One Dimensional Lattice Dynamics

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Section 1
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I. ABSTRACT

A linear air track is used as a model for a 1-D lattice, which sliders of different masses acting as atoms. Monoatomic and diatomic cases are investigated, and dispersion relations are created. The speed of sound is determined to be $1.636 \pm 0.018 \frac{m}{s}$ in the monoatomic lattice, and $1.364 \pm 0.016 \frac{m}{s}$ through the diatomic one. The Debye cut-off is found to occur at at $\omega_D = 9.40Hz$, and $k_m = 9.03m^{-1}$ in the monoatomic lattice. The diatomic lattice's band gap is determined to be $2.067 \pm 0.056Hz$ in theory, while the experimental results produce a value of $0.4875 \pm 0.0029Hz$. The limitations of the theoretical model are discussed and used to justify the discrepancy.

II. INTRODUCTION

Studying Lattice dynamics, even if only in on the One Dimensional has many real world applications and some of the fundamental lessons learned in this lab can be carried forward to much more complicated situations. Through the use of the sliders and springs, we can study the propagation of phonons, which are quanta of sound travelling though a medium we can create a model and derive the dispersion relation related to atoms in a solid for both monoatomic lattices, and diatomic lattices. We will also be looking at the speed of sound though these mediums and observe the band gap between the acoustic and optical branches in the diatomic lattice dispersion relation. By studying phonons we can broaden our understanding and apply the concepts we learn to important fields of study such as thermal and electrical conductivity, as well as being an important part in Solid State physics.

III. THEORETICAL BACKGROUND

A. Vibrations in a Monoatomic Lattice

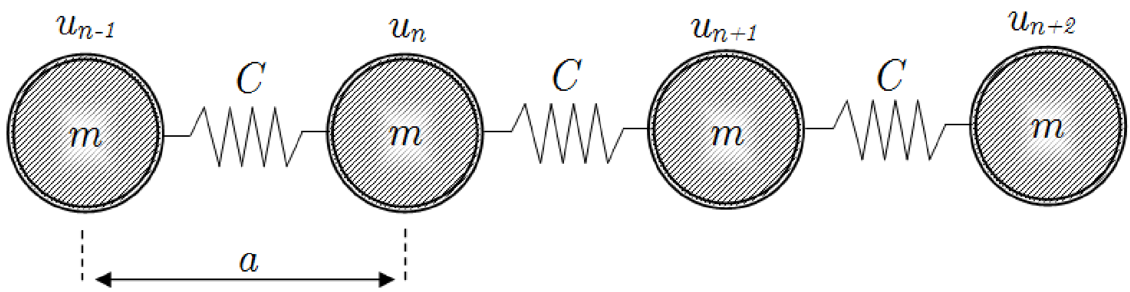

FIG. 1: Monoatomic lattice model of atoms u, with mass m, spring constant C, and spacing a.

We can begin to derive the equations of motion for the monoatomic 1D lattice by assuming each atom in the lattice moves due the nearest-neighbour interaction, for example, in an array of couple atoms, atom n would be acted upon by the coupled atoms $n-1$ and $n+1$. Using Hooke's law, $F = Cu$, where C is the spring constant and u is the displacement from equilibrium, we can describe the force acting on atom n by:

$$F_n = C(u_{n+1} - u_n) + C(u_{n-1} - u_n) \tag{1}$$

We can then derive from (1), using the fact that $F = ma = m\ddot{u}$,

$$m\ddot{u_n} = m\frac{d^2u_n}{dt^2} = -C(2u_n - u_{n+1} - u_{n-1}) \tag{2}$$

We can solve this differential equation by looking for solutions of the form

$$u_n = Ae^{i(kna - \omega t)} \tag{3}$$

where k is the wave number, and a is the spacing between planes in the monoatomic lattice, then differentiating (3) twice w.r.t time we get,

$$\ddot{u_n} = -\omega^2 \cdot Ae^{i(kna-\omega t)} = -\omega^2 u_n \tag{4}$$

By substituting (3) and (4) into (2), we get as follows:

$$m\ddot{u_n} = -C(2u_n - u_{n+1} - u_{n-1})$$
$$-m\omega^2 \cdot \cancel{Ae^{i(kna-\omega t)}} = -C(2\cancel{Ae^{i(kna-\omega t)}} - \cancel{Ae^{i(kna-\omega t)}}e^{ika} - \cancel{Ae^{i(kna-\omega t)}}e^{-ika})$$
$$-m\omega^2 = -C(2 - e^{ika} - e^{-ika})$$
$$-m\omega^2 = -C(2 - (2\cos ka))$$

