One Dimensional Lattice Dynamics

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***Abstract*—In this experiment, the monatomic and diatomic 1D lattices are examined. In each case, the normal modes are found, and the dispersion relation is plotted. The speed of sound through the medium of the lattice was then found for the monatomic case to be $1.73m/s$, and the Debye frequency was found to be $15.5\frac{1}{s}$. Finally, the band gap between the acoustic and optical branches was found experimentally to be $2.45\frac{1}{s}$, which is 12.9% from the theoretical value of 2.17.**

I. Introduction

Lattice vibration is an important basis for studying the macroscopic properties and microscopic processes of solids. It plays an important role in the physical properties of optical properties, superconductivity, magnetism, structural phase transitions, etc. Studying those properties depends on the dynamics of atoms (lattice vibrations). Atoms in crystal lattice are never at rest as the quantum mechanics studies show, such that atoms vibrate around it's equilibrium position under the elastic force (Hook's law), this force leads to vibrations in the crystal lattice. This motion propagates through the lattice simultaneously. These vibrations which are called normal modes and they are harmonic waves. We will study these normal modes from a classical point of view, however, from a quantum mechanics point of view, the quanta energy of these normal modes are called phonons and they have particle-like properties too.

In this experiment, we will study two cases of lattice vibrations: Monoatomic case and Diatomic case. In the Monoatomic case, we will study a linear chain of atoms with the same mass, every atom is in a single unit cell. In our experiment, we can represent this case in a classical way by using same masses in the system which are connected by springs with spring constant κ. In this case, we are examining the dispersion relation of the normal modes, such that these vibrations corresponds to the displacements from the equilibrium position are identical which is same as the propagation of a sound wave through the lattice; these for these normal modes are names acoustic branches.

However, in the diatomic case, we consider a model where we have two atoms in each unit cell with different masses. For the lower modes, we get acoustic branches like in monoatomic case, however, for higher modes, the lattice vibrations in this case corresponds to the displacement of the opposite atoms in the same unit cell in opposite directions such that the centre of mass stays stationary. These modes are called optical branches.

II. Theoretical Background [1]

A. Vibrations in a mono-atomic chain:

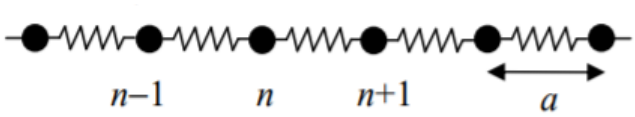

Fig. 1. one-dimentional linear mono-atomic lattice [2]

In the figure 1, consider a chain of atoms, with lattice constant a, we define the equilibrium position of atom n, as x_eq na. The spring constant between the adjacent atoms is denoted by κ. If we allow vibration (longitudinal vibrations) of this chain, we can define the deviation from the equilibrium position by: δx_n. [3]

such that:

$$\delta x_n = x_n - x_{eq}$$

To determine the force on spring n, we use Hooke's law such that:

$$F_n = \kappa(\delta x_{n+1} - \delta x_n) - \kappa(\delta x_n - \delta x_{n-1})$$

$$= \kappa(\delta x_{n+1} + \delta x_{n-1} - 2\delta x_n)$$

Then the equation of motion of an atom is given by:

$$m\frac{d^2(\delta x_n)}{dt^2} = F_n = \kappa(\delta x_{n+1} + \delta x_{n-1} - 2\delta x_n)$$

Now lets assume a wave solution:

$$\delta x_n = Ae^{i\omega t - iKx_{eq}} = Ae^{i\omega t - iKna}$$

where A is the amplitude, and K is the wavevector The we substitute and solve:

$$m\frac{d^2(Ae^{i\omega t - iKna})}{dt^2} = F_n = \kappa(\delta x_{n+1} + \delta x_{n-1} - 2\delta x_n)$$

$$\omega^2 = \frac{4\kappa}{m} sin^2(\frac{Ka}{2})$$

therefore,

$$\omega = 2\sqrt{\frac{\kappa}{m}} \| sin(\frac{Ka}{2}) |$$

Such that, this relationship is called Dispersion relation.

