Fall semester 2013

Solid State Physics

Lattice Dynamics, theory & experiment

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Introduction

In this report, we will investigate a physical phonon model for a linear one dimensional chain. We will begin doing some theoretical analysis and then proceed to compare the model to a experimental setup. To simulate the 1D crystal lattice, we will connect several masses with springs on a track that minimizes newtonian friction. One end of the chain is held in place and at the other end is connected to a motor that drives force into the spring mass system. Throughout this report, we will refer to a worksheet called *Lattice Dynamics, Theoretical and experimental examination of normal modes in a mechanical one dimensional multy body system*, from *Stockholm University*, that was handed to us before the experiment.

Theory

Assignment #1

We will calculate the relative relative amplitudes and frequencies for a 3 mass chain. Disregarding friction, we write the force on each mass m (with respect to their equilibrium postion) connected to springs with a spring constant C.

$$
\begin{aligned}
m\ddot{x}_1 &= -Cx_1 + C(x_2 - x_1) &&= C(x_2 - 2x_1) && (1)\\
m\ddot{x}_2 &= -C(x_2 - x_1) + C(x_3 - x_2) &&= C(x_1 - 2x_2 + x_3) && (2)\\
m\ddot{x}_3 &= -C(x_3 - x_2) - Cx_3 &&= C(x_2 - 2x_3) && (3)
\end{aligned}
$$

We educatedly guess the solution of the differential equation to be,

$$
x_j = A_j e^{i\omega t} \quad \Rightarrow \quad \frac{d^2}{dt^2}x_j = \ddot{x}_j = -\omega^2 A_j e^{i\omega t} \tag{4}
$$

The natural frequency $\omega_0 \equiv \sqrt{\frac{C}{m}}$ and for convenience, we define $\gamma \equiv \frac{m\omega^2}{C} = \frac{\omega^2}{\omega_o^2}$
Plugging equation 4 in to eqs. (1-3) yields

$$
\begin{aligned}
-\gamma A_1 &= A_2 - 2A_1 && (5)\\
-\gamma A_2 &= A_1 - 2A_2 + A_3 && (6)\\
-\gamma A_3 &= A_2 - 2A_3 && (7)
\end{aligned}
$$

therefore

$$
\begin{aligned}
A_1(\gamma - 2) + A_2 &&&= 0 && (8)\\
A_1 \quad + A_2(\gamma - 2) + A_3 &&&= 0 && (9)\\
A_2 \quad + A_3(\gamma - 2) &&&= 0 && (10)\\
&&&& (11)
\end{aligned}
$$

we can then represent the problem in the following way

$$\begin{pmatrix} \gamma-2 & 1 & 0 \\ 1 & \gamma-2 & 1 \\ 0 & 1 & \gamma-2 \end{pmatrix} \begin{pmatrix} A_1 \\ A_2 \\ A_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \tag{12}$$

lets call the matrix in equation 12, $\mathbf{A}$ and find its determinant,

$$\det \mathbf{A} = \begin{vmatrix} \gamma-2 & 1 & 0 \\ 1 & \gamma-2 & 1 \\ 0 & 1 & \gamma-2 \end{vmatrix} = (\gamma-2)((\gamma-2)^2-1)-(\gamma-2) = 0$$

it's pretty obvious that $\gamma = 2$ fulfills our criteria, next we divide through our latest result with $(\gamma - 2)$ and simplify

$$\det \mathbf{A} = (\gamma^2 - 4\gamma + 4 - 1) - 1 = \gamma^2 - 4\gamma + 2 = 0$$

we then use the quadratic equation to find solutions for γ,

$$\gamma = -\frac{b}{2a} \pm \frac{\sqrt{b^2-4ac}}{2a} = -\frac{(-4)}{2\cdot 1} \pm \frac{\sqrt{(-4)^2 - 4\cdot 1\cdot 2}}{2\cdot 1} = 2 \pm \frac{\sqrt{8}}{2} = \underline{2 \pm \sqrt{2}} \tag{13}$$