$$\omega^2 = 2\frac{C}{m}(1 - \cos ka) \tag{5}$$

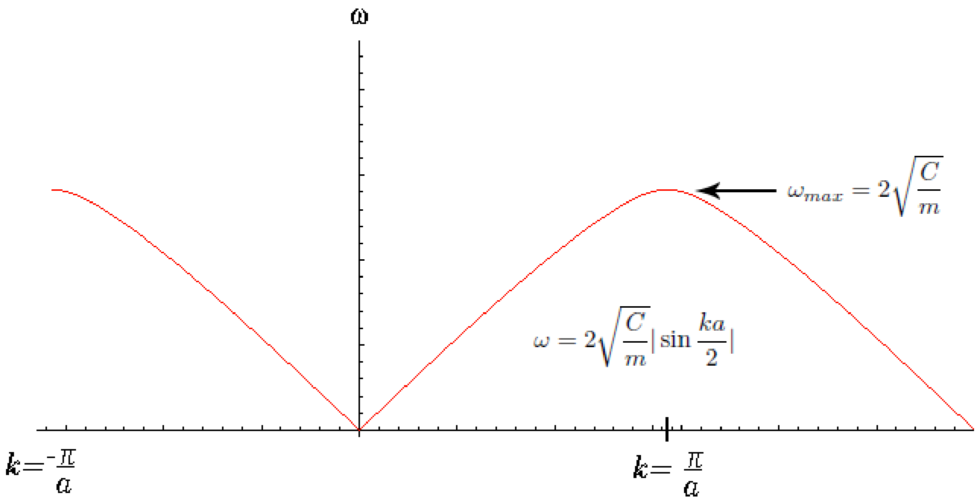

FIG. 2: The dispersion relation for a Monoatomic lattice, showing the Acoustic branch and ω_{max}.

and using the double angle formula for $1 - \cos ka = 2\sin^2\frac{ka}{2}$, from (5) we derive the Dispersion law as,

$$\omega = \pm 2\sqrt{\frac{C}{m}}|\sin\frac{ka}{2}| \tag{6}$$

Taking the continuum limit as $k \to 0$, using the small angle approximation:

$$\sin\frac{ka}{2} \approx \frac{ka}{2} \tag{7}$$

substituting (7) into (6), we can get an expression for the speed of sound in the lattice v

$$\frac{\omega}{k} = v = \sqrt{\frac{C}{m}}a \tag{8}$$

1. *Behaviour of Dispersion Curve at* $k = \pm\frac{\pi}{a}$

When the wave number is a multiple of $\frac{\pi}{a}$, this is where there will be the maximum vibration frequency in the monoatomic lattice.

$$\omega_{max} = 2\sqrt{\frac{C}{m}} \tag{9}$$

this is the edge of the Brillouin zones for this lattice, the first Brillouin zone spans $-\frac{\pi}{a} \leq k \leq \frac{\pi}{a}$, as seen in Fig. 2 between maxima.

B. Vibrations in a Diatomic Lattice

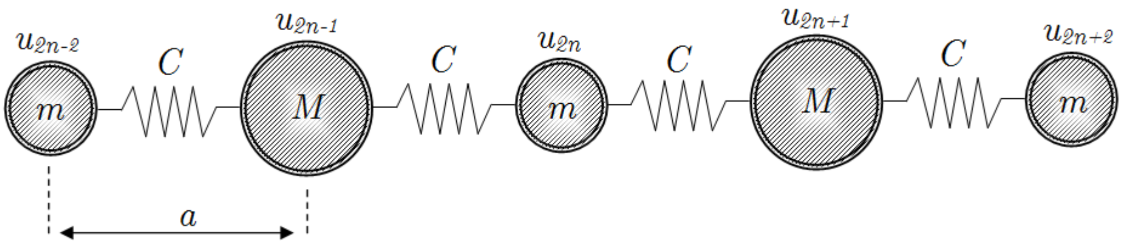

FIG. 3: Diatomic lattice model of atoms u, with masses m and M where $m < M$, spring constant C, and spacing a.

Similar to a monoatomic lattice, we can derive the equations for a diatomic lattice which, in one dimension, has two different atoms of different masses in a unit cell, repeating. We now have two coupled differential equations that need to be solved,

$$m\ddot{u}_{2n} = m\frac{d^2 u_{2n}}{dt^2} = -C(2u_{2n} - u_{2n+1} - u_{2n-1}) \tag{10}$$

$$M\ddot{u}_{2n+1} = M\frac{d^2 u_{2n+1}}{dt^2} = -C(2u_{2n+1} - u_{2n+2} - u_{2n}) \tag{11}$$

and similarly subbing in (3) into the two equations, we get the set of equations,

$$\begin{bmatrix} u_{2n} \\ u_{2n+1} \end{bmatrix} = \begin{bmatrix} Ae^{ik2na} \\ Be^{ik(2n+1)a}e^{ika} \end{bmatrix} e^{-i\omega t} \tag{12}$$

