, 1993.

[2] U. Kausik. Some puzzles (for students) regarding infinite lattices of masses and springs. University Lecture, 2022.

[3] R. D. V. Meade, S. G. Johnson, and J. N. Winn. Photonic crystals: Molding the flow of light, 2008.

[4] A. Maradudin. Theoretical and experimental aspects of the effects of point defects and disorder on the vibrations of crystals—1. In *Solid state physics*, volume 18, pages 273–420. Elsevier, 1966.

[5] A. A. Maradudin, E. W. Montroll, G. H. Weiss, and I. Ipatova. *Theory of lattice dynamics in the harmonic approximation*, volume 3. Academic press New York, 1963.

[6] R. J. Elliott, W. Hayes, G. Jones, H. Macdonald, and C. Sennett. Localized vibrations of h–and d–ions in the alkaline earth fluorides. *Proceedings of the Royal Society of London. Series A. Mathematical and Physical Sciences*, 289(1416):1–33, 1965.

[7] B. Simon. The bound state of weakly coupled schrödinger operators in one and two dimensions. *Annals of Physics*, 97(2):279–288, 1976.

[8] K. Yang and M. de Llano. Simple variational proof that any two-dimensional potential well supports at least one bound state. *American Journal of Physics*, 57(1):85–86, 1989.

[9] A. Parzygnat, K. K. Lee, Y. Avniel, and S. G. Johnson. Sufficient conditions for two-dimensional localization by arbitrarily weak defects in periodic potentials with band gaps. *Physical Review B*, 81(15):155324, 2010.

[10] K. K. Lee, Y. Avniel, and S. G. Johnson. Rigorous sufficient conditions for index-guided modes in microstructured dielectric waveguides. *Optics Express*, 16(13):9261–9275, 2008.

[11] J. Hofbauer. A simple proof of and related identities. *The American mathematical monthly*, 109(2):196–200, 2002.

[12] S. G. Johnson. Notes on waveguide localization by slow-wave regions (a.k.a. "total internal reflection"), Nov 2014.

A Diatomic Lattice

Building upon the findings from the previous section, we will model the movement of atoms in a 1-D diatomic crystal. Specifically, we could consider a harmonic chain consisting of two different atoms within a unit cell, as depicted in figure 7. The harmonic constants are G and g, the mass of the atoms are M and m, the displacement of first and second atom in the nth unit cell is $U_{n,1}$ and $U_{n,2}$ ($n \in \mathbb{Z}^+$), and the distance between two neighbour unit cells are a.

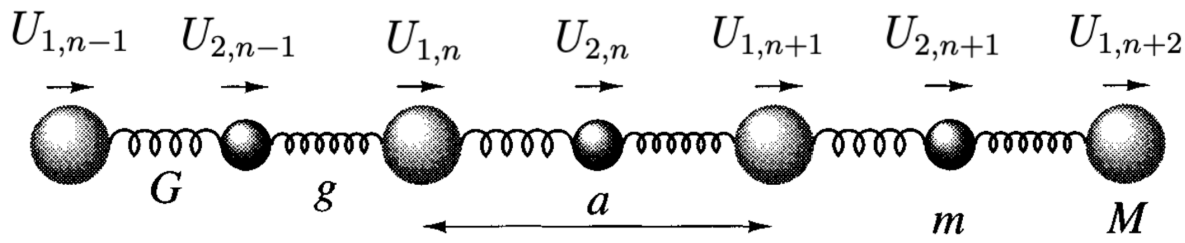

Figure 7: Linear chain model of diatomic lattice. This figure is from [1] and the notations have been modified.

Similar to the monatomic case, we would apply Hooke's Law, Newton's Law and the normal mode equation to model the atoms' displacements. Note that We only consider the interaction between the nearest neighbour atoms in the chain. The force between the nearby atoms is simulated by strings. According to Hooke's Law, the energy obtained by two atoms in the nth unit cells is $E_{1,n}$ and $E_{2,n}$:

$$E_{1,n} = \frac{1}{2}G\left(U_{1,n} - U_{2,n}\right)^2 + \frac{1}{2}g\left(U_{1,n} - u_{2,n-1}\right)^2, \quad E_{2,n} = \frac{1}{2}G\left(U_{2,n} - U_{1,n}\right)^2 + \frac{1}{2}g\left(U_{2,n} - u_{1,n+1}\right)^2.$$

