Study of Lattice Vibration using Electronic Circuits

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In this experiment, we explore the concept of lattice vibrations using an electrical circuit analogy. We construct circuits simulating both monoatomic and diatomic lattice structures using inductors and capacitors. For both the setups, we analyzed their dispersion relation, by measuring how the phase changes depending on the oscillation frequency. We also observed the emergence of a bandgap in the diatomic lattice case. Measurements were carried out using a function generator and an oscilloscope in XY mode, with precise phase difference recordings. The results were compared with theoretical predictions to validate the models. This experiment demonstrates the effectiveness of electronic circuits in visualizing and understanding the fundamental principles of lattice dynamics.

I. OBJECTIVE

- 1. To study the dispersion relation for the monoatomic lattice and determine the cutoff frequency.
- 2. To study the dispersion relation for the di-atomic lattice and analyse the optical and acoustic modes and obtain the energy gap.

II. THEORY

Almost all solids with the exception of amorphous solids and glasses have periodic arrays of atoms which form a crystal lattice. The existence of the periodic crystal lattice in solid materials provides a medium for characteristic vibrations. Between the lattice spacing, there are quantized vibrational modes called a phonon. The study of phonon is an important part of solid state physics, as they play an essential role in the physical properties of solids, the thermal and electrical conductivity of the materials. The long wavelength property of phonon also gives attributes to sounds in solids.

A. Monoatomic One Dimensional Lattice

Consider the mono-atomic 1D crystal lattice. It can be modelled with an infinite spring mass system with particles having mass m connected by spring constant f. The equilibrium distance between the particles is a. Assuming only the nearest neighbour interaction, the equation of motion of the n-th atom is given by,

$$m\frac{d^2U_n}{dt^2} = f(U_{n+1} - U_{n-1} - 2U_n)$$
 (1)

which when solved gives the angular frequency,

$$\omega = \sqrt{\frac{2f}{m}(1 - \cos\theta)} \tag{2}$$

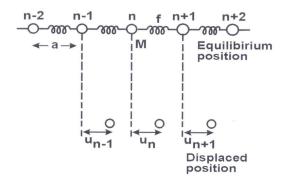


FIG. 1: A one-dimensional monoatomic lattice

where, $\theta = ka$ is the phase change per unit cell. The above equation shows that there exists a maximum frequency

$$\nu_{\text{max}} = \frac{\omega_{\text{max}}}{2\pi} = \frac{1}{\pi} \sqrt{\frac{f}{m}} \tag{3}$$

beyond which no transmission occurs. The array may be considered as a low-pass filter which transmits only in the range 0 to $\nu_{\rm max}$.

B. Diatomic One Dimensional Lattice

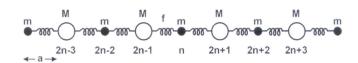


FIG. 2: A one-dimensional diatomic lattice

The spring-mass analogy of di-atomic lattice can be given by assuming two different masses connected by springs in series alternatively. For di-atomic lattice we can use same spring-mass formulation to find as a function of phase angle.

$$m_1 \frac{d^2 U_{2n}}{dt^2} = f(U_{2n+1} - U_{2n-1} - 2U_{2n})$$
 (4)

$$m_2 \frac{d^2 U_{2n+1}}{dt^2} = f(U_{2n+2} - U_{2n} - 2U_{n+1})$$
 (5)

Solving for U_{2n} and U_{2n+1} by taking,

$$U_{2n} = Ae^{-i\omega t - 2ikna}$$
 and $U_{2n+1} = Be^{-i\omega t - 2ikna}$ (6)

we get an eigenvalue equation, where k is the wavenumber, ω is the angular frequency and a is the distance between two atoms on the chain. On solving for ω , we get

$$\omega_{\pm}^{2} = \frac{f}{mM} \left[m + M \pm \sqrt{(m - M)^{2} + 4mM \cos^{2}(ka)} \right]$$
(7)

The resulting dispersion relation is sketched in Fig. 3 for the first Brillouin zone (where $k \in [-\pi/2a, \pi/2a)$). Note that there is a gap in the spectrum on the boundary of the Brillouin zone, $k = \pm \pi/2a$, given by

$$\Delta E = \hbar \sqrt{2f} \left| \frac{1}{\sqrt{m}} - \frac{1}{\sqrt{M}} \right| \tag{8}$$

Thus, in a diatomic lattice, where two different atomic species alternate, the frequency spectrum divides into two distinct branches -

- The acoustic branch which is characterized by low-frequency oscillations where adjacent atoms move in unison. It os called so because its dispersion relation is of the form $\omega = ck$ characteristic of sound waves, at small k.
- and the **optical branch** which is characterized by by high-frequency oscillations where adjacent atoms oscillate out of phase. It is called so because the long wavelength optical modes in ionic crystals can interact with electromagnetic radiation, and are responsible for much of the characteristic optical behavior of such crystals.