And substituting into (10) and (11) and cancelling out the factor of $e^{-i\omega t}e^{ik2na}$, we get:

$$\begin{bmatrix} -mA\omega^2 \\ -MB\omega^2 \end{bmatrix} = \begin{bmatrix} -C(2A - B(e^{-ika} + e^{ika})) \\ -C(2B - A(e^{ika} + e^{-ika})) \end{bmatrix} = \begin{bmatrix} -C(2A - 2B\cos ka) \\ -C(2B - 2A\cos ka) \end{bmatrix} \tag{13}$$

then rearranging (10) grouping like terms A and B we get the system of equations:

$$\begin{bmatrix} A(-m\omega^2 + 2C) \\ -2AC\cos ka \end{bmatrix} = \begin{bmatrix} 2BC\cos ka \\ B(-2C + M\omega^2) \end{bmatrix} \tag{14}$$

$$\begin{bmatrix} (2C - m\omega^2) & -2C\cos ka \\ -2C\cos ka & (2C - M\omega^2) \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} = 0 \tag{15}$$

and taking the determinant of the matrix in (15) we can solve for ω we get:

$$(2C - m\omega^2)(2C - M\omega^2) - 4C^2 \cos^2 ka = 0$$
$$(2\tfrac{C}{m} - \omega^2)(2\tfrac{C}{M} - \omega^2) - 4\tfrac{C^2}{mM} \cos^2 ka = 0$$
$$4\tfrac{C^2}{mM} - 2\tfrac{C}{m}\omega^2 - 2\tfrac{C}{M}\omega^2 + \omega^4 - 4\tfrac{C^2}{mM} \cos^2 ka = 0$$

$$(\omega^2)^2 - (\omega^2)[2(\frac{C}{m} + \frac{C}{M})] + 4\frac{C^2}{mM}(1 - \cos^2 ka) = 0 \tag{16}$$

Solving for the value of ω^2 in (16) using the quadratic equation, we get a value of:

$$\omega^2 = (2(\tfrac{C}{m} + \tfrac{C}{M}) \pm \sqrt{(2(\tfrac{C}{m} + \tfrac{C}{M}))^2 - 4 \cdot 4\tfrac{C^2}{mM}(1 - \cos^2 ka)}) \cdot \tfrac{1}{2}$$
$$\omega^2 = (\cancel{2}C(\tfrac{1}{m} + \tfrac{1}{M}) \pm \cancel{2}C\sqrt{(\tfrac{1}{m} + \tfrac{1}{M})^2 - 4\tfrac{1}{mM}(1 - \cos^2 ka)}) \cdot \cancel{\tfrac{1}{2}}$$

$$\omega^2 = C(\frac{1}{m} + \frac{1}{M}) \pm C\sqrt{(\frac{1}{m} + \frac{1}{M})^2 - 4\frac{\sin^2 ka}{mM}} \tag{17}$$

Equation (17) is the dispersion relation, the negative branch is known as the Acoustic branch and is when all the atoms in the lattice vibrate in phase with each other, as seen in Fig. 4. Alternatively, we can take the positive branch of (17) which is known as the Optical branch and is described as when all atoms in the lattice vibrate out of phase by π, and the diatomic pair vibrate against eachother as seen in Fig. 5.

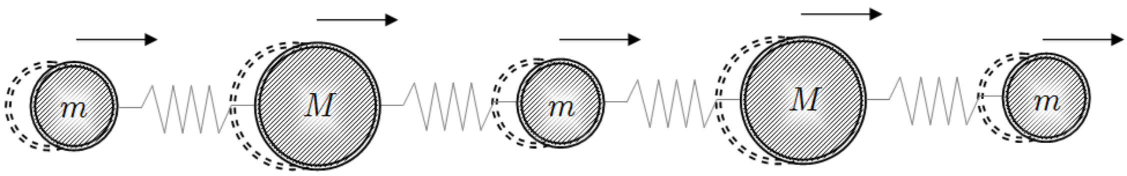

FIG. 4: The Acoustic branch motion of atoms in the diatomic lattice, when all the atoms vibrate in phase with each other.

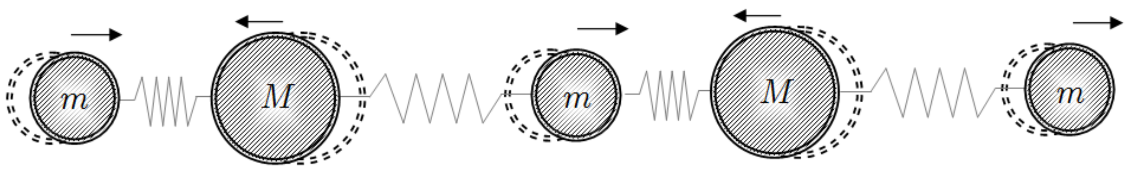

FIG. 5: The Optical branch motion of atoms in the diatomic lattice, when all the atoms vibrate out of phase with each other by a phase difference of π.