We next need to deal with Newton's Second Law: $Force = Mass \times Acceleration$. The force can also be calculated by the derivative of the energy with respect to displacement:

$$M\frac{\partial^2 U_{1,n}}{\partial t^2} = -(G+g)U_{1,n} + gU_{2,n-1} + GU_{2,n}, \quad m\frac{\partial^2 U_{2,n}}{\partial t^2} = -(G+g)U_{2,n} + gU_{1,n+1} + GU_{1,n}.$$

For the displacement of atoms, we can employ the same general solutions that were previously utilized for the monatomic chain.

$$U_{n,1}(t) = \sum_k \tilde{U}_1 \exp\left(i\left[kna - \omega_k t\right]\right), \quad U_{n,2}(t) = \sum_k \tilde{U}_2 \exp\left(i\left[kna - \omega_k t\right]\right),$$

where $\tilde{U}_1$ and $\tilde{U}_2$ denotes the two amplitudes of a single given mode, and ω_k is the angular frequency. The acceleration of an atom is given as the second time derivative of the atomic

displacement. By substituting the acceleration and normal mode equation into Newton's Second Law, we could acquire the dispersion relation:

$$M\omega_k^2\tilde{U}_1 = (G+g)\tilde{U}_1 - (G+g\exp(-ika))\tilde{U}_2, \quad m\omega_k^2\tilde{U}_2 = (G+g)\tilde{U}_2 - (G+g\exp(ika))\tilde{U}_1.$$

These equations can also be written in matrix form:

$$\begin{pmatrix} -(G+g) & G+g\exp(-ika) \\ G+g\exp(ika) & -(G+g) \end{pmatrix} \begin{pmatrix} \tilde{U}_1 \\ \tilde{U}_2 \end{pmatrix} = \begin{pmatrix} M & 0 \\ 0 & m \end{pmatrix} w_k^2 \begin{pmatrix} \tilde{U}_1 \\ \tilde{U}_2 \end{pmatrix},$$

$$D(k) \cdot \begin{pmatrix} \tilde{U}_1 \\ \tilde{U}_2 \end{pmatrix} = w_k^2 \begin{pmatrix} \tilde{U}_1 \\ \tilde{U}_2 \end{pmatrix}.$$

It is clear that w_k^2 is the eigenvalue and $\begin{pmatrix} \widetilde{U}_1 \\ \tilde{U}_2 \end{pmatrix}$ is the eigenvector in this equation.

Appendix B Waveguide Localization by Slow-wave Regions

In this section, we describe the proof of existence of bounded states(localization) in waveguides in the context of scaler wave equation using Min-max theorem.

A waveguide is a special form of transmission line consisting of a hollow, metal tube that allows waves to propagate along one or more directions while confining them in one or more other "transverse" directions. Waveguide can be seen in many different wave equation, each employing different mechanisms to achieve transverse confinement. One prominent confinement mechanism, widely recognized as "total internal reflection," involves trapping waves within a region of higher refractive index. In essence, this phenomenon prevents waves arriving at the interface between two media from being refracted into the second medium and instead reflects them entirely back into the first medium. Surprisingly, this mechanism is not exclusive to optics but extends to other wave phenomena, leading to a general principle: waves can be confined within a medium where their phase velocity (wave speed) is slower than that of the surrounding medium. We describe the proof of this general principle in 2-D scaler wave equation; related proofs can be applied to other wave equations.

We define the linear operator $\hat{A} = c^2\nabla^2$, where c denotes the wave speed, $c(\mathbf{x}) > 0$ and c is some function of x. $\hat{A}$ is a Hermitian and semidefinite matrix. The scalar wave equation can be written as:

$$-\hat{A}u = c^2\nabla^2 u = \frac{\partial^2 u}{\partial t^2}.$$

For reasonable $c(x)$ we will have *spectral theorem*, which means we can understand the the eigenfunctions $u(x)$ satisfying $\hat{A}u = \lambda u$. Since $\hat{A}$ is self-adjointed, λ would be real; all $\lambda \geq 0$ due to $\hat{A}$'s positive semidefiniteness. Therefore, we can write λ as ω^2, where ω has the units of angular frequency. Plugging these back to the wave equations, $-\hat{A}u = -\omega^2 u = \ddot{u}$, we see that every eigensolution $u(\mathbf{x})e^{\pm i\omega t}$ describes the normal modes with angular frequency ω.