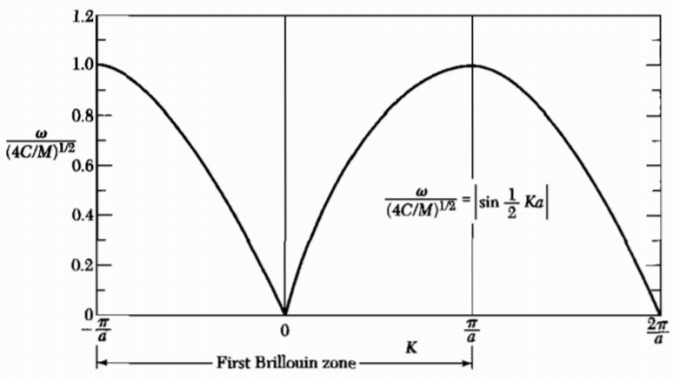

Fig. 2. Plot of ω versus K. in this plot, C is κ [1]

There are few points to make here regarding this plot. First, this range is called the first Brillouin zone of the linear lattice, The extreme values are $K = \pm\frac{\pi}{a}$. values of K outside of the first brillouin zone merely reproduce lattice motions described by values within the limits $\pm\frac{\pi}{a}$, such that, the wave becomes standing wave, this means that the wave moves neither to the left or to the right. in figure 2, it looks like sound waves for small K. For small K:

$$\omega = 2\sqrt{\frac{\kappa}{m}}\|sin(\frac{Ka}{2})| \approx 2\sqrt{\frac{\kappa}{m}}\|\frac{Ka}{2}|$$

$$a\sqrt{\frac{\kappa}{m}}|K|$$

such that, velocity is:

$$\nu_s = \frac{\omega}{K}$$

So we can say that the sound's velocity is :

$$\nu_s = a\sqrt{\frac{K}{m}}$$

B. Vibrations in a di-atomic chain:

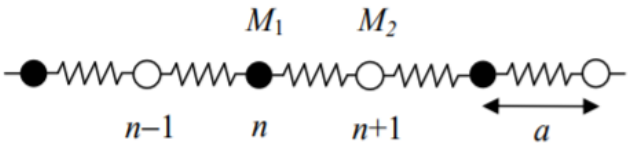

Fig. 3. one-dimentional linear di-atomic lattice [2]

Now we will consider a model where we have two atoms in each unit cell, in the diatomic case, we will have two different spring constants, κ_1 and κ_2. same as we did in the monoatomic case, we obtain equations of motion from Newton's law:

$$m\frac{d^2(\delta x_n)}{dt^2} = \kappa_2(\delta y_n - \delta x_n) + \kappa_1(\delta y_{n-1} - \delta x_n)$$

$$m\frac{d^2(\delta y_n)}{dt^2} = \kappa_1(\delta x_{n+1} - \delta y_n) + \kappa_2(\delta x_n - \delta y_n)$$

Now lets assume a wave solution:

$$\delta x_n = A_x e^{i\omega t - iKna}$$

$$\delta y_n = A_y e^{i\omega t - iKna}$$

Now we substitute and solve for the equation of motions, we found that:

$$\omega = \sqrt{\frac{\kappa_1 + \kappa_2}{m} \pm \frac{1}{m}\sqrt{\kappa_1^2 + \kappa_2^2 + 2\kappa_1\kappa_2 cos(Ka)}}$$

there are two different solutions corresponding to two different dispersion curves depending on the sign of this Equation. [3] Considering a diatomic chain instead of a monoatomic chain, we get additional branches in the dispersion relation.

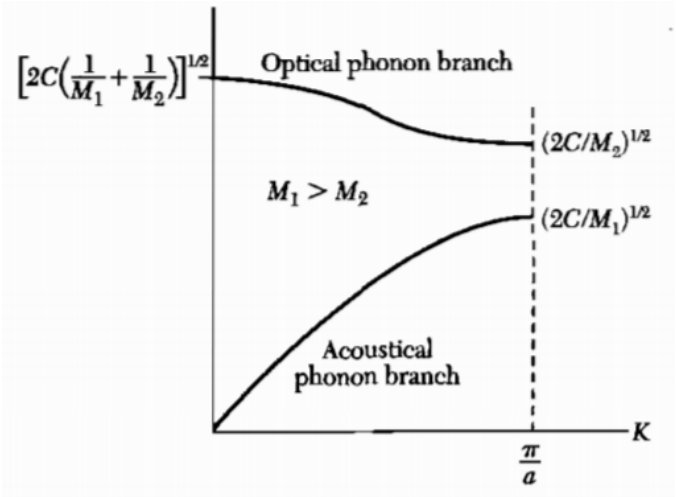

Fig. 4. Optical and acoustic branches of the dispersion relation for a diatomic linear lattice. [1]

For the acoustic branch, the two atoms in the are in phase and have the same amplitude, and it has this name (acoustic) because it gives long wavelength vibrations which correspond to elastic waves or sound, and to excite this frequency mode, we just need small amount of energy. However, for the optical branch, the wave has higher energy, so to excite this high frequency mode, we need certain amount of Energy, the two atoms move in out of phase.