For the solution $\gamma = 2 \pm \sqrt{2}$, equation 12 can then take the following forms

$$\begin{pmatrix} \pm\sqrt{2} & 1 & 0 \\ 1 & \pm\sqrt{2} & 1 \\ 0 & 1 & \pm\sqrt{2} \end{pmatrix} \begin{pmatrix} A_1 \\ A_2 \\ A_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \Rightarrow 0 = \begin{cases} \pm\sqrt{2}A_1 + A_2 \\ A_1 \pm \sqrt{2}A_2 + A_3 \\ A_2 \pm \sqrt{2}A_3 \end{cases} \tag{14}$$

so we can then find the relation between the amplitudes.

$$\begin{aligned} \mp\sqrt{2}A_1 = A_2 = \mp\sqrt{2}A_3 \quad &\Rightarrow \quad \boxed{A_1 = A_3} \\ 2A_1 = \mp\sqrt{2}A_2 \quad &\Rightarrow \quad \boxed{A_2 = \mp\sqrt{2}A_1 = \mp\sqrt{2}A_3} \end{aligned}$$

and the solution $\gamma = 2$ yields $A_1 = -A_3$ and $A_2 = 0$

we have $\omega = \sqrt{\gamma}\omega_0$ (only the positive solutions because $\{\gamma, C, m\} > 0$), we get

$$\omega = \left\{ \sqrt{2}\omega_0, \sqrt{2+\sqrt{2}}\omega_0, \sqrt{2-\sqrt{2}}\omega_0 \right\}$$

For the solution $A_1 = A_3$, we can arbitarily choose $A_2 = 1$ combined with the $A_2 = 0$ solution, we get the set of mutually orthogonal eigenvectors

$$\begin{pmatrix} A_1 \\ A_2 \\ A_3 \end{pmatrix} \in \left\{ \begin{pmatrix} 1/\sqrt{2} \\ 1 \\ 1/\sqrt{2} \end{pmatrix} , \begin{pmatrix} -1/\sqrt{2} \\ 1 \\ -1/\sqrt{2} \end{pmatrix} , \begin{pmatrix} 1/\sqrt{2} \\ 0 \\ -1/\sqrt{2} \end{pmatrix} \right\} \tag{15}$$

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Assignment #2

Let $S \equiv$ *number of masses in the system + 1 = number of springs in the system.* We get the amplitude A_j of each mass located at postion j to be,

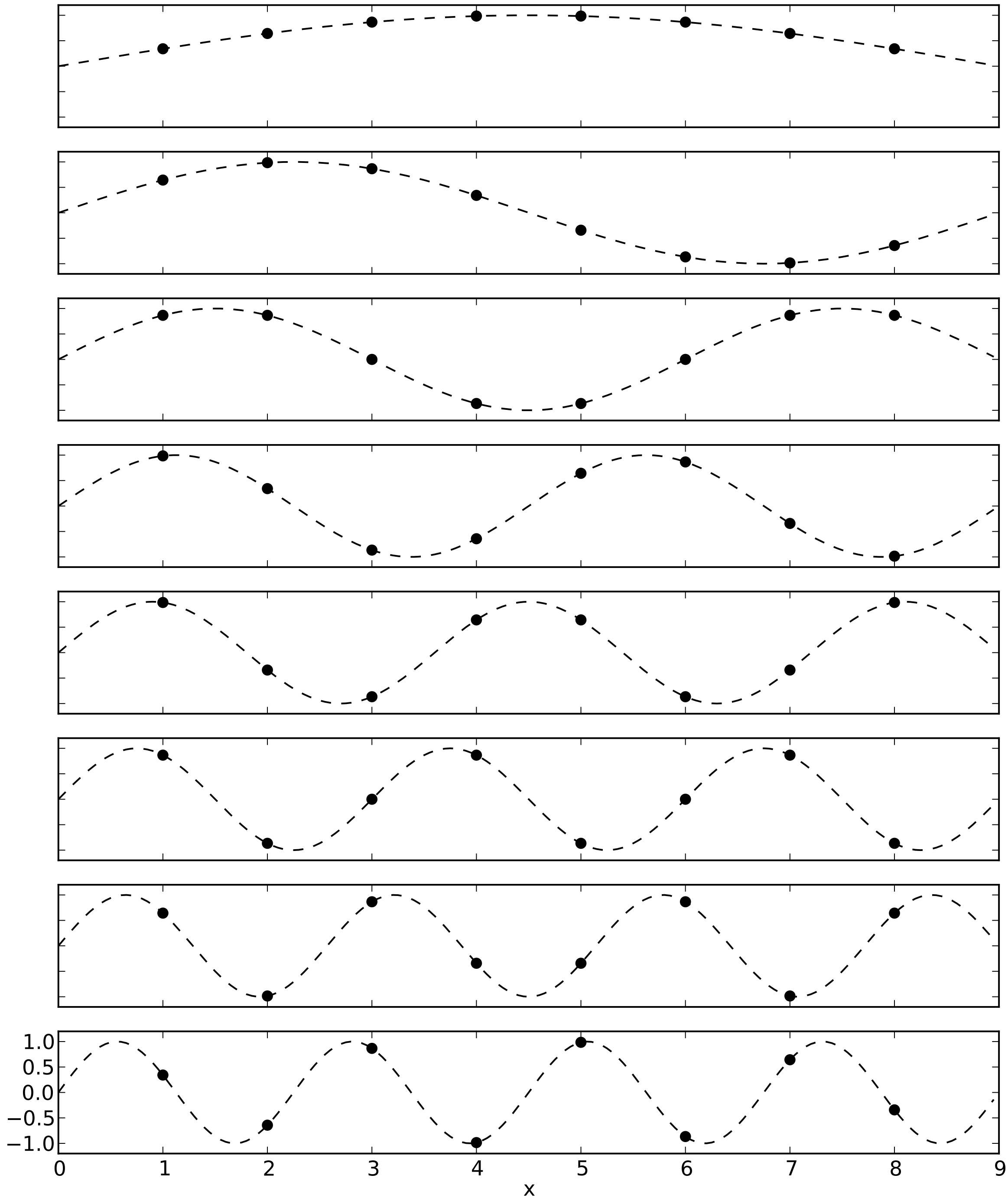
$$A_j = A \sin(jn\pi/S) = \sin(jn\pi/S) \tag{16}$$

