STUDY OF LATTICE VIBRATIONS USING ANALOGOUS ELECTRONIC CIRCUITS

Aritra Mukhopadhyay
National Institute of Science Education and Research
Bhubaneswar, Odisha 751005, India
3rd year, Integrated M.Sc. Physics
Roll No.: 2011030
(Dated: January 24, 2023)

Using an LC low pass filter, we investigated the lattice vibration of a monoatomic and diatomic crystal in the provided experiment. We discover that a lattice spring and mass model is akin to an LC circuit, and the equation for the resonant frequency yields a similar dispersion relation, so demonstrating the analogy. We have now discovered the maximum resonant frequency of vibration in a monoatomic lattice similar circuit and the frequency band gap in a diatomic lattice analogous circuit.

I. THEORY

Each atom in an equilibrium crystal lattice is precisely positioned at its lattice location. The morse potential, which has the lowest energy at the bond length internuclear distance when the lattice is in equilibrium, gives the potential energy for two particles. The lattice vibrations can be approximated to that of a harmonic oscillator in its most stable state, as seen in the image below. As a result, the lattice may be described as a spring and mass system, with atoms acting as the mass. As a result, when the atoms are pushed by a little amount from the equilibrium point, they tend to return to their original location. Due to interparticle interactions, these movements are subsequently imparted to all atoms, resulting in lattice vibrations.

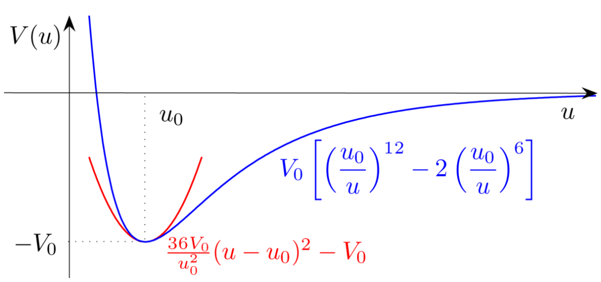


FIG. 1: Harmonic Approximation for Lattice Dynamics

A. Monatomic Lattice Vibrrations

The harmonic approximation for a monoatomic crystal lattice is shown in Figure 2. In Figure 2 these are the relevant constants:

- **a** → Lattice Constant
- **f** → Force constant
- **M** → Mass of the atom

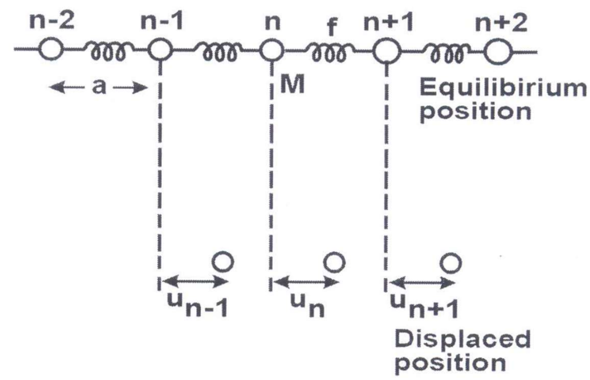


FIG. 2: Spring Mass model of One Dimentional Linear Mono-atomic Lattice

On applying Newton's second law of motion and Hook's law for the sprin-mass system, we get the differential equation for the n^{th} atom:

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

where f corresponds to the force constant and U_n is the displacement of the n^{th} atom. Similarly, for N number of particles at equilibrium particle distance r, there will n coupled differential equations. Resonance would occur for the relation between length of the atomic chain in one dimension ($L = (N+1)r$) and the wavelength of vibration, for an integer m given as $2L = m\lambda$.

Now, let us assume that the solution be of the form $U_n = A\exp(kx_n - \omega t)$. Substituting this in the differential equation with the boundary conditions of $x_N = x_0 = 0$, we get the following equation:

$$\omega = \sqrt{\frac{4f}{m}}\left|\sin\frac{ka}{2}\right|$$

This is the dispersion relation, with k denoting the ${}^{wavenumber}/_{wavevector}$. The Brilluoin zone for the newest (the independent values of k, values for which are indentical to other zones in the lattice) is supplied by the sin term as:

$$\frac{-\pi}{a} \leq k \leq \frac{\pi}{a}$$

$$\nu_{max} = \frac{1}{\pi}\sqrt{\frac{f}{m}}$$

B. Electrical Analogue of Monoatomic Lattice Vibrations

The electronic circuit that is an equivalent for these monoatomic vibration is that on an LC low pass filter as shown in figure, the output voltage of which is measured around the capacitor.

