STUDY OF LATTICE DYNAMICS USING EQUIVALENT ELECTRONIC CIRCUITS

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ABSTRACT

This report is mainly focused on the phenomenon of lattice vibrations observed in the case of monoatomic and diatomic 1-D lattices. Specifically, we studied the associated lattice vibrations in an imaginary 1-D lattice of monoatomic and diatomic lattices by creating electrical circuits analogous to the same using inductors and capacitors. This could be the basis for thinking of more complex lattices in the real world where the lattices are of higher dimensions, mostly 3-D. Using the data observed, we verified the dispersion relation, plotted the required graphs, found some relation between the frequency of the vibration and the corresponding change in phase per unit cell, and finally studied the acoustical and optical branches, band gap energy, etc.

1 OBJECTIVES

- Study the dispersion relation in the case of monoatomic 1-D lattice by building an analogy of the same using inductors and capacitors (same).
- Study the dispersion relation and band gap energy in the case of diatomic 1-D lattice by building an analogy of the same using inductors and capacitors (two different).

2 THEORY

2.1 Introduction

Except for amorphous solids and glasses, almost all solids have periodic arrays of atoms that form a crystal lattice. This periodic crystal lattice in solid materials serves as a medium for characteristic vibrations.
There are quantized vibrational modes called **phonons** that exist between the lattice spacing. The study of phonons is an important part of solid-state physics because they play an important role in determining the physical properties of solids, as well as the thermal and electrical conductivity of the materials. The phonon's long wavelength property confers properties on sounds in solids. Phonons are a quantum mechanical representation of a specific type of vibrational motion, known as a normal mode (elementary blocks of lattice vibration).
An example of a normal mode is a standing wave, which is a continuous form of normal mode, and all space elements, (x, y, and z coordinates) are oscillating at the same frequencies, and phases but with different amplitudes.

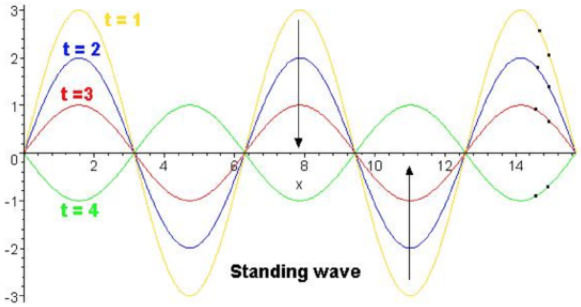


Figure 1: Example of a normal mode: Standing wave

2.2 Lattice vibration

The oscillations of atoms in a solid about the equilibrium position are referred to as **lattice vibration**. Because the atoms are bound to neighbor atoms, the equilibrium positions form a regular lattice in a crystal. These neighboring atoms' vibrations are not independent of one another.
Lattice waves are formed by a regular lattice with har-

monic forces between atoms and normal modes of vibration. These lattice waves have frequencies ranging from low to high in the order of 1 kHz or higher. However, at extremely high frequencies, the wavelengths are on the order of interatomic spacing. Because these wavelengths are so short, the motion of neighboring atoms is uncorrelated, with each atom moving about its average position in three dimensions.

2.3 Working principle of the Experiment

When the lattice is at equilibrium, each atom is positioned exactly at its lattice site. Now suppose that an atom is displaced from its equilibrium site by a small amount. Due to the force acting on this atom, it will tend to return to its equilibrium position. This results in lattice vibrations. Due to interactions between atoms, various atoms move simultaneously, so we have to consider the motion of the entire lattice.