The two branches are named optical and acoustic since optical waves consist of the ionic bonds within a crystal lattice storing vibrational energy. This can usually be achieved by using the the electromagnetic oscillation of a light beam in real crystals. For larger waves, where there is little to no vibration between the ionic bonds of substance, this is usually caused by sound waves flowing through the substance.

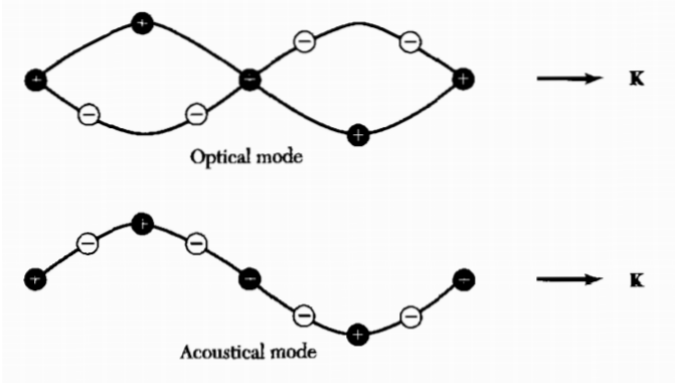

Fig. 5. Traverse optical and acoustical waves [1]

III. EXPERIMENTAL DESIGN AND PROCEDURE

A. Description of the apparatus

The used apparatus consists of :

A) Airtrack
B) Sliders.
C) Air blower.
D) function generator.
E) Eccentric cam motor.
F) Springs.

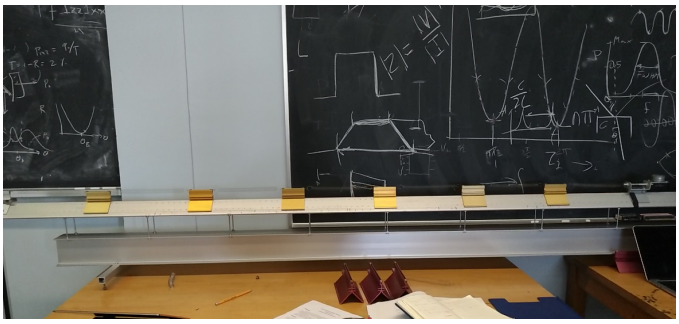

Fig. 6. Monoatomic experiment setup

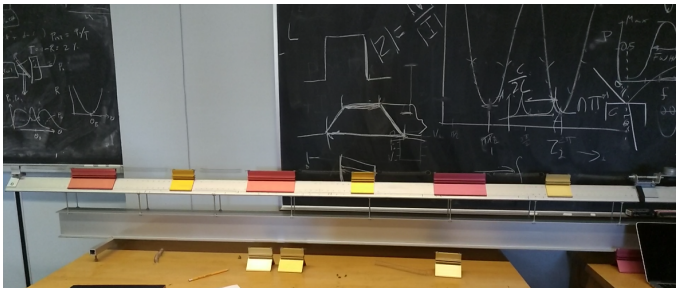

Fig. 7. Diatomic experiment setup

B. Description of the experimental procedure

First, we selected 4 springs to determine the spring constants and then we averaged them, we measured the extension of the springs by hanging a mass from one spring and measure the associated displacement. We repeated this procedure for 6 masses for each spring. Then we attached the springs back to the system, we put a spring between each cart and to the end of the air-track. Next, we wanted to determine the equilibrium position of the carts, so we turned on the air blower and left if for the couple of minutes to make sure the carts barely moving, then we turned the air blower off to measure the distance between the end of each cart to determine the equilibrium position.

Then we turned on the air blower and the function generator which is connected to the motor mounted on the air track and it's attached to the first spring in the chain. We slowly started changing the generated frequency of the motor and observed the system for the normal modes. We recorded these frequencies for further analysis. However, we needed to convert the function generator frequency to the motor frequency using this equation

$$f_{motor} = (0.02150) f_{scope} - 0.01236 Hz$$

Finally, for the Diatomic setup, we replaced each alternating yellow cart with the red one which is different in mass and then we repeated the same procedures for measuring the equilibrium position and the normal modes frequencies.

IV. ANALYSIS

A. Monatomic Lattice

Before starting the experiment, the average spring constant, mass and lattice distance were determined to be the following:

- Total Distance $L = 2.398m$
- Average Spring Constant $C = 3.31 \frac{N}{m}$
- Mass of Small Slider $M_1 = 0.136kg$
- Mass of Large Slider $M_2 = 0.286kg$
- Average Spaceing (Monatomic) $a = 0.351m$
- Average Spaceing (Diatomic) $A = 0.721m$

Note for the one dimensional case, the wave vector has the magnitude of $\frac{n+1}{L}$ where n is the number of nodes in a standing wave. The dispersion relation of the monatomic case is displayed by Figure 8.