1. *Behaviour of Dispersion Curve at $k \ll 1$*

We can explore the behaviour of this dispersion relation in solids by taking the continuum limit as $k \to 0$, we can derive expressions for the acoustic and optic branch dispersion relations. We use the small angle approximation for sin, and we take the Taylor expansion of the root term in (17),

$$C\sqrt{(\tfrac{1}{m} + \tfrac{1}{M})^2 - 4\tfrac{\sin^2 ka}{mM}}$$
$$\Rightarrow C\sqrt{(\tfrac{1}{m} + \tfrac{1}{M})^2}[1 - \tfrac{4}{2}\tfrac{\frac{(ka)^2}{mM}}{(\frac{1}{m} + \frac{1}{M})^2}]$$
$$\Rightarrow C(\tfrac{1}{m} + \tfrac{1}{M})[1 - \tfrac{4}{2}\tfrac{\frac{(ka)^2}{mM}}{(\frac{m+M}{mM})^2}]$$
$$\Rightarrow C(\tfrac{m+M}{mM})[1 - 2\tfrac{(ka)^2 mM}{(m+M)^2}]$$

Taking the positive branch of (17), for $k \ll 1$ we get,

$$\omega^2 \approx C(\tfrac{1}{m}+\tfrac{1}{M}) + C(\tfrac{1}{m}+\tfrac{1}{M})[1-2\tfrac{(ka)^2 mM}{(m+M)^2}]$$
$$\omega^2 \approx 2C(\tfrac{1}{m}+\tfrac{1}{M}) + C\tfrac{\cancel{m+M}}{\cancel{mM}}[2\tfrac{(ka)^2\cancel{mM}}{(m+M)^{\cancel{2}}}]$$

$$\omega^2 \cong 2C(\frac{1}{m}+\frac{1}{M}) \tag{18}$$

Equation (18) describes the root of the Optical branch of the dispersion relation, which can be seen in Fig. 6 as the maximum value of the Optical branch.

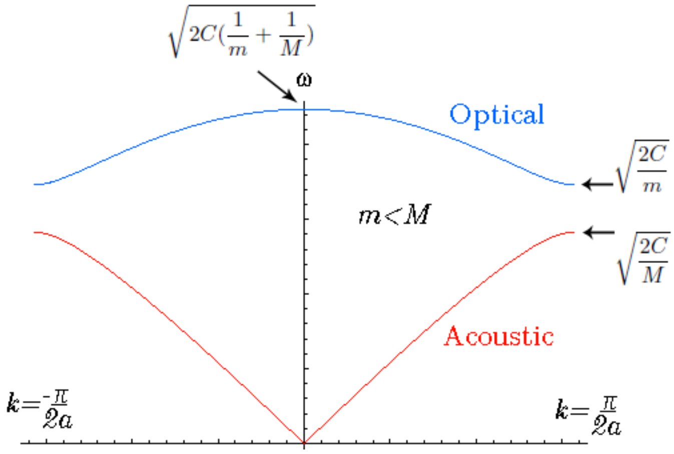

FIG. 6: The dispersion relation for a Diatomic lattice, showing the Acoustic and Optical branches with some key values.

$$\omega^2 \approx C(\tfrac{1}{m}+\tfrac{1}{M}) - C(\tfrac{1}{m}+\tfrac{1}{M})[1-2\tfrac{(ka)^2 mM}{(m+M)^2}]$$
$$\omega^2 \approx C(\tfrac{\cancel{m+M}}{\cancel{mM}})[2\tfrac{(ka)^2\cancel{mM}}{(m+M)^{\cancel{2}}}]$$

$$\omega^2 \cong 2C\frac{(ka)^2}{m+M} \tag{19}$$

using (19), we derive the speed of sound though a Diatomic lattice as similarly to how we did for the monoatomic lattice.

$$\frac{\omega}{k} = v = a\sqrt{\frac{2C}{m+M}} \tag{20}$$

2. *Behaviour of Dispersion Curve at $k = \pm\frac{\pi}{2a}$*

We can explore what happens when the wave number k in (17) is a value of $\pm\frac{\pi}{2a}$, this area is known as the edge of the first Brillouin Zone, which spans $-\frac{\pi}{2a} \leq k \leq \frac{\pi}{2a}$. At the edges the sin term in (17) has a value of 1, and the roots will allow us to find the band gap energy of the system.