and we're supposed to show that for $n > S$ there are no new solutions. Let $j \to j + S$, then equation 16 becomes.

$$A_j = A \sin(jn\pi/S + n\pi) = \begin{cases} A \sin(jn\pi/S) & n \text{ is even} \\ -A \sin(jn\pi/S) & n \text{ is odd} \end{cases} \tag{17}$$

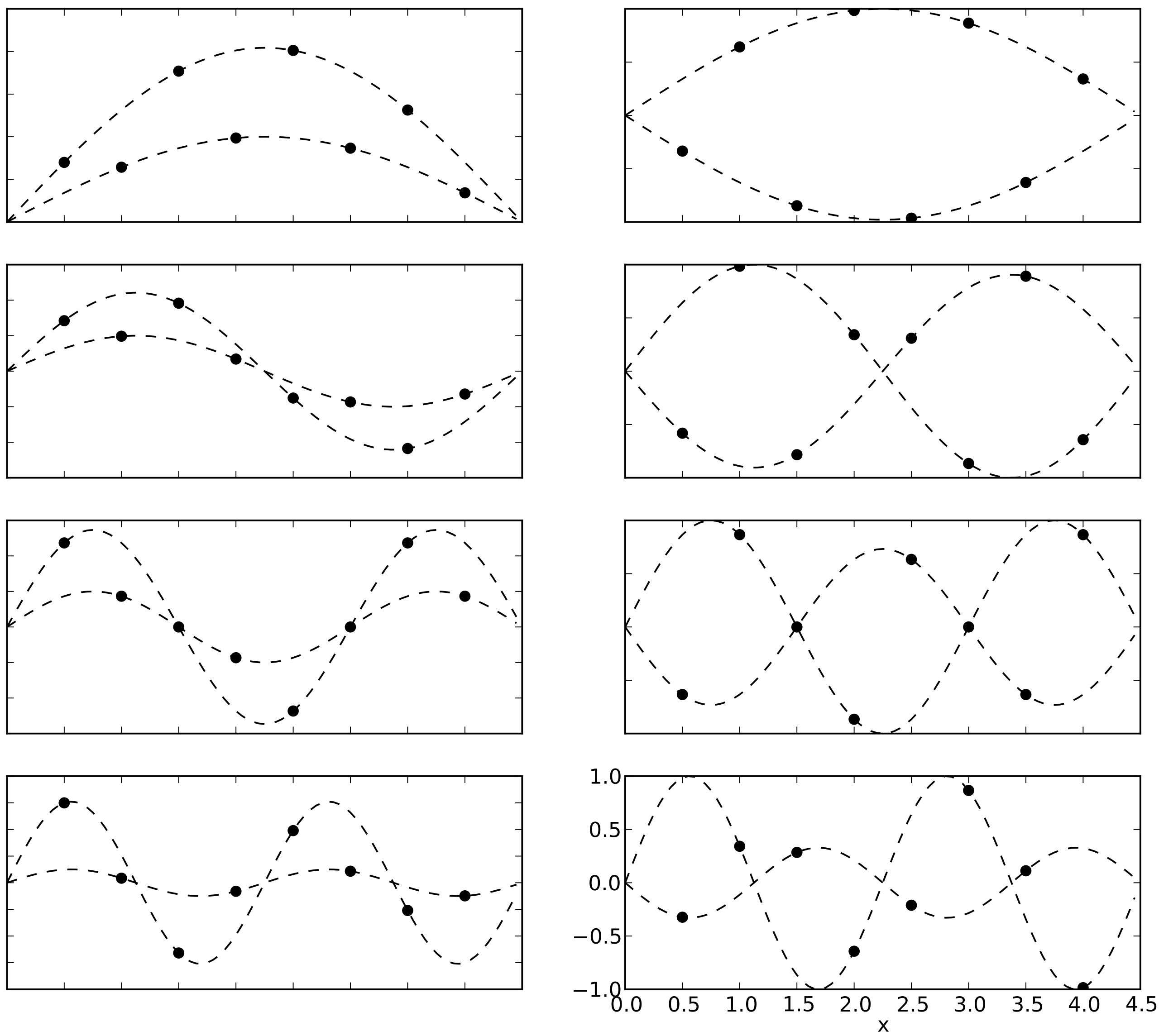
We really only care about the relative amplitudes, so like at the end of assignment #1, we choose an arbitrary magnitude for A and the rest of them follow from that.
As for assignments #3 & #4, we put the phonon lattice model up in a Python script and plot it for different parameters.

Assignment #3



Mynd 1: All 8 normal modes n for 8 equal masses m sketched at $t = 0$

Assignment #4



Mynd 2: Diatomic linear chain with mass ratio= 2 at $t = 0$ for $n \in \{1, 2, 3\}$. The acoustic solutions are on the left and the optical on the right.

Experimental

Estimating the uncertainty

There are various sources of errors, we are first of all trying to simulate a 1D crystal lattice, in reality the vibrations are usually in a linear combination of many normal modes and the energy dissipates due to heat conversion, in contrast our experimentla Spring constant

$$C = \omega^2 m = \left(\frac{2\pi}{T}\right)^2 m \tag{18}$$

