Phonons in a one-dimensional crystal

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The Kronig-Penney model for electron wavefunctions in a crystal predicts that there will be "gaps" in the energy: energy regions for which there are no solutions to the Schrödinger equation.[3, 467–470] For very similar reasons, there are forbidden *frequency regions* in the vibrational spectra of a one-dimensional diatomic crystal lattice. We will use a "crystal" formed from alternating masses (fishing weights) attached at regular intervals on a vibrating wire. By measuring the amplitude of vibration as we scan the driving frequency in the wire, we can determine the resonant angular frequencies of the "phonons" allowed in the wire. We can also observe the forbidden region, where there are no allowed resonant frequencies.[2]

Mathematical Background

Begin by considering a series of masses on a wire, as shown in figure 1.[1, 104–107] The "lattice constant" is the distance between equivalent points on the lattice, as shown by a. The masses of the larger and smaller weights are m_u and m_v, respectively. The transverse displacement of the larger and smaller masses is represented by u and v, respectively, with s an index to indicate which mass we're talking about. The transverse spring constant is k.

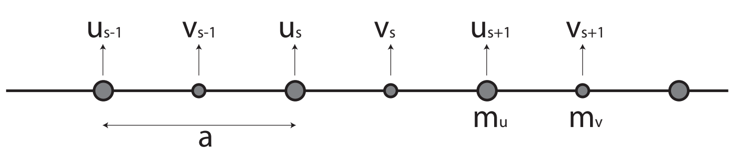

Figure 1: Diatomic 1-D crystal, with notation indicated

Newton's second law for u_s and v_s on this wire becomes

$$\begin{aligned} m_u \frac{d^2 u_s}{dt^2} &= k(v_s - u_s) + k(v_{s-1} - u_s) \\ &= k(v_s + v_{s-1} - 2u_s) \quad (1) \\ m_v \frac{d^2 v_s}{dt^2} &= k(u_{s+1} - v_s) + k(u_s - v_s) \\ &= k(u_{s+1} + u_s - 2v_s)\ . \quad (2) \end{aligned}$$

We will look for plane-wave solutions, of the form

$$u_s = ue^{isKa}e^{-i\omega t} \tag{3}$$

$$v_s = ve^{isKa}e^{-i\omega t} \tag{4}$$

where u and v are the maximum amplitudes of m_u and m_v, and K is the wavenumber, related to the wavelength λ by

$$K \equiv \frac{2\pi}{\lambda} \ .$$

Substituting equation 3 into 1 gives

$$m_u \left(-\omega^2 ue^{iska}e^{-i\omega t}\right) = k(v_s + v_{s-1} - 2u_s)$$

$$-\omega^2 m_u ue^{isKa}e^{-i\omega t} = k\left[ve^{isKa}e^{-i\omega t} + ve^{i(s-1)Ka}e^{-i\omega t} - 2ue^{isKa}e^{-i\omega t}\right]$$

$$-\omega^2 m_u u = k\left[v + ve^{-iKa} - 2u\right]$$

or

$$(2k - \omega^2 m_u)u - k(1 + e^{-iKa})v = 0 \ . \tag{5}$$

A similar substitution and manipulation gives, for m_v,

$$-k(e^{iKa} + 1)u + (2k - \omega^2 m_v)v = 0 \ . \tag{6}$$

Equations 5 and 6 can be solved exactly, but it is more instructive to write them in matrix form:

$$\begin{bmatrix} 2k - \omega^2 m_u & -k(1 + e^{-iKa}) \\ -k(e^{iKa} + 1) & 2k - \omega^2 m_v \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = 0$$

From this we see that in order for a solution to exist, the determinant of the left-hand matrix must be zero:

$$\begin{vmatrix} 2k - \omega^2 m_u & -k(1 + e^{-iKa}) \\ -k(e^{iKa} + 1) & 2k - \omega^2 m_v \end{vmatrix} = 0$$

$$\implies 2k^2(1 - \cos(Ka)) - 2k\omega^2(m_u + m_v) + \omega^4 m_u m_v = 0 \tag{7}$$

Solving equation 7 for $\cos(Ka)$ gives

$$\cos(Ka) = 1 - \frac{\omega^2}{k}(m_u + m_v) + \frac{\omega^4}{2k^2} m_u m_v \tag{8}$$

In order for equation 8 to be true, the magnitude of the right hand side must be less than or equal to one. We're not particularly interested in the limit at $Ka = 0$, so we instead look at the other limit to $\cos(Ka)$ at $Ka = \pi$, for which

$$-\frac{\omega^2}{k}(m_u + m_v) + \frac{\omega^4}{2k^2} m_u m_v \geq -2$$

This has no real solutions on the range between $\omega = \sqrt{\frac{2k}{m_u}}$ and $\omega = \sqrt{\frac{2k}{m_v}}$.