2.4 Monoatomic 1-D lattice

The whole system of mass and spring for a 1-D monoatomic model shown in Figure 2 can be transformed into an LC circuit (electrical analogue) shown in Figure 3 after comparing the solutions of equations we get by solving the corresponding equations. Consider the array

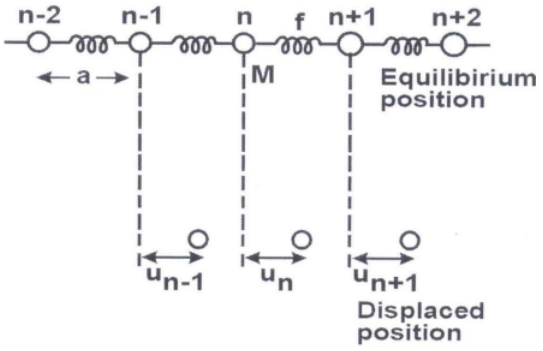


Figure 2: Mass-spring model of monoatomic 1-D lattice
a: Lattice constant
M: Mass of the atom
f: force constant

to be infinitely long. Assuming only the nearest neighbor interaction, the equation of the motion of the nth atom is given by:

$$m\frac{d^2x_n}{dt^2} = f[u_{n+1} + u_{n-1} - 2u_n] \tag{1}$$

A similar equation should be written for each atom in the lattice, resulting in N-coupled differential equations, which should be solved simultaneously (N: is the total number of atoms in the lattice). The boundary conditions applied to the end atom in the lattice should be taken into account.
Now let us attempt a trial solution of the form

$$u_n = Ae^{i(qx_n - \omega t)} \tag{2}$$

x_n: equilibrium position of the n-th atom so that $x_n = na$.
This equation represents a traveling wave, in which all the atoms oscillate with the same frequency ω and the same amplitude A and have wavevector q. Note that a solution of form (2) is only possible because of the translational symmetry of the lattice.
Now substituting Eq.(2) into Eq.(1) and simplifying, we obtain the dispersion relation of the frequency as:

$$\omega = \sqrt{\frac{4f}{M}}sin|\frac{qa}{2}| \tag{3}$$

which is the relationship between the frequency of vibrations and the wavevector q.
Eqn. (3) can also be written as:

$$\omega^2 = \frac{2f}{M}(1 - cos\theta) \tag{4}$$

where θ(=qa): phase change per unit cell.
The equation shows that there exists a maximum frequency ν_{max} beyond which no transmission occurs and thus can be considered as a low pass filter.

$$\nu_{max} = \frac{\omega_{max}}{2\pi} = \frac{1}{\pi}\sqrt{\frac{f}{m}} \tag{5}$$

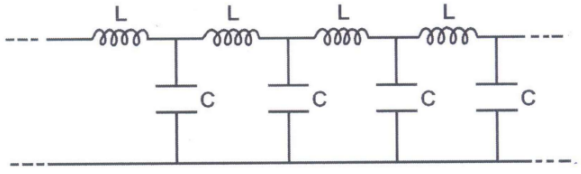


Figure 3: Electrical analogue of Figure 2

The dispersion relation of the circuit is given by:

$$\omega^2 = \frac{2}{LC}(1 - cos\theta) \tag{6}$$

Thus, we have a precise analogy with 1-D monoatomic lattice with $(f/m) \rightarrow (1/LC)$.
By measuring the phase difference between input and output voltages as the function of frequency, the dispersion relation can be verified.

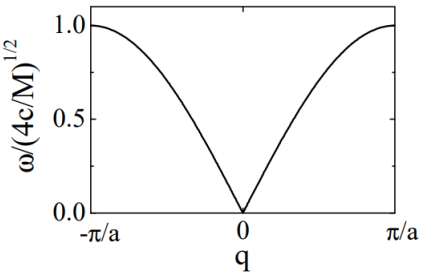


Figure 4: Frequency vs wave vector for monoatomic 1-D lattice

2.5 Diatomic 1-D lattice

The whole system of mass and spring for a 1-D diatomic model shown in Figure 4 can be transformed into an LC circuit (electrical analogue) shown in Figure 5 after comparing the solutions of equations we get by solving the corresponding equations.
The di-atomic lattice with alternative masses 'm' and 'M' shown in Figure 4 can be simulated by the transmission line with alternative capacitors 'C' and 'C1' shown in Figure 5.