we'll assume the uncertainty is relatively small, for the fractional uncertainty in C is,

$$\Delta C = \left|\frac{d}{dm}C\right|\Delta m + \left|\frac{d}{dT}k\right|\Delta T = \left|\frac{2\pi}{T}\right|^2 \Delta m + \left|\left(-2\frac{1}{T^3}\right)4\pi m\right|\Delta T \tag{19}$$

$$= \left(\frac{2\pi}{T}\right)^2\left(\Delta m + \frac{2m}{T}\Delta T\right) = \underbrace{\left(\frac{2\pi}{T}\right)^2 m}_{C}\left(\frac{\Delta m}{m} + 2\frac{\Delta T}{T}\right) \tag{20}$$

therefore

$$\Delta C = C\left(\frac{\Delta m}{m} + 2\frac{\Delta T}{T}\right) \tag{21}$$

We used measured the spring constants C with test mass of (40 ± 1) g, so $\Delta m = 1$g. The period T is measured with a stopwatch, so ΔT is based on the reaction time to start and stop the watch, we estimate $\Delta T = 0.1$s Now we figure how much the uncertainty in $\omega = \sqrt{\frac{C}{m}}$ is, we get similar as before

$$\Delta\omega = \left|\frac{1}{2}\left(\frac{C}{m}\right)^{-1/2}\frac{1}{m}\right|\Delta C + \left|\frac{1}{2}\left(\frac{C}{m}\right)^{-1/2}\left(-\frac{1}{2}\frac{C}{m^2}\right)\right|\Delta m \tag{22}$$

$$= \frac{1}{2m}\sqrt{\frac{m}{C}}\left(\Delta C + \frac{C}{m}\Delta m\right) = \frac{1}{2}\sqrt{\frac{C}{m}}\left(\frac{\Delta C}{C} + \frac{\Delta m}{m}\right) \tag{23}$$