$$\omega^2 = C(\tfrac{1}{m}+\tfrac{1}{M}) \pm C\sqrt{(\tfrac{1}{m}+\tfrac{1}{M})^2 - 4\tfrac{\sin^2 ka}{mM}}$$
$$\omega^2 = C(\tfrac{m+M}{mM}) \pm C\sqrt{(\tfrac{m+M}{mM})^2 - \tfrac{4}{mM}}$$
$$\omega^2 = C(\tfrac{m+M}{mM}) \pm C\sqrt{(\tfrac{m^2+M^2+2mM}{(mM)^2}) - \tfrac{4mM}{(mM)^2}}$$
$$\omega^2 = C(\tfrac{m+M}{mM}) \pm C\sqrt{(\tfrac{m^2+M^2-2mM}{(mM)^2})}$$
$$\omega^2 = C(\tfrac{m+M}{mM}) \pm C\sqrt{(\tfrac{M-m}{mM})^2}$$

$$\omega^2 = C(\frac{m+M}{mM}) \pm C(\frac{M-m}{mM}) \tag{21}$$

Taking the positive branch of (21), we get the lowest frequency in the optical branch

$$\omega = \sqrt{\frac{2C}{M}} \tag{22}$$

and similarly taking the negative branch of (21), we get the highest frequency of the acoustic branch,

$$\omega = \sqrt{\frac{2C}{m}} \tag{23}$$

The difference between (22) and (23) will give us the band gap for $m < M$ equal to,

$$\omega_{gap} = \sqrt{\frac{2C}{m}} - \sqrt{\frac{2C}{M}} \tag{24}$$

IV. EXPERIMENTAL DESIGN AND PROCEDURE

Apparatus:

- Air-track with vacuum
- 6 Small Air-track sliders
- 3 Large Air-track sliders
- 7 identical springs
- Eccentric cam motor and power supply
- Oscilloscope
- Spring weights
- Electronic weight scale

First the spring constant was measured by applying weights sequentially and measuring the displacement of the spring using a ruler and recorded the values. We then measured the weight three small and three large air-track sliders individually using the electronic weight scale and recorded the values.

We first began with the monoatomic lattice set-up using the 6 small sliders each fastened together with the springs, with the end sliders attached to the mounting bracket and the eccentric cam motor respectively. Then, with the vacuum on, we waited for the system to stabilize and come to equilibrium, we then turned off the vacuum so the sliders wouldn't move and measured the inter-atomic distance between sliders, by measuring the relative displacement on the air-track of two of the same ends of two adjacent sliders (both right edges for example). Then continuing with the experiment, the vacuum was turned on again and using the control knob on the eccentric cam motor power supply (with it first set to the lowest setting), the frequency of the motor was adjusted in small amounts, being sure to wait to give the system enough time to react, until we found a frequency at which the amplitude of the displacement of the sliders was comparatively large compared to previous frequencies (a normal mode harmonic). We then recorded the frequency from the oscilloscope readout. We did this until we found 4-6 harmonic frequencies of the system.

For the second part of the experiment, the diatomic lattice set-up, we replaced 3 of the small sliders on the track with large sliders, having them arranges in alternating sizes so the sliders are evenly distributed in the lattice, again connected with the springs. The vacuum was turned on and the system allowed to reach equilibrium before turning it off and measuring the relative displacement on the air-track of both edges of a small and both edges adjacent large slider, such that the center of masses and separation of center of masses could be calculated. Similar to the monoatomic lattice procedure, with the vacuum on again and with the eccentric motor power supply control knob in its lowest setting, the frequency of the motor was slowly increased until harmonic modes were achieved. The frequencies of motor at the excited modes was recorded from the oscilloscope readout. Once 3-4 acoustic modes and 2-3 optic modes were found and recorded, all the equipment was shut off and the station tidied.