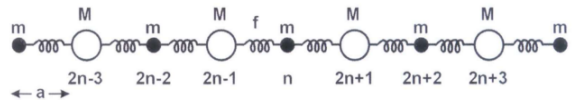


Figure 5: Mass-spring model of diatomic 1-D lattice

In this case, the set of equations needed to solve are:

$$m\frac{d^2x_n}{dt^2} = f[u_{n+1} + u_{n-1} - 2u_n] \tag{7}$$

$$M\frac{d^2x_n}{dt^2} = f[u_{n+2} + u_n - 2u_{n+1}] \tag{8}$$

After solving these sets of equations we get the frequency as:

$$\omega^2 = f\left(\frac{1}{m} + \frac{1}{M}\right) \pm f\sqrt{\left(\frac{1}{m} + \frac{1}{M}\right)^2 - \frac{4sin^2qa}{mM}} \tag{9}$$

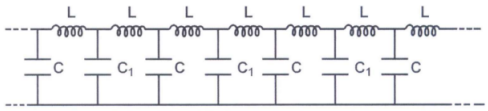


Figure 6: Electrical analogue of diatomic 1-D lattice

In contrast to the mono-atomic lattice, there are now two frequencies ω_+ and ω_- corresponding to a particular value of the wave vector 'q'. In a plot of ν versus θ, this leads to two branches; the acoustical branch and the optical branch.

The lower curve is called the acoustic branch, while the upper curve is called the optical branch. The optical branch begins at q=0 and ω=0. Then with increasing q, the frequency increases in a linear fashion. This is why this branch is called acoustic, similar to elastic waves or sound. Eventually this curve saturates at the edge of the Brillouin zone.
On the other hand, the optical branch has a nonzero frequency at zero q:

$$\omega_0 = \sqrt{2f\left(\frac{1}{m} + \frac{1}{M}\right)} \tag{10}$$

and it does not change much with q.
The distinction between the acoustic and optical branches

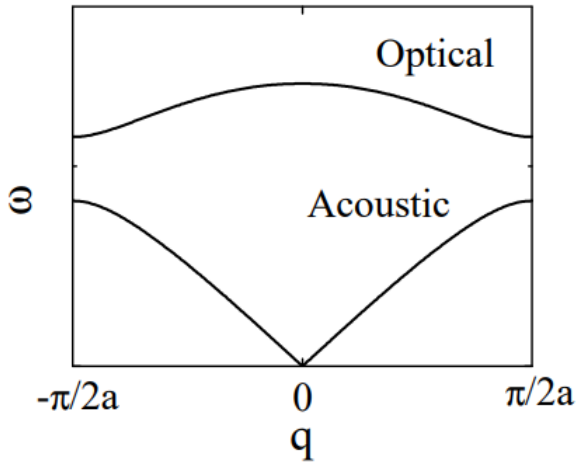


Figure 7: Frequency vs wave vector for diatomic 1-D lattice

of lattice vibrations can be seen most clearly by comparing them at q=0 (infinite wavelength).
For the acoustic branch, the two atoms in the cell have the same amplitude in the phase. Therefore, the molecule oscillates as a rigid body, as shown in Figure 8 for the acoustic mode. On the other hand, for optical vibrations, the optical oscillation takes place in such a way that the center of mass of a molecule remains fixed. The two atoms move in out of phase as shown in Figure 8.

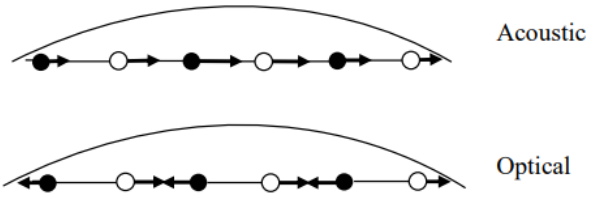


Figure 8: Visualization of vibration corresponding to the two branches

3 APPARATUS

- **Capacitors:** of capacitance 50 nF (For monoatomic lattice circuit) and 160 nF (For diatomic lattice circuit).
- **Inductors:** of inductance 1mH.
- **Breadboard and connecting wires:** to arrange electrical circuits on it.
- **Function generator:** to provide input pulse to the circuits.
- **Oscilloscope:** to measure the phase of the input and output voltages.