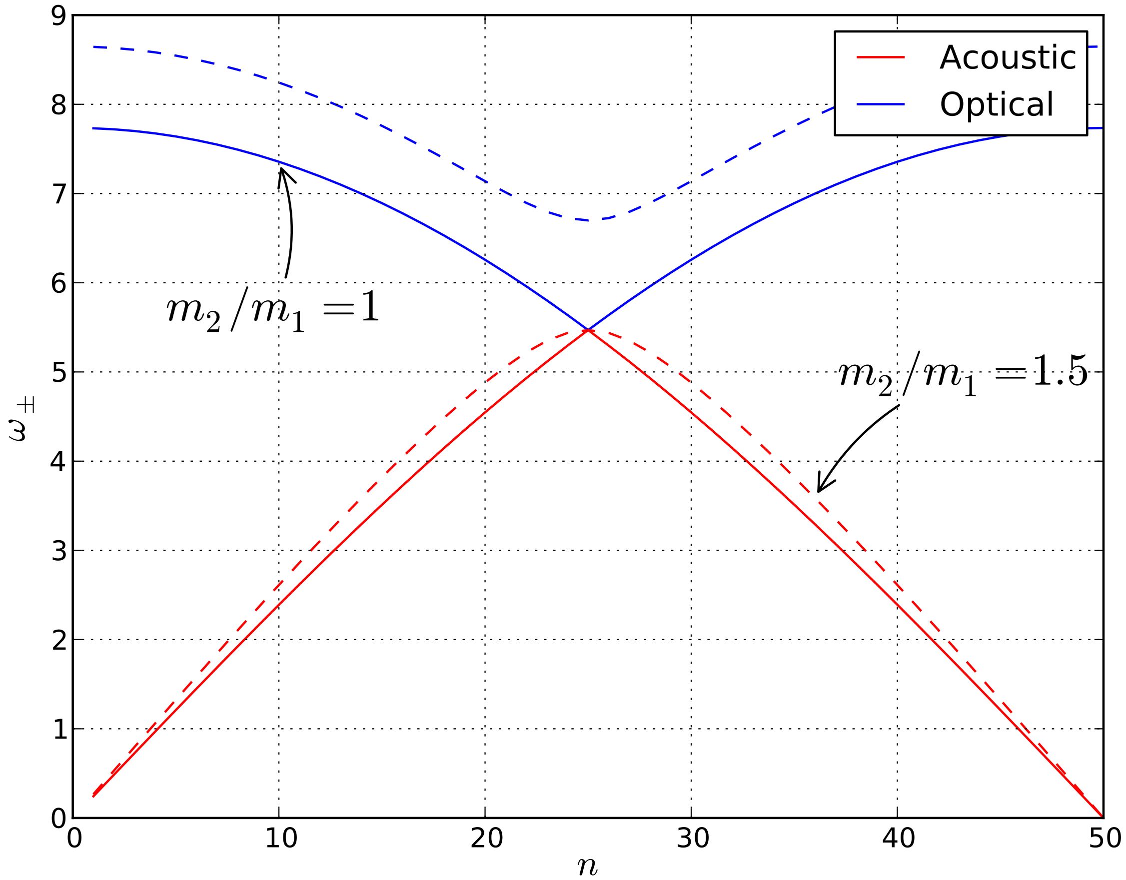
We can plug in ΔC from equation 21 to the latter part of equation 23. We still have $\Delta m =$ 1g.

$$\Delta\omega = \frac{1}{2}\sqrt{\frac{C}{m}}\left(\frac{\Delta m}{m} + 2\frac{\Delta T}{T} + \frac{\Delta m}{m}\right) = \boxed{\omega\left(\frac{\Delta m}{m} + \frac{\Delta T}{T}\right)} \tag{24}$$