We have assumed an infinitely long wire, for which the allowed solutions are essentially continuous. The actual equipment is not infinite in extent, of course, so within the region of allowed frequencies there are discrete resonant frequencies rather than a continuum. But the forbidden region between $\omega = \sqrt{\frac{2k}{m_u}}$ and $\omega = \sqrt{\frac{2k}{m_v}}$ exists, regardless.

Lock-In Amplification

A lock-in amplifier is a powerful tool for extracting very small periodic signals from a comparatively large noise background. In this experiment, we want for the oscillations of the wire to remain small, so that the linear approximations used in the preceding derivation hold. A lock-in amplifier is perfect for this situation: here's how it works.

The integral of the product of two sine functions,

$$\int_{-\infty}^{\infty} \sin(\omega_1 t) \sin(\omega_2 t) \, dt$$

is usually zero. This is because the two functions are each positive (and negative) half the time, so their product is positive (and negative) half the time and the integral is then zero. The exception to this is if $\omega_1 = \omega_2 \equiv \omega$, in which case the integral becomes

$$\int_{-\infty}^{\infty} \sin^2(\omega t) \, dt$$

which is always positive.

Any signal can be expressed as the sum of some carefully-chosen set of sine waves.

$$\mathcal{S}(t) = \sum_i A_i \sin(\omega_i t)$$

So if we took an arbitrary signal and multiplied it by a signal at the frequency we wanted to see, and integrated, most of the components of the signal would go away, leaving only the component with the reference frequency.

$$\int_{-\infty}^{\infty} \mathcal{S}(t)\sin(\omega_o t) = \int_{-\infty}^{\infty} \sum_i A_i \sin(\omega_i t)\sin(\omega_o t)\ dt$$
$$= 0 + 0 + \cdots + \int_{-\infty}^{\infty} \sin^2(\omega_o t)\ dt + 0 + \cdots$$

This is, in essence, what is done by a lock-in amplifier.

Of course, there are some complications. For starters, it takes awhile to integrate over all time. Instead, we integrate over some time constant τ. This results in a somewhat broader peak: the integration does not go completely to zero for values of ω near ω_o. The peak is still centered at ω_o, but the width is inversely related to τ. There is a trade-off: you can get fast results with a short time constant, or precise results with a long one. In general, use as long a value of τ as you can, and at least make sure it's much greater than $1/\omega$.

Another complication is that the *phase* of the signal affects the result. We've ignored phase so far in this discussion, but consider what happens if the desired frequency component in the signal is out of phase with the reference signal by 90°.

$$\int_{-\tau}^{\tau} \sin\left(\omega t + \frac{\pi}{2}\right)\sin(\omega t)\ dt = \int_{-\tau}^{\tau} \cos(\omega t)\sin(\omega t)\ dt = 0$$

It turns out that we can use this to our advantage, though, by use of a dual-channel lock-in. One channel multiplies the signal by $\sin(\omega t)$ and integrates: the other multiplies by $\cos(\omega t)$ and integrates. The resulting two components correspond to the y and x components of the signal in phasor representation. We can then use this to obtain not only the original signal amplitude R, but also the phase difference ϕ between the signal and the reference.

$$R = \sqrt{x^2 + y^2} \qquad \phi = \tan^{-1}\frac{y}{x}$$

If phase measurement is an important consideration in your experiment, try to set the phase angle to about 45° so as to minimize the effect of small errors in x or y.

Experimental Procedure

1. Begin by checking the alignment of the masses on the wire, as they can easily be knocked out of position. There should be *pairs* of masses,

one large and one small, in keeping with the idea that this is a one-dimensional "crystal" of some material. The masses should be at a uniform spacing of 15 cm or more, and the supports at the ends of the wire should be located half this spacing from the nearest mass. The tension in the wire should be as high as the wire can safely bear, so that the frequencies are higher and the time constant on the lock-in can be correspondingly shorter.

2. Align the driving and detection coils so that they are directly below (about 1-2 mm) the first and last masses. The detection coil (the one that looks suspiciously like an electric guitar pick-up) should be attached to the 'A' input of the lock-in amplifier, and the driving coil should be attached to the 'sin out' frequency output.