4 EXPERIMENTAL SETUP

Schematics of the experimental setup are shown in Figures 3 and 6 of the Theory section. The exact experimental setups we are working on are attached below.

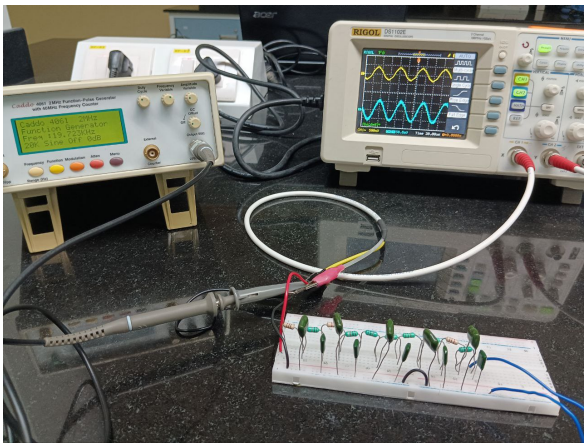


Figure 9: Experimental setup

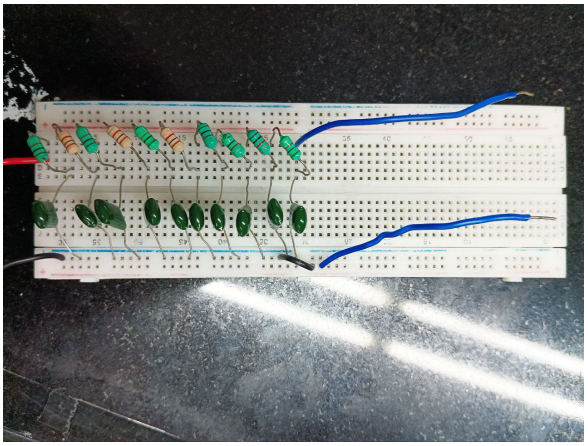


Figure 10: Setup on the breadboard

5 OBSERVATIONS AND PLOTS

The various parameters of the components measured using a digital multimeter are shown in Table 1.

Table 1: Important parameters of the various individual components used

	Monoatomic	Diatomic	
Inductance(mH)	Capacitance (nF)	C(nF)	C_1(nF)
0.975	53	53.4	160.4
1.021	53.3	52	166
1.062	52.5	51	166.1
1.055	54.5	52.6	161.9
1.088	50.9	52.2	166.3
1.009	52.9		
1.04	54.8		
0.921	52.2		
0.95	52		
0.947	54.2		

5.1 Monoatomic 1-D lattice

The inductors have the value of inductance to be:
$L = (1.0068 \pm 0.053)$ mH
The capacitors have the value of capacitance to be:
$C = (53.03 \pm 1.154)$ nF