Measurements

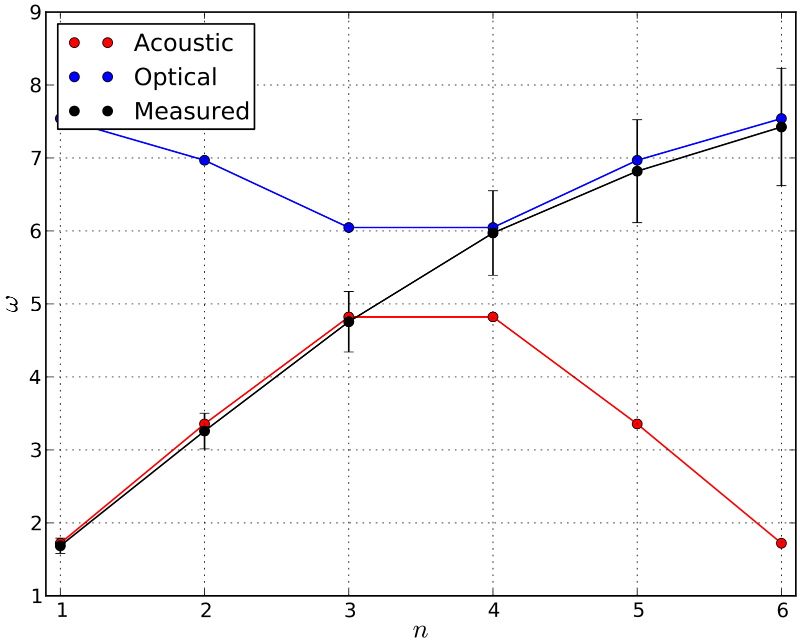
We started out measuring a value for the spring constant C for each of the springs, with a test mass $m_0 = 0.04 \pm 0.01$ kg. All the springs were measured with similar periods, the estimate the spring constant to be $C = 0.030 \pm 0.0076$ kg/s^2

To demonstrate how the frequency spectrum of a mono- & di- atomic chain behaves, we plot it as a function of the normal mode number for 100 masses (to get a decently continuous path).

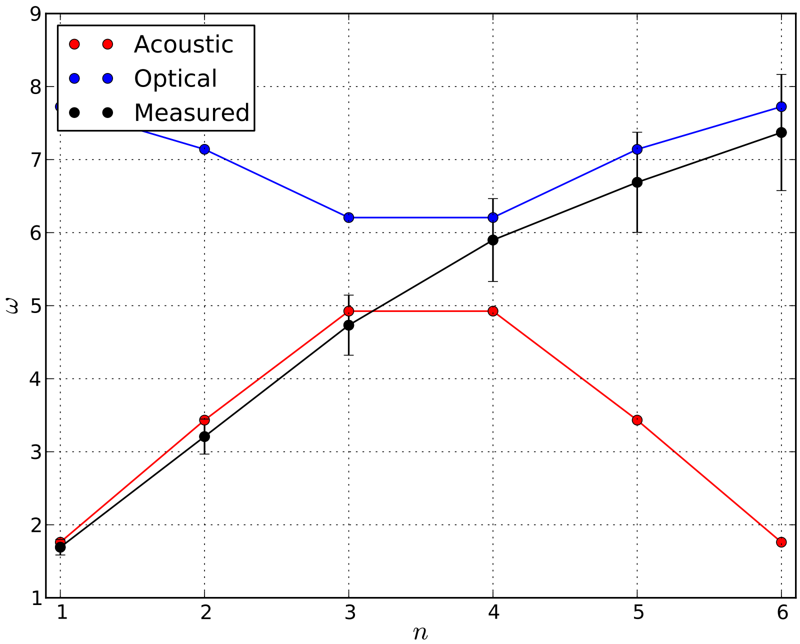


Mynd 3: Frequency spectrum of a 100 mass chain, dotted line with mass-ratio 1.5 and solid line mass-ratio 1.0

The results for the mono-atomic chain are well within the estimated uncertainty. For the di-atomic chain we measured the frequency to be similiar. It probably would have been better to have a mass ratio of atleast ≈ 1.5 instead of ≈ 1.1 which we had for this experiment.



Mynd 4: Our measurements of ω for the mono-atomic linear chain sketched with the corresponding theoretical values.



Mynd 5: Our measurements of ω for the di-atomic linear chain sketched with the corresponding theoretical values.