V. ANALYSIS

Mass (kg)	Displacement ($\pm 0.05cm$)
50	35.3
70	41.3
90	47.5
100	50.4
110	55.6

TABLE I: Spring constant displacement versus mass applied

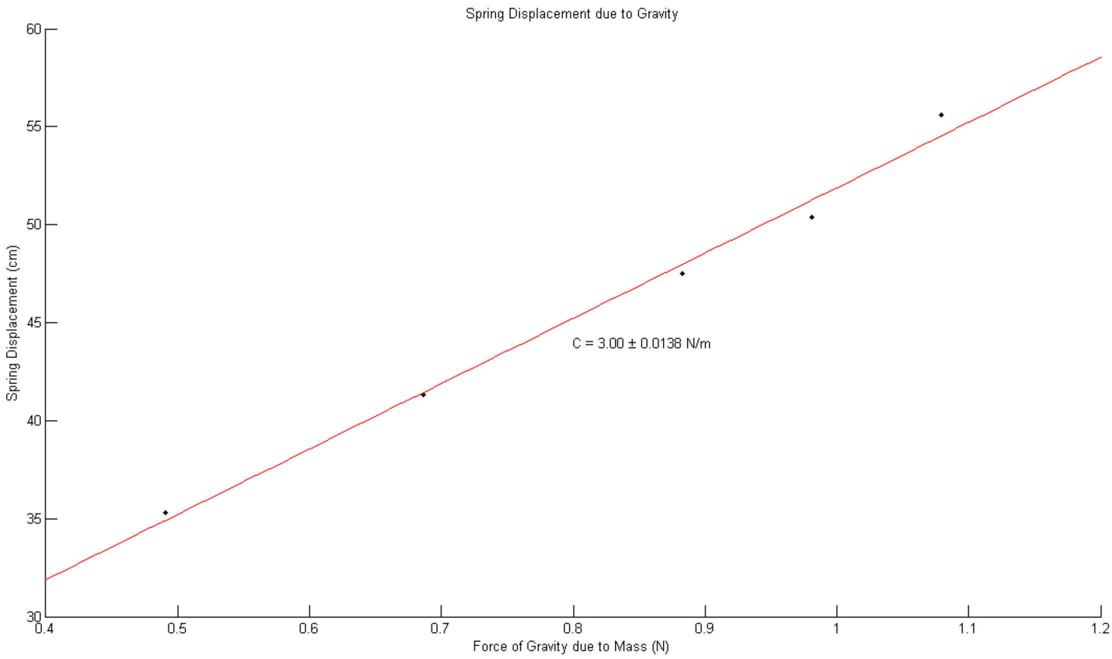

FIG. 7: Plot of spring displacement versus force on the spring from the masses applied. Resulting is the determination of the Spring constant as $C = 3.00 \pm 0.0138 \frac{N}{m}$.

Small Slider Masses (with error) (g)			Average
Trial 1	**Trial 2**	**Trial 3**	
135.4	136.5	135.3	135.7
0.05	0.05	0.05	0.0866

TABLE II: Slider masses for the small slider carts and average

Small Slider Masses (with error) (g)			Average
Trial 1	**Trial 2**	**Trial 3**	
286.2	284.9	286.5	285.9
0.05	0.05	0.05	0.0866

TABLE III: Slider masses for the larger slider carts and average

Mode	Monatomic Frequencies ($48 \times Hz$)	Diatomic Frequencies ($48 \times Hz$)
1	16.61	—
2	31.8	26.04 (acoustic)
3	46.3	34.7 (acoustic)
4	58.8	58.1 (optical)

TABLE IV: Excited modes for the Monoatomic lattice and diatomic lattice configurations respectively

The error for all frequency measurements is 0.1 Hz, due to some uncertainty as to the precise locations of the modes. It was also difficult to obtain values for the diatomic lattice, for both the acoustic and optical branches. The acoustic branch appeared to have a node close to 14/48 Hz, but the equipment was not capable of obtaining data at lower frequencies. There also appeared to be several modes above or below the one at 58.1/48 Hz, but it was difficult to ascertain whether they were true modes, or just beats. It was decided to only use data points about which there was a high degree of certainty.