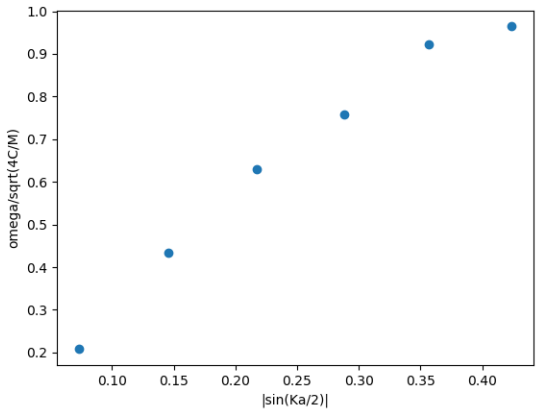

Fig. 8. Dispersion Relation for Monatomic Lattice

As described in the Theory section, the speed of sound through this lattice with the assumption of a small K:

$$\nu_s = a\sqrt{\frac{\kappa}{m}} \tag{1}$$

Where κ is the force constant of Hooke's law, and m is the mass of the atom. If the experimental values of these variables are plugged in, we obtain:

$$\nu_s = 1.73m/s \tag{2}$$

For atomic scales, the force constant to mass ratio is much larger, causing the speed of sound for most substances to be much faster than this experiment.

The Debye frequency is defined to be the following.

$$\omega_D = \nu_s \frac{\pi}{a} \tag{3}$$

The experimental result is given by:

$$\omega_D = 15.5\frac{1}{s} \tag{4}$$

B. Diatomic Lattice

When plotting the angular frequency ω against the wavenumber K for the case of the diatomic case, the following plot is obtained.

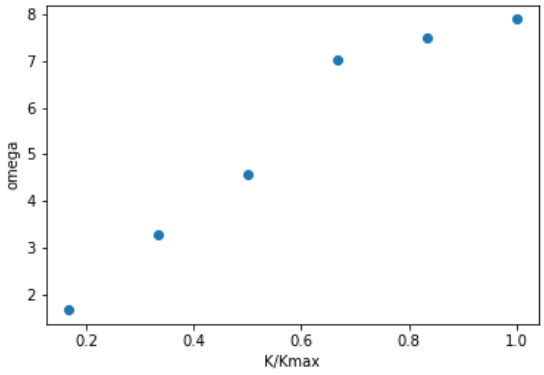

Fig. 9. Dispersion Relation for Diatomic Lattice

From this, we may see the clear distinction between the optical and acoustic branches of the the frequency. The gap in between the two branches is called the band gap. This gap can be approximately found experimentally by taking the difference in frequency between the leap from acoustic to optical branches. By taking the difference between the frequency of the fourth and third point, we find the experimental value of the band gap to be from $4.58\frac{1}{s}$ to $7.03\frac{1}{s}$. The width of the calculated band gap is $2.45\frac{1}{s}$.

The theoretical values of the edges of the band gap is given by the following:

$$\omega_{lower} = \sqrt{\frac{2C}{M_1}} \tag{5}$$

$$\omega_{higher} = \sqrt{\frac{2C}{M_2}} \tag{6}$$

By using the measured values of the force constant C (This is also represented as κ for the speed of sound measurement), and M, the theoretical values of the edges of the band gap are:

$$\omega_{lower} = 4.81\frac{1}{s} \tag{7}$$

$$\omega_{higher} = 6.98\frac{1}{s} \tag{8}$$

The width of the gap being:

$$\omega_{gap} = 2.17\frac{1}{s} \tag{9}$$

The Percentage error between the calculated gap and the theoretical gap is as follows:

$$\%error = \frac{2.45 - 2.17}{2.17} \times 100\% \tag{10}$$

$$\%error = 12.9\% \tag{11}$$

V. CONCLUSION

The monatomic and diatomic one dimensional lattice lattice was observed and experimented on in this lab. The dispersion relations were found, and for the monatomic case, the speed of sound through the medium was found to be $1.73m/s$, and the Debye frequency was found to be $15.5\frac{1}{s}$. For the diatomic case, the band gap between the acoustic branch and optical branch was found to be $2.45\frac{1}{s}$.

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[2] Tsymbal, E. (2005). Lattice Vibrations. Lecture, NEBRASKA CENTER FOR MATERIALS AND NANOSCIENCE.

[3] Frolov, S. (2015). One-dimensional models of vibrations in solids. Presentation, University of Pittsburgh.