Hence a bandgap, emerges between these branches, prohibiting wave propagation with certain energies.

C. The Electrical Analogue of Lattice Vibrations

The point is that both the LC circuit and a lattice of atoms (in the limit of small displacements) are harmonic oscillators, and as such, they obey similar dynamics. With just change the symbols to go from one system to the other, but the equations of motion are formally the same.

The dispersion relation for the electrical analogue circuit for monoatomic lattice is

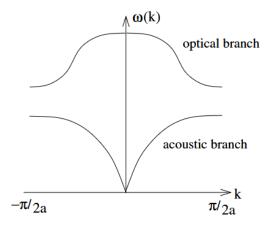


FIG. 3: Phonon dispersion relation for a diatomic chain.

$$\omega_{\text{mono}} = \sqrt{\frac{2}{LC}(1 - \cos \theta)} \tag{9}$$

Here, the highest possible frequency in the circuit will be

$$\omega_{\text{max}} = \frac{2}{\sqrt{LC}} \tag{10}$$

In the analogy, inductance L represents the atomic mass m and the reciprocal of capacitance 1/C represents the force constant f.

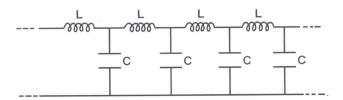


FIG. 4: Circuit diagram representing a monoatomic lattice with L and C

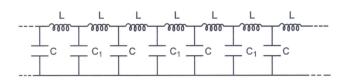


FIG. 5: Circuit diagram representing a diatomic lattice with L and two values of capacitance C_1 and C_2

Here, the bandgap is represented by a frequency gap, prohibiting wave propagation in a certain frequency range. The electrical circuit analogy enables controlled tuning of the bandgap by adjusting component values. The dispersion relation for the electrical analogue circuit for diatomic lattice is

$$\omega_{\rm di}^2 = \frac{1}{L} \left(\frac{1}{C_1} + \frac{1}{C_2} \right) \pm \frac{1}{L} \left[\left(\frac{1}{C_1} + \frac{1}{C_2} \right)^2 - \frac{4\sin^2 \theta}{C_1 C_2} \right]^{1/2} \tag{11}$$

Thus the frequency gap for the diatomic lattice system is the difference between the minimum optical frequency and the maximum acoustic frequency, given by,

$$f_{\rm gap} = \frac{1}{2\pi} \sqrt{\frac{2}{LC_1}} - \frac{1}{2\pi} \sqrt{\frac{2}{LC_2}}$$
 (12)

When the alternating elements in a diatomic lattice become identical, the system behaves as a monoatomic lattice, leading to a continuous frequency spectrum without a bandgap.

III. EXPERIMENTAL SETUP

The circuit diagrams used in the experiment are shown in Fig. 4 and 5.

Apparatus

- 1. Inductors
- 2. Capacitors with 2 different values
- 3. Signal generator
- 4. Oscilloscope
- 5. Breadboard
- 6. DC Power Supply
- 7. Connecting Wires
- 8. Multimeter and LCR Multimeter

IV. OBSERVATION AND CALCULATIONS

A. Monoatomic Lattice

The experimentally obtained data for the monotomic lattice is shown in Table II. The phase difference was observed using the oscilloscope in XY mode, with one input being from the signal generator and the other from the LC circuit output. Measurements were taken at every phase change of $\pi/2$ where the oscilloscope display switched between an ellipse (phase difference $\pm \pi/2$; Fig. 6) and a straight line (phase difference 0 or π ; Fig. 7).