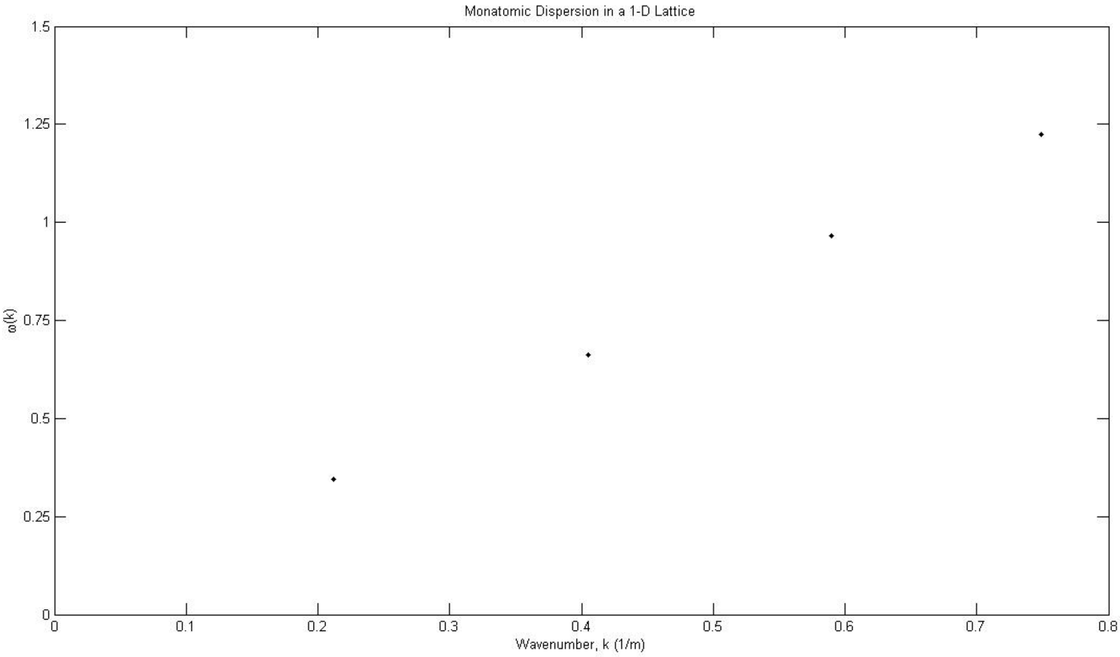

FIG. 8: Plotted excited modes for the Monoatomic lattice configuration on Frequency versus wavenumber

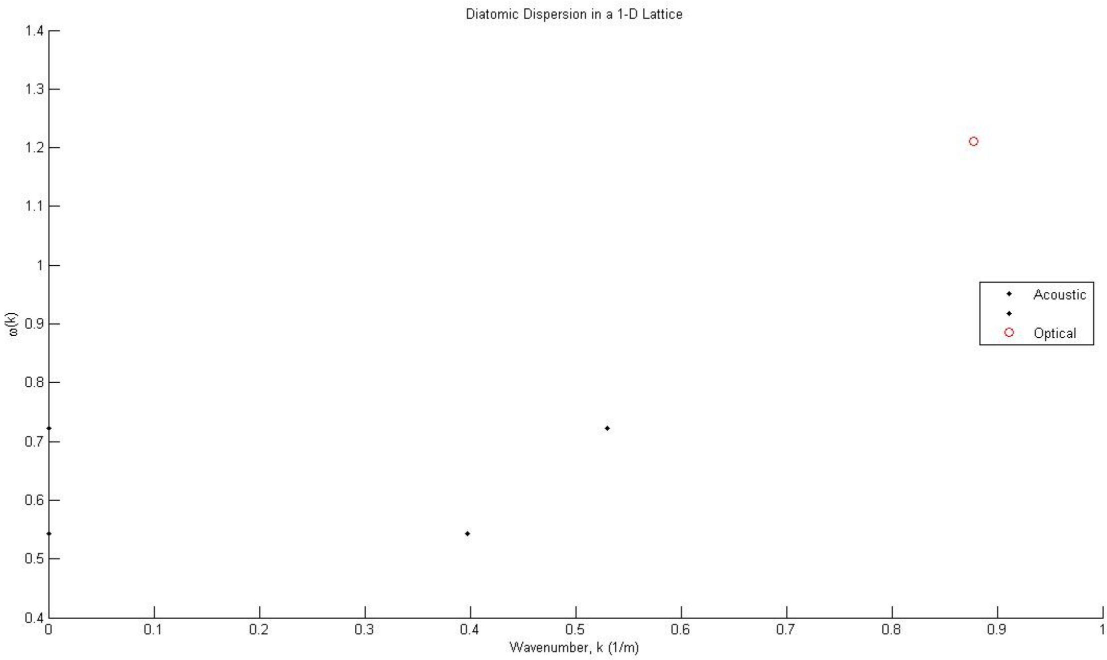

FIG. 9: Plotted excited modes for the Diatomic lattice configuration on Frequency versus wavenumber

The absence of error bars in the dispersion plots is due to the error being negligibly small (small enough that their inclusion did not produce any visible effect on the plots).

The Debye Frequency is understood to be the maximum frequency allowable in the 1-D monoatomic lattice. It occurs at $\omega_D = \omega_{max}$, and $k = \frac{\pi}{a}$, as depicted in equation (9). This maximum is a property related to the speed at which sound waves can propagate through a lattice. Its calculation is as follows:

$$\omega_{max} = 2\sqrt{\frac{C}{m}} = 2\sqrt{\frac{3.00\frac{N}{m}}{0.1357kg}} = 9.40Hz$$
$$k_m = \frac{\pi}{a_{mon}} = \frac{\pi}{0.348} = 9.03m^{-1}$$

With the spring constant, slider masses, and separations, it becomes a simple matter to calculate the speed of sound in each lattice, as well as the associated errors. Sample calculations are provided below.