3. Rather than sweeping the frequency by hand (a somewhat lengthy and boring process) we will be using LabView to control the lock-in amplifier, via a GPIB interface.

   Start LabView, and load frequency-sweep.vi from the shared directory. Adjust the program settings to the desired values: I recommend a sweep range of 1–200 Hz, 1000 points, a time constant of at least 300 ms, and a time interval between frequency steps of several times the time constant. The sensitivity required will depend on the exact spacing between the coils and the wire, but 200 μV is a good first guess. Set the driving amplitude to 5.00V.

   The driving coil attracts the wire twice per cycle, not once, so the driving frequency that the wire sees is actually *twice* the driving frequency generated by the lock-in. For this reason, set the harmonic number to 2. This makes the lock-in look at the amplitude of the $2f$ signal rather than f.

   Make sure that the lock-in displays and reports R and θ rather than x and y. This is the default behavior for the program, but worth checking anyway.

4. Run the scan. This takes awhile, so find something useful to do while you're waiting. Save the data when the sweep is complete.

5. Plot amplitude *vs* Frequency, and observe the gap between the first and second clusters of frequency peaks. Note that the lock-in will report spurious peaks at multiples of 60 Hz, due to pick-up of the AC mains and related harmonics — ignore these peaks in your analysis.

6. From the graph in step 5, extract ω and K data. the first resonance peak is the fundamental, the next the first harmonic, etc. from the length of the wire and the harmonic number, you can obtain the wavelength λ and thus wavenumber K. Remember that the driving frequency at the wire is twice the frequency reported by the lock-in amplifier.

   Plot ω *vs* K. Note the frequency gap at $K = \frac{\pi}{a}$. Make a qualitative comparison to the plot of energy *vs* K in your textbook.

Instructor's notes

This lab, as written, uses a lock-in amplifier (LIA). This is a rather expensive bit of equipment, but it can be used for many applications in numerous fields of research.

One could presumably do this experiment with a spectrum analyzer or other tool to make a plot of amplitude v. frequency. It has also been done by hand, determining the resonances by looking at the amplitude of an oscilloscope trace, but I would not wish this on anyone.

Equipment Sources

Lock-in amplifier The best ones are made by Stanford Research Systems.

`http://www.thinksrs.com`

My personal favorite is the SR850, but the SR830 is an excellent choice for this experiment and many others.

`http://www.thinksrs.com/products/SR810830.htm`

Signal Recovery also makes a good digital LIA, the 7225.

`http://www.signalrecovery.com/7225.htm`

While not as good as the SR830 at higher frequencies,[1] it is quite adequate for this experiment, and costs about half as much as the SR830.

Do make sure that whatever LIA you purchase allows GPIB control.

Wire It has to be ferromagnetic, for obvious reasons. The best signal is obtained using soft iron wire, usually sold as "stovepipe wire" in a hardware store. Steel wire, such as what I used in the workshop, works with a good pick-up coil and allows more tension, but some steels are not particularly magnetic...

Weights Fishing weights purchased from the local fly-fishing shop. Avoid the "removable" weights with the extended tabs, such as the ones sold at Walmart: the asymmetry of the tabs allows significant torsional modes, which cause no end of confusion.

[1] The Signal Recovery LIA's, as of 1999–2000 or so at least, claimed to operate at frequencies of up to 120 kHz. The Stanford Research Systems LIA's go only to 102 kHz. However, the Signal Recovery models actually only go to 60 kHz, and then look at the second harmonic for 60-120 kHz. This increases the noise level significantly in the higher frequency range. The process of discovering, isolating, and working around this bit of chicanery on their part delayed my Ph.D by about two months. Not that I am bitter.

Drive coil I used a solenoid coil salvaged from a 8.5” floppy drive. (Yes, we have some OLD equipment in our back storage room!) The exact details are not the least bit critical, it just needs to be a coil of some sort.

Pick-up coil You can spend a lot of time winding a great pick-up coil. I did. When you’re done, call the local music store and see if they have any spare electric-guitar pickups. I bought one for $10, and it increased the signal/noise ratio by a factor of 5–10 or so. Get a “humbucker” pickup if it’s available, as they pick up less 60-cycle AC noise.

Hardware Lab clamps, rods, hanging masses, cables, etc... All standard lab hardware.