To define a waveguide, we shall examine a 2-D $\mathbb{R}^2$ domain that is defined by the xz plane. The wave speed, denoted as $c(x)$, solely relies on the x-coordinate and remains independent of the z-coordinate. Therefore, we have separable eigensolutions of the form $u(x,z,t) = u_k(x)e^{i(kz-\omega t)}$, where k denotes the propagation constant. The eigenfrequencies $\omega(k)$ are the dispersion relations, and satisfy a reduced eigenproblem:

$$\hat{A}_k u_k = \omega(k)^2 u_k, \text{ with } \hat{A}_k = e^{-ikz}\hat{A}e^{ikz} = c^2\left(-\frac{\partial^2}{\partial x^2} + k^2\right).$$

Therefore, for each k, we have a 1-D eigenproblem for $u_k(x)$. Note that $\hat{A}_k$ is also self-adjoint and positive semidefinite, like $\hat{A}$. We define the 1-D inner product $\langle u(x), v(x)\rangle = \int \frac{\bar{u}v}{c^2}$ (where $\bar{u}$ denotes complex conjugation of u). $\langle u, \hat{A}v\rangle = \langle \hat{A}u, v\rangle$ and $\langle u, \hat{A}u\rangle = \int |\nabla u|^2 \leq 0$ for all u, v.

Consider that there is a width-h strip of "slower" material running along the z axis. The speed of wave $c(x)$ is

$$c(x) = \begin{cases} c_1 & |x| < h/2 \\ c_0 & |x| \geq h/2 \end{cases}, \text{ where } c_1 < c_0.$$

The possible dispersion relation $\omega(k)$ can be categorized into two types: the light cone and guided modes.

- **The light cone**: A continuous spectrum encompassing all potential situations that can exist in the homogeneous c_0 medium(infinitely far away from the "slow" strip). Shown as the shaded area in the left graph of figure 8. In c_0 region, frequencies in light cone correspond to any real $k_\perp$.
- **The guided modes**: Discrete sets of bands of $\omega_n(k)$ lying below the light cone, $\omega_n(k) < c_0|k|$. Shown as the red lines in the left graph of figure 8. In c_0 region, frequencies below light cone would all correspond to purely imaginary $k_\perp = \pm i\sqrt{k^2 - (\omega/c_0)^2}$, which means that it would expotienally decay away.

Appendix B.1 Variational Proof of Slow-wave Guiding

We aim to prove that the fundamental $\omega_1(k)^2 < c_0|k|$. Instead of determining the exact value, a simpler approach is to find the upper limit of $\omega_1(k)^2$ and demonstrate that it is smaller than $c_0|k|$. According to Min-max theorem, $\omega_1(k)^2 < R\{u\}$ for any $u(x)$. Therefore, we only need to find a $u(x)$ such that $R\{u\} < c_0^2k^2$. Then, it will follow that $\omega_1(k)^2 < c_0^2k^2$, which demonstrate the existence of guided modes.

In order to apply Min-max theorem, we first need to prove that $\langle u, u\rangle$ and $\langle u, \hat{A}u\rangle < \infty$. Then we find a $u(x)$ such that $R\{u\} < c_0^2k^2$.

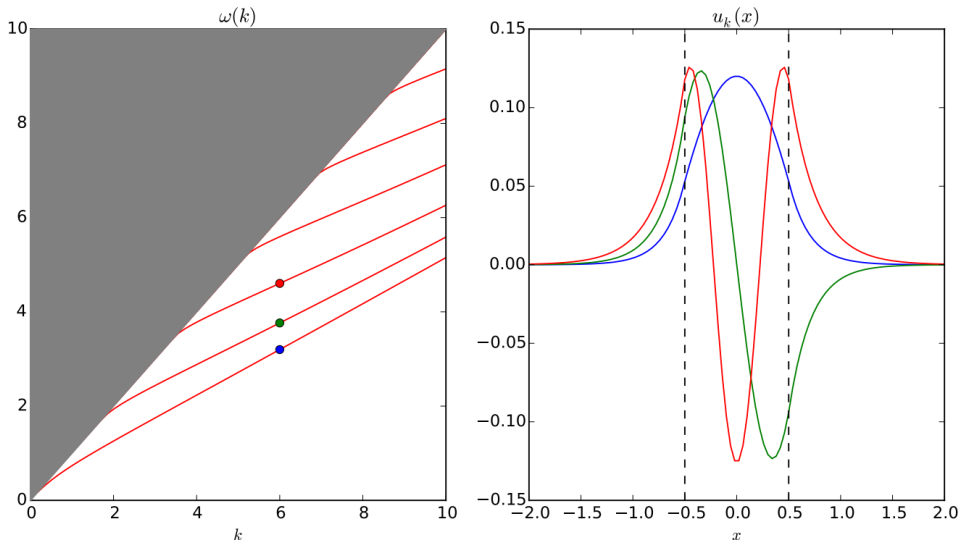

Figure 8: Linear chain model of diatomic lattice. This figure is obtained from [12].