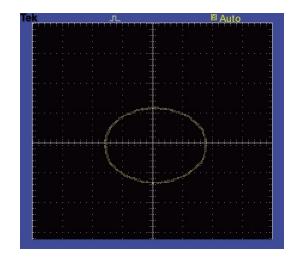


FIG. 6: Oscilloscope output in XY mode showing a phase difference $\pm \pi/2$

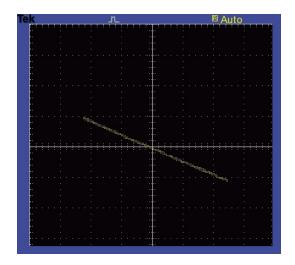


FIG. 7: Oscilloscope output in XY mode showing a phase difference 0 or π

The corresponding inductance and capacitance values used are given in Table I. The graph of θ vs f for the monoatomic lattice is shown in Fig. 8.

Now, using Eq. 10, the theoretical value of ω_{\max} can be calculated from the measured average values of L and C as,

$$\begin{split} \omega_{\rm max} &= \frac{2}{\sqrt{0.976 \times 10^{-3} \times 48.72 \times 10^{-9}}} \\ &= 290.00 \ {\rm krad/s} \\ {\rm or}, \, f_{\rm max} &= 46.16 \ {\rm kHz} \end{split}$$

From the experimental, the maximum frequency observed is 50.68 kHz or 318.43 krad/s.

S.No.	L (mH)	C (nF)
1	0.993	48.52
2	0.981	48.88
3	0.965	48.06
4	0.982	50.15
5	0.959	48.33
6	0.965	50.75
7	0.978	49.93
8	0.992	47.19
9	0.980	48.01
10	0.967	47.39
Mean	0.976	48.721
Std. Dev.	0.011	1.136

TABLE I: Measured values of the component of the circuit for a monoatomic lattice

Total phase	Phase change	Frequency	ω
Change (°)	per unit cell (°)	(Hz)	(krad /s)
90	9	2.151	13.52
180	18	6.771	42.54
270	27	10.250	64.40
360	36	13.870	87.15
450	45	17.100	107.44
540	54	20.580	129.31
630	63	23.740	149.16
720	72	27.210	170.97
810	81	30.270	190.19
900	90	33.300	209.23
990	99	36.030	226.38
1080	108	38.830	243.98
1170	117	41.270	259.31
1260	126	43.410	272.75
1350	135	45.300	284.63
1440	144	47.130	296.13
1530	153	48.730	306.18
1620	162	50.680	318.43

TABLE II: Observed frequencies and their corresponding phase changes in the circuit for a monoatomic lattice

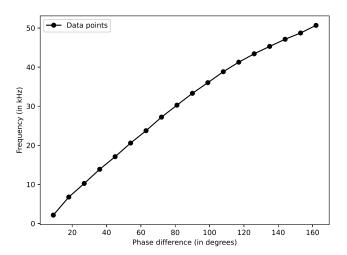


FIG. 8: Plot showing θ vs. f for the monoatomic lattice

S.No.	L (mH)	C_1 (nF)	C_2 (nF)
1	0.993	48.52	157.18
2	0.981	48.88	152.36
3	0.965	48.06	152.20
4	0.982	50.15	148.54
5	0.959	48.33	150.74
6	0.965		
7	0.978		
8	0.992		
9	0.980		
10	0.967		
Mean	0.976	48.570	152.20
Std. Dev.	0.011	0.705	2.84

TABLE III: Measured values of the component of the circuit for a diatomic lattice

Total phase	Phase change	Frequency	ω
Change (°)	per unit cell (°)	(Hz)	(krad /s)
90	9	2.160	13.57
180	18	4.725	29.69
270	27	7.247	45.53
360	36	9.715	61.04
450	45	12.030	75.59
540	54	14.300	89.85
630	63	16.330	102.60
720	72	18.140	113.98
810	81	20.130	126.48
900	90	25.220	158.46
990	99	28.310	177.88
1080	108	31.950	200.75
1170	117	34.900	219.28
1260	126	36.470	229.15
1350	135	37.680	236.75
1440	144	38.820	243.91
1530	153	40.030	251.52

TABLE IV: Observed frequencies and their corresponding phase changes in the circuit for a diatomic lattice

B. Diatomic Lattice

The experimentally obtained data for the diatomic lattice is shown in Table IV. The corresponding inductance and capacitance values used are given in Table III. The graph of θ vs f for the diatomic lattice is shown in Fig. 8.