Figure 2: Photograph of the driver-end of the wire

Figure 3: Photograph of the receiver-end of the wire

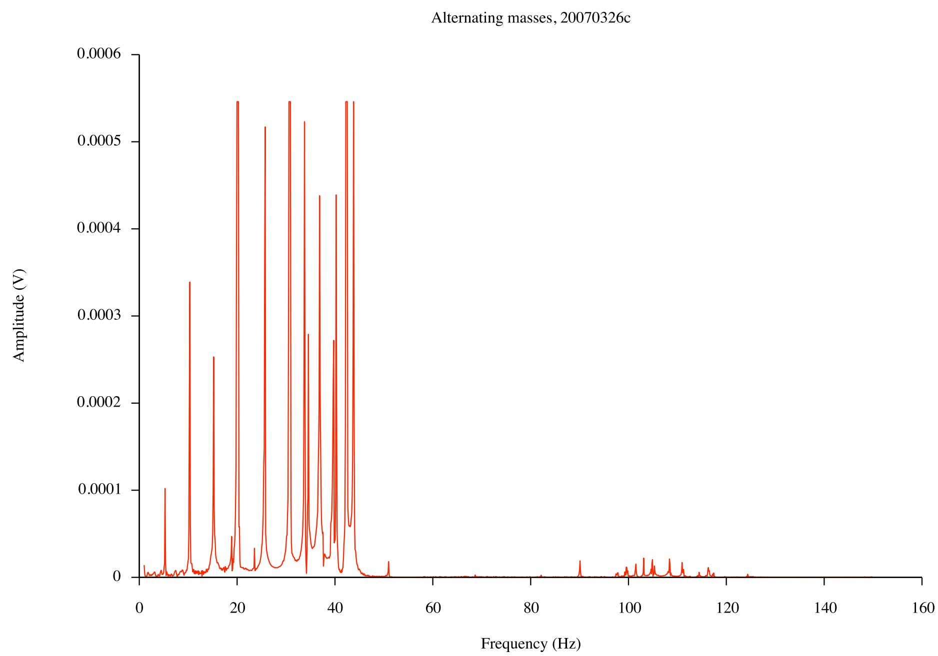

Figure 4: Frequency response of the "one-dimensional crystal". Note that the frequency scale is the *driving* frequency to the excitation coil: the frequency of the wire is twice this value.

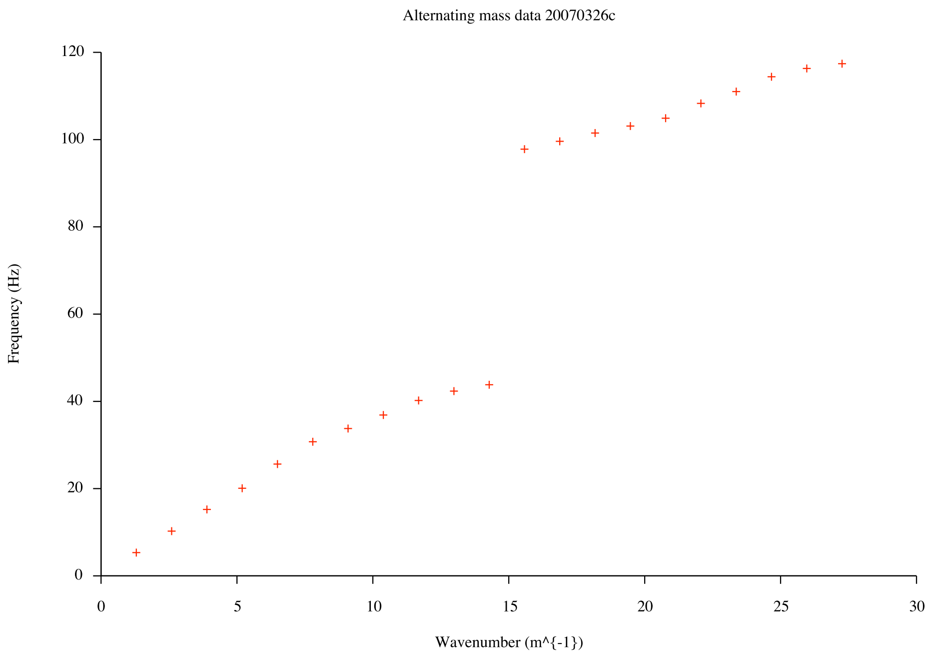

Figure 5: Plot showing actual modes, with bandgap

Bibliography

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[2] Dietrich Lüerßen. A demonstration of phonons that implements the linear theory. *American Journal of Physics*, 72(2):197–202, Feb 2004.

[3] Paul Allan Tipler and Ralph A. Llewellyn. *Modern Physics*. W. H. Freeman, 4^{th} edition, 2004.