On solving for the current arcoss the n-th capacitor, we find a differntial equation similar to that of Equation 1 given as:

$$C\frac{d^2V_n}{dt^2} = \frac{1}{L}(V_{n+1} - 2V_n + V_{n-1})$$

where capacitance C is equivalent to the mass, inductance L to $1/_{forceconstant}$, and V_i is the voltage across the i^{th} capacitor. Similar solution leads us to the equations of the dispersion equation and the cut off frequency which is equivalent to substituting the corresponding values of their electrical analogue.

$$\omega = \sqrt{\frac{4}{LC}}|\sin\theta|$$

$$v_{max} = \frac{1}{\pi\sqrt{LC}} \tag{2}$$

Where θ is the phase change introduced by the ach of the filter. By measuring the phase difference between the input and output voltages of the circuit as the function of frequency, the dispersion relation may be verified.

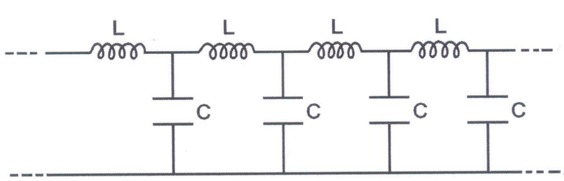


FIG. 3: Monatomic lattice Analogous Circuit

C. Diatomic Lattice Vibrations

For the diatomic case, the model (shown in Figure 2) is changed ever so slightly. Here we have atoms of alternating masses m and M aligned in a row with lattice parameter a, and force constant f. The design is illustrated in Figure 3.

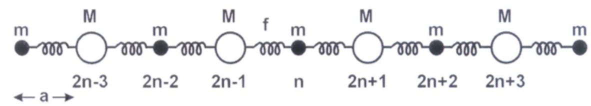


FIG. 4: Diatomic lattice

Thus the coupled differential equations for the n^{th} atom are given as:

$$m\frac{d^2U_n}{dt^2} = f(U_{n+1} - 2U_n + U_{n-1}) \tag{3}$$

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

Solving the Equation 3 and Equation 4 we obtain:

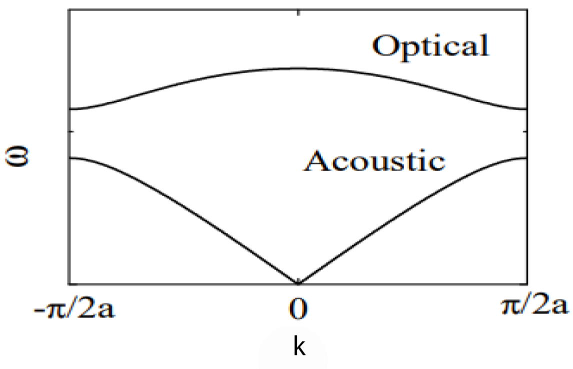
$$\omega = f\left(\frac{1}{m} + \frac{1}{M}\right) \pm f\sqrt{\left(\frac{1}{m} + \frac{1}{M}\right)^2 - 4\frac{\sin^2 ka}{mM}}$$

As seen in the image above, the lower curve is known as the acoustic branch, while the top curve is known as the optical branch. The optical branch starts at $k = 0$ and ends at $\omega = 0$. The frequency then rises in a linear way as k grows. This is why this branch is known as acoustic: it relates to elastic waves or sound at lower frequencies. Near the cut off frequency, this curve eventually saturates at the boundary of the Brillouin zone. At $k = 0$, the optical branch has a nonzero frequency. It has a higher frequency and is created as a result of vibrations caused by electromagnetic waves; the frequency is in the infrared region.

For acoustic brach at $k = \omega = 0$, the relation between the amplitude of oscillation of the two particles is given as $A_1 = A_2 \cdot n$. Therefore the molecule oscillates as a rigid body for the acoustic mode. For the optical vibrations, it yeilds the relation $mA_1 + MA_2 = 0$. This implies that the optical oscillation takes place in such a way that the center of mass of a molecule remains fixed.