5.2 Diatomic 1-D lattice

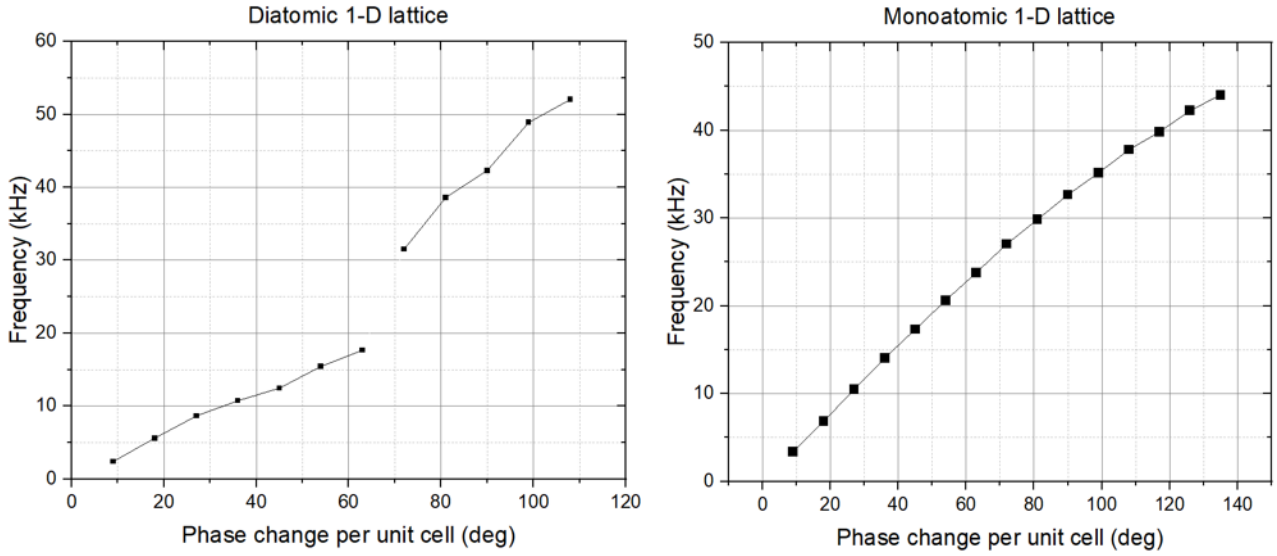
The inductors have the value of inductance to be:
$L = (1.0068 \pm 0.053)$ mH
The smaller capacitors have the value of capacitance to be:
$C = (52.24 \pm 0.554)$ nF
The larger capacitors have the value of capacitance to be:
$C_1 = (164.14 \pm 5.565)$ nF
NOTE: The plots are made using the signed data attached on the next page.

Diatomic				
C	C1		Frequency(kHz)	Phase per unit cell
53.4	160.4		2.397	9
52	166		5.606	18
51	166.1		8.644	27
52.6	161.9		10.732	36
52.2	166.3		12.46	45
			15.436	54
			17.68	63
			31.513	72
			38.59	81
			42.315	90
			48.9	99
52.24	164.14		52.033	108

Verified

Monoatomic				
Inductance(mH)	Capacitance (nF)		Frequency(kHz)	Phase per unit cell
0.975	53		3.393	9
1.021	53.3		6.845	18
1.062	52.5		10.493	27
1.055	54.5		14.065	36
1.088	50.9		17.331	45
1.009	52.9		20.636	54
1.04	54.8		23.794	63
0.921	52.2		27.06	72
0.95	52		29.842	81
0.947	54.2		32.67	90
			35.144	99
1.0068	53.03		37.8	108
			39.83	117
			42.246	126
			44.04	135
			48.085	144

Figure 11: Signed raw data



Plots of Frequency vs phase difference per unit cell for both monoatomic and diatomic 1-D lattices

6 CALCULATIONS and ERRORS

6.1 Monoatomic 1-D lattice

For the monoatomic 1-D lattice, we observed only one branch, called the acoustical branch which gets cut at a frequency with theoretical value:

$$\nu_{max}^{th} = \frac{1}{\pi}\sqrt{\frac{1}{LC}} = 43.52kHz \tag{11}$$

The experimental value of this cut-off frequency we observed from the plot is:

$$\nu_{max}^{exp} = 44.04kHz \tag{12}$$

[We have rejected the last data point as we couldn't figure out whether it was a good data or not due to scaling issues]

6.1.1 Error calculation:

$$d\nu = \frac{\partial\nu}{\partial L}\delta L + \frac{\partial\nu}{\partial C}\delta C \tag{13}$$

After calculating the above eqn. and dividing it by eqn. 11,

$$\frac{d\nu}{\nu} = \frac{1}{2}[(\frac{\delta L}{L}) + (\frac{\delta C}{C})] \tag{14}$$