Again, using Eq. 12, the calculated band gap value is,

$$f_{\text{gap}} = \frac{1}{2\pi} \sqrt{\frac{2}{LC_1}} - \frac{1}{2\pi} \sqrt{\frac{2}{LC_2}}$$
$$= 32.79 - 18.52$$
$$= 14.27 \text{ kHz}$$

From Fig. 9, we can see than the lowest frequency in the optical branch is $25.22~\rm kHz$ and the highest frequency in the acoustic branch is $20.13~\rm kHz$. Hence, the experiment band gap is $5.09~\rm kHz$.

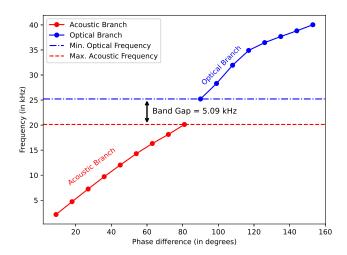


FIG. 9: Plot showing θ vs. f for the diatomic lattice

V. ERROR ANALYSIS

Based on Eq. 10, the error in f_{max} for the monoatomic lattice can be calculated using

$$\Delta f_{\text{max}} = f_{\text{max}} \sqrt{\left(\frac{\Delta L}{2L}\right)^2 + \left(\frac{\Delta C}{2C}\right)^2}$$
 (13)

Using the values of standard deviation in the above equation, the error comes out to be $\Delta f_{\text{max}} = 0.60 \text{ kHz}$.

Similarly using the above equation for the diatomic lattice, the individual errors in the maximum acoustic and minimum optical frequencies amount to the final error in $\Delta f_{\rm max}$,

$$\begin{split} \Delta f_{\rm gap} &= |\Delta f_{\rm acoustic,\ max}| + |\Delta f_{\rm optical,\ min}| \\ &= 0.03 + 0.02 \\ &= 0.05\ \mathrm{kHz} \end{split}$$

VI. DISCUSSION & CONCLUSION

In this experiment, we explored the vibrational properties of one-dimensional monoatomic and diatomic lattices using an electrical circuit analogy. By constructing equivalent LC circuits, we analyzed the dispersion relation by observing the phase change in the circuit using Lissajous figures, across a range of frequencies.

For the monoatomic lattice, the maximum theoretical and observed frequencies are,

$$f_{\text{max, th}} = (46.16 \pm 0.60) \text{ kHz}$$

 $f_{\text{max, obs}} = (50.68 \pm 0.01) \text{ kHz}$

This confirms the expected behavior of the system as a natural low-pass filter. The minor deviation, which amounted to $\approx 9.7\%$, can be attributed to component tolerances and measurement uncertainties.

For the diatomic lattice, the emergence of a frequency bandgap was observed, validating theoretical predictions. The cutoff frequencies for the acoustic and optical branches are,

$$f_{
m acoustic, \ th} = (18.52 \pm 0.03) \
m kHz$$

 $f_{
m acoustic, \ obs} = (20.13 \pm 0.01) \
m kHz$
 $f_{
m optical, \ th} = (32.79 \pm 0.02) \
m kHz$
 $f_{
m optical, \ obs} = (25.22 \pm 0.01) \
m kHz$

And the theoretical and observed frequency bandgaps are,

$$f_{
m gap, \ th} = (14.27 \pm 0.05) \ {
m kHz}$$

 $f_{
m gap, \ obs} = (5.09 \pm 0.01) \ {
m kHz}$

The deviation in $f_{\rm gap}$ is much higher, around 64%. We can see that this is because of the heavy deviation in the cutodd frequency of the optical branch. Errors in measurement and practical component variations likely contributed to the discrepancies.

VII. PRECAUTIONS AND SOURCES OF ERROR

- 1. Ensure that all connections share a common ground to prevent signal interference.
- 2. Avoid loose connections and ensure secure wiring to prevent fluctuations in circuit behavior.
- 3. Verify that all inductors and capacitors remain within their specified tolerance limits to reduce deviations from theoretical predictions.
- 4. Handle circuit components carefully to prevent damage or changes in their electrical properties.
- 5. Use properly calibrated measuring instruments such as oscilloscopes and multimeters to obtain pre-cise readings.

SPS, Study of lattice vibrations using electronic circuits, NISER (2023).

^[2] D. Tong, Applications of quantum mechanics.

^[3] N. W. Ashcroft and N. D. Mermin, *Solid State Physics* (Cengage Learning, 1976).