The electronic analogue for the circuit is given as shown with one unit cell comprising of two capacitors of capacitance C and C_1 which acts as a band stop filter, where the gap is dependent on the $\frac{C}{C_1} \leftrightarrow \frac{m}{M}$. The analogous dispersion relation is given as:

$$\omega = \frac{1}{L}\left(\frac{1}{C} + \frac{1}{C_1}\right) \pm \frac{1}{L}\sqrt{\left(\frac{1}{C} + \frac{1}{C_1}\right)^2 - 4\frac{\sin^2\theta}{CC_1}}$$



On putting $k = \pm\pi$, we can obtain the range of the band gap, which lies between:

$$\nu_{upperbound} = \frac{1}{2\pi\sqrt{LC}} \tag{5}$$

$$\nu_{lowerbound} = \frac{1}{2\pi\sqrt{LC_1}} \tag{6}$$

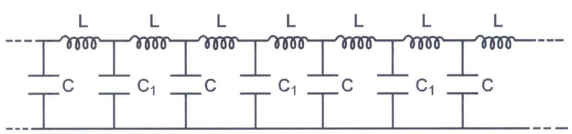


FIG. 5: Diatomic lattice Analogous Circuit

II. OBSERVATIONS

A. Monatomic Lattice

The experimentally obtained data for the monatomic lattice is shown in Table 1. The graph of θ vs ν for the monatomic lattice is shown in Graph 1.

B. Diatomic Lattice

The experimentally obtained data for the diatomic lattice is shown in Table 2. The graph of θ vs ν for the diatomic lattice is shown in Graph 2.

9.206 11.706 13.836 16.136 18.246 20.246 21.966 23.868 25.768 26.968 40.668 41.768

III. CALCULATION

A. Monatomic Lattice

- $C = 50nF$

Frequency (ν) (KHz)	$10 \times \theta(^\circ)$	$\theta(^\circ)$
1.8	90	9
7	180	18
12.1	270	27
15.4	360	36
19.5	450	45
21.8	540	54
27.07	630	63
30.5	720	72
34	810	81
38.8	900	90
42	990	99
48	1080	108
57	1170	117
63	1260	126
77	1350	135

TABLE I: Monoatomic Lattice

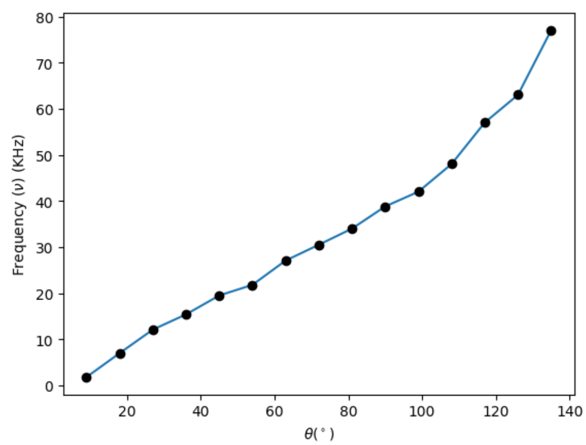


FIG. 6: Graph of θ vs ν for monatomic lattice

- $L = 1mH$

From Table 1 we have the maximum angular frequency of the monatomic lattice as $f_{max} = 38.8kHz$. And from Equation 2 the theoretical value is:

$$\nu_{max} = \frac{1}{\pi\sqrt{LC}} = 45.016kHz$$

B. Diatomic Lattice

- $C = 50nF$
- $C_1 = 165nF$
- $L = 1mH$

From Table 2 we find the frequency band gap is between $26.968kHz$ and $40.668kHz$. And from Equation 2 the theoretical value is:

$5 \times \theta$ (°)	θ (°)	**Frequency (ν) (KHz)**
90	18	9.206
180	36	11.706
270	54	13.836
360	72	16.136
450	90	18.246
540	108	20.246
630	126	21.966
720	144	23.868
810	162	25.768
900	180	26.968
990	198	40.668
1080	216	41.768