Substituting the values we got as the mean and standard deviation of inductance and capacitance, we get the relative error percentage to be:

$$\frac{d\nu}{\nu} = 0.0372 = 3.72\% \tag{15}$$

6.2 Diatomic 1-D lattice

For the diatomic 1-D lattice, we observed two branches as it is expected to be, the lower one corresponding to the acoustical branch and the upper one corresponding to the optical branch with frequencies having theoretical values:

$$\nu_1 = \frac{1}{2\pi}\sqrt{\frac{2}{LC_1}} = 17.44kHz \tag{16}$$

$$\nu_2 = \frac{1}{2\pi}\sqrt{\frac{2}{LC}} = 31.05kHz \tag{17}$$

The corresponding experimental values are:

$$\nu_1 = 17.68kHz \tag{18}$$

$$\nu_2 = 31.513kHz \tag{19}$$

Band gap energy: Since phonons are analogous to photons, the energy corresponding to one phonon is equivalent to $h\nu$. So, the band gap energy:

$$\Delta E = h[\nu_2 - \nu_1] = 0.916 \times 10^{-29}J \tag{20}$$

6.2.1 Error calculation:

Using eqn. (14),

$$\frac{d\nu_1}{\nu_1} = 0.0316 = 3.16\% \tag{21}$$

$$\frac{d\nu_2}{\nu_2} = 0.0432 = 4.32\% \tag{22}$$

$$\frac{d\Delta E}{\Delta E} = \frac{d\nu_1}{\nu_1} + \frac{d\nu_2}{\nu_2} = 7.48\% \tag{23}$$

7 RESULTS

- Monoatomic 1-D lattice:

$$\nu = (44.04 \pm 1.64)kHz$$

- Diatomic 1-D lattice:

$$\nu_1 = (17.68 \pm 0.56)kHz$$

$$\nu_2 = (31.513 \pm 1.36)kHz$$

$$\Delta E = (0.916 \pm 0.068) \times 10^{-29}J$$

8 CONCLUSIONS AND DISCUSSIONS

- Comparing the theoretical and experimental results, we got similar values of the required frequencies in both the cases of monoatomic and diatomic 1-D lattices with some error bars which are caused due to the reasons mentioned in the Sources of errors section. Thus the dispersion relations are sufficiently verified.
- Since in this experiment, we are considering a hypothetical 1-D lattice that is impossible to be found in the real world where everything is in higher dimensions, it would be much more difficult to generalize these observations to the real materials scenario. Also, we have considered only the effect of the nearest neighboring atoms and derived all the related formulas, which is not the case in real-world materials.
- As expected after studying the theory part, we got a good plot for both the cases of monoatomic and the diatomic 1-D lattice. We observed a branch cut that occurs in the case of a diatomic 1-D lattice.
- The band gap energy we got is a very small amount of energy in the order of $10^{-11}eV$. So, a small extra energy at the end of the acoustical branch can excite a phonon to the optical region.
- The data would have been more accurate if we had considered more unit cells and calculated the phase difference per unit cell corresponding to a frequency.
- For 2-D lattices (for both monoatomic and diatomic atoms), we need to consider all types of vibration that are possible in a unit cell and the effect of neighboring atoms which would give coupled second-order differential equations for each vibrational mode. After solving those, we could get a complex relation between frequency and phase change per unit cell.
- The only ambiguity found was that we considered the inductor to correspond to mass and the capacitors to correspond to 1/f of the spring-mass model. Is it really true? This hasn't been verified. For the time being, it has been considered to be true. But, the surety is 1/LC corresponds to f/m.

9 SOURCES OF ERRORS

- Non-ideal nature of inductors and capacitors used.
- Non-ideal instruments like oscilloscopes, multimeters, etc.
- We took the data when the approximate phase difference is around 0° or 90° by ensuring an approximately straight line or circle as viewed in the oscilloscope x-y mode, as there was much fluctuation in the value of phase difference displayed on the oscilloscope screen.
- Random errors, personal errors while taking data, etc.
- Non-ideal environmental conditions should have caused some errors as a small amount of heat in the system can create much change in data as the band gap energy is very low to handle.

10 REFERENCES

- NISER Lab Manual
- Lattice vibration theory: `https://unlcms.unl.edu/cas/physics/tsymbal/teaching/SSP-927/Section%2005_Lattice_Vibrations.pdf`
- Lattice vibration theory:`https://www.sciencedirect.com/topics/physics-and-astronomy/lattice-vibration`