$$\Delta a_{mon} = \sqrt{(0.05cm)^2 + (0.05cm)^2} = \pm 0.071cm$$
$$\Delta a_{di} = \sqrt{(0.05cm)^2 + (0.05cm)^2 + (0.05cm)^2} = \pm 0.10cm$$

$$v_{mon} = \sqrt{\frac{C}{m}} a_{mon} = \sqrt{\frac{3.00\frac{N}{m}}{0.1357kg}}(0.348m) = 1.636\frac{m}{s}$$

$$\Delta\frac{C}{m} = \frac{1}{2}\frac{C}{m}\sqrt{(\frac{\Delta C}{C})^2 + (\frac{\Delta m}{m})^2} = \frac{1}{2}\frac{3.00\frac{N}{m}}{0.1357kg}\sqrt{(\frac{0.0138\frac{N}{m}}{3.00\frac{N}{m}})^2 + (\frac{2.9\times10^{-5}kg}{0.1357kg})^2} = \pm 0.051(\frac{N}{m\cdot kg})^{\frac{1}{2}}$$

$$\Delta v_{mon} = v_{mon}\sqrt{(\frac{\Delta C/m}{C/m})^2 + (\frac{\Delta a_{mon}}{a_{mon}})^2} = (1.636\frac{m}{s})\sqrt{(\frac{0.051}{4.702})^2 + (\frac{0.00071}{0.348})^2} = \pm 0.018\frac{m}{s}$$

$$v_{di} = a_{di}\sqrt{\frac{2C}{M+m}} = (0.3615m)\sqrt{\frac{2(3.00\frac{N}{m})}{0.2859kg+0.1357kg}} = 1.364\frac{m}{s}$$

$$\Delta v_{di} = 0.016\frac{m}{s}$$

The calculation of the error in the diatomic sound speed was omitted since it was similar to that of the monoatomic case. The energy gap is similarly straightforward to calculate using the previously derived equation (24).

$$\omega_{gap} = \sqrt{\frac{2C}{m}} - \sqrt{\frac{2C}{M}} = \sqrt{\frac{2(3.00\frac{N}{m})}{0.1357kg}} - \sqrt{\frac{2(3.00\frac{N}{m})}{0.2859kg}} = 2.067Hz$$

$$\Delta\omega_{gap} = \sqrt{(\Delta\frac{C}{m})^2 + (\Delta\frac{C}{M})^2} = \sqrt{(0.024)^2 + (0.051)^2} = \pm 0.056Hz$$

The experimental value of the band gap is calculated from the highest frequency observed on the acoustic branch, and from the lowest frequency observed on the topical branch.

$$\omega_{gap} = \frac{58.1Hz - 34.7Hz}{48} = 0.4875Hz$$

$$\Delta\omega_{gap} = \sqrt{(\frac{0.1}{48})^2 + (\frac{0.1}{48})^2} = \pm 0.0029Hz$$

VI. CONCLUSION

The springs used in the experiment were found to have a Hook's law spring constant of $3.00N/m \pm 0.0138\frac{N}{m}$. This was used in all subsequent calculations. Dispersion relation plots were then created for the monoatomic and diatomic lattices (see the Analysis section for the plots).

As mentioned in the derivation of the diatomic dispersion relation, the terms "acoustic" and "optical" refer to the phase difference between the oscillations of the two atom types (the two varieties of slider). The acoustic branch is so called as the in-phase oscillations are akin to sound travelling through a medium. Whether or not the displacement is in the direction of the propagation or perpendicular to it is irrelevant to the classification (the perpendicular case is similar to waves travelling through water). The optical branch corresponds to oscillations out of phase by π. Its suggestive name relates to lattice vibrations that result from interactions between radiation and atoms (i.e. excitations from photons being absorbed). For more information about these vibrations, refer to paper [2].

As k is made to go to zero, and becomes much smaller than one, the speed in the lattices is found according to equations (8) and (20). Thus, it is determined that sound propagates at $1.636 \pm 0.018\frac{m}{s}$ through the monoatomic lattice, and at $1.364 \pm 0.016\frac{m}{s}$ through the diatomic one. The theoretical value of the diatomic lattice's band gap was determined to be $2.067 \pm 0.056Hz$. In the dispersion plot, and hence also in the experimental data, the difference between the acoustic and optical branches is $0.4875 \pm 0.0029Hz$. As these two values lie outside of one another's error ranges, it is likely that the discrepancy arises from another factor. One possibility is that the springs used in the experiment did not all have the same spring constant, or that the springs did not oscillate perfectly, as when they compressed they noticeably relaxed and hung from the sliders (instead of remaining horizontal to the track and compressing). While likely insignificant, it is also worth noting that the masses of the springs themselves were neglected.

VII. REFERENCES

1. Jeff Gardiner. One Dimensional Lattice Dynamics. Waterloo, Ontario: University of Waterloo; c2014. 1p.
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