TABLE II: Diatomic Lattice

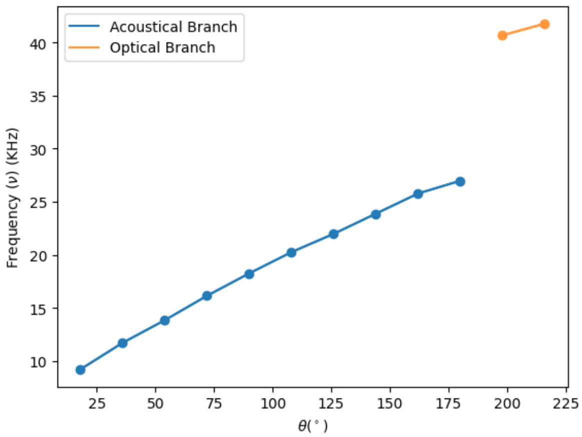


FIG. 7: Graph of θ vs ν for dinatomic lattice

$$\frac{1}{\pi\sqrt{LC}} = 45.016kHz$$

$$\frac{1}{\pi\sqrt{LC_1}} = 24.780kHz$$

IV. ERROR ANALYSIS

A. Monoatomic Lattice

Comparing the experimental value of ν_{max} with the theoretical value:

$$\Delta\nu = \frac{|\nu_{theoretical} - \nu_{experimental}|}{\nu_{theoretical}} \times 100\%$$

$$\therefore \Delta\nu = \frac{|45.016 - 38.8|}{45.016} \times 100\% = 13.8\%$$

B. Diatomic Lattice

Comparing the experimental value of band gap with the theoretical value:

$$\Delta\nu = \frac{|45.016 - 40.668|}{45.016} \times 100\% = 9.66\%$$

$$\Delta\nu = \frac{|24.780 - 26.968|}{24.780} \times 100\% = 8.83\%$$

V. CONCLUSION

- For monatomic case the threshold frequency is, $38.8kHz$ with a 13.8% error.
- For diatomic case the band gap lies between $26.968kHz$ and $40.668kHz$ with a 9.66% and 8.83% error respectively.
- The cutoff frequency is the value at which the vibration's wavelength is in the order of the average internuclear distance.
- In the monoatomic situation, 10 unit cells were employed, whereas in the diatomic example, 5 unit cells were used. To reproduce the lattice, the LC components should ideally be quite big. Furthermore, having a greater number of cells provides for a bigger cutoff wavelength since there are more resonant frequencies accessible before the resonant frequency hits the cutoff value, as indicated in the preceding paragraph.
- We can also find the dispersion relation for a 2-d and 3-d lattice. Consider the monoatomic lattice with atoms in a membrane arranged in a two dimensional square lattice. The membrane is stretched such the equation of motion for the atoms is given as:

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

  $$+(U_{n,m+1} + U_{n,m-1} - 2U_{n,m})]$$

  where $U_{n,m}$ position, leading to $n \times m$ coupled differential equations. Since there are two possible motions, transverse and longitudinal, we get two lines on the frequency versus phase plot. This is due to the two nodes of vibration as shown in figure below. Similarly for the diatomic case case, we will get 4 lines, two each for acoustic and optical branch.
- In terms of experiment findings, we discover that the phase difference caused in the signal by one unit cell is equal to 9°. The data on the oscilloscope accords with the result when we tested the signal

for only one unit cell, as shown in the picture below. However, we know that the phase difference between the input and output signal in an ideal (resistance-less) LC circuit is $90°$. The defects in the LC circuit due to the resistances present might explain this, as resonance corresponds to a 90 degree phase difference, resulting in a circle or oval picture on the oscilloscope for the X-Y mode. The oval form appears at higher frequencies, as the circuit's attenuation rises. The lattice's cutoff wavelength matches to the LC filter's bandwidth edge.

A. Conclusion

Hence the analogy between the Monoatomic, diatomic lattice and the corresponding LC circuits have been established with errors for the parameters being around $1 - 10\%$. The scope of errors and the necessary precautions include:

- The unstable value of the frequency on the oscilloscope. Although the values could be made static using the "Stop" button, we still got around the 3-4 slightly different readings for the same value.
- Experimenter's error in discerning the shape of the plot in the X-Y mode.
- Small differences in the values of the circuit's capacitance and inductance when measured separately outside the circuit and jointly while inside the circuit.
- Noise should be avoided by using suitable connections. We discovered that connecting the function generator and the oscilloscope input channel with the same wire on the breadboard might result in more noise entering into the circuit.

[1] SPS, Sps lab manual, Website (2022), https://www.niser.ac.in/sps/sites/default/files/basic_page/p347_2023/5.Study_of_lattice_vibrations_using_electronic_circuits_v2.pdf.

[2] E.Y.Tsymba, Lattice vibrations, Website https://unlcms.unl.edu/cas/physics/tsymbal/teaching/SSP-927/Section%2005_Lattice_Vibrations.pdf.