

A demonstration of phonons that implements the linear theory

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Beads on a vibrating wire are used to simulate the discrete structure of a solid-state material. The novel idea of the experiment is to use very small oscillation amplitudes of the wire to avoid nonlinearities in the interaction. We achieve a good signal-to-noise ratio using a lock-in technique. We find quantitative agreement between theory and experiment for not only a mono- and a diatomic chain, but also for the bare wire. The latter agreement is the crucial aspect that distinguishes our experiment from previous ones. This agreement assures that the fundamental assumption of the theory (Hooke's law) is satisfied. We show that the properties of phonon dispersion curves are not special, and that the same band structures occur when the wavelength of any wave becomes comparable to the length scale of a discrete periodicity. © 2004 American Association of Physics Teachers. [DOI: 10.1119/1.1625923]

I. INTRODUCTION

Lattice vibrations are covered to some extent in every textbook on solid state physics.^{1–3} They are important for understanding phenomena as diverse as the specific heat and the inelastic scattering of neutrons. Because the underlying phenomena and calculations are entirely mechanical in nature, the treatment of lattice vibrations also provides a relatively simple means of introducing the concepts of energy bands and forbidden gaps.

The theoretical tool of a linear chain calculation⁴ is covered in classical mechanics textbooks because students have a good background in mechanics at this point, and the calculations that lead to the solution are familiar. More important, this tool is invaluable for many applications, for example, the calculation of phonon dispersion curves in crystals. For more advanced students, the theoretical tools provided by quantum mechanics can be successfully used to describe the behavior of waves in macroscopic, periodic media, and detailed band structures can be calculated.⁵

It is helpful for students to not only see the theoretical derivation of, for example, phonon dispersion curves in the classroom, but also to do some associated experiments. In the past, there have been several efforts to visualize lattice vibrations in large-scale demonstrations.^{6–9} However, there is one aspect that has not been addressed satisfactorily in Refs. 6–9. Although the theory relies on the assumption that the interaction between adjacent beads/atoms is linear, earlier demonstrations either do not check the linearity of the interaction or show explicitly that the interaction is not linear. In the following, we propose a demonstration that shows explicitly that the interaction is linear and in accordance with the fundamental assumption of the theory.

If the subject of lattice vibrations is introduced properly, students can obtain additional insight into complex phenomena such as the behavior of a single electron in a periodic potential as well as photonic band gaps¹⁰ and acoustic crystals.¹¹ The underlying idea of all these phenomena is that the wavelength of the excitation is comparable to the length scale of the periodicity of the medium in which the wave travels. We can start from a familiar experiment (for example, standing waves on a string), and then impose a periodicity comparable to the wavelength on the system. The transition from the familiar dispersion relation to one that shows the bending of the dispersion relation and band gaps

present in lattice vibrations can help students realize the fundamental concept that leads to these features: a spatial periodicity that is comparable to the wavelength of the excitation. In addition, other interesting phenomena such as disorder-induced localization of wave packets (Anderson localization) can be realized.^{9,12,13}

The demonstration we propose specifically addresses the transition from the linear dispersion relation to a more complicated one. The expected proportionality between frequency and wave number for a simple stretched wire is found in our experiment. This agreement ensures that the foundation for both the theory and the demonstration is the same, and that we can therefore expect reasonable consistency between theory and experiment for the complex cases that can be studied, of which only a few are explored in this paper.

Some of the pedagogical uses of the experiment are that it can be used to show the difference between a linear and nonlinear dispersion relation, the cut-off frequency of a linear chain, and the forbidden gap for a diatomic lattice. It is best used in an advanced undergraduate laboratory setting. In addition, the experimental setup is of potential interest in undergraduate research projects.

II. THEORY

The properties of phonons are usually introduced using a model that is based on two assumptions: (1) The interaction between neighboring atoms is based on Hooke's law: the force is proportional to the displacement of the atoms. (2) Only the interaction between adjacent atoms is taken into account. In addition, the "springs" that connect the atoms are assumed to be massless.

The benefits of this theoretical approach for lattice vibrations are easy to see. First of all, these assumptions lead to simple solutions for the phonon dispersion relation $\omega(k)$ which are in qualitative agreement with phonon dispersion curves measured in real crystals. For the purpose of the demonstration proposed in this paper, there is a second and often overlooked benefit: students are already familiar with the continuous case (vibrations of a stretched string), and they will be able to verify that the first assumption is satisfied in the demonstration.

We will consider only one polarization of the transverse

waves. Hence, the number of modes is reduced by a factor of 3 in comparison with a solid, where there are one longitudinal and two transverse modes.

The resonance frequencies ω of the system are extracted from the measured data. They are then paired with the corresponding wave vector k to obtain the dispersion relation $\omega(k)$. The wave vectors are calculated knowing the geometry of the experimental setup. For a stretched string (continuum) of length L , they can be found easily. The allowed wave vectors are given by

$$k_n = \frac{\pi}{L} \times n, \quad n = 1, 2, 3, \dots, \quad (1)$$

where the integer n does not have an upper limit.

If the bare string is loaded with beads made of split shot (a special kind of fishing lead) with a well-checked periodicity, we call this arrangement a “uniformly loaded string.” This uniformly loaded string can be used to simulate vibrations of, for example, a crystalline lattice. For such an arrangement, we want to look at vibrations that can be distinguished from each other by looking only at the amplitudes of the individual beads in contrast to looking at the string.¹⁴ Consequently, the number of beads gives the number of vibrational patterns that can be distinguished, and the wave vector has an upper limit. For N identical beads with spacing (lattice constant) a , the wave vectors k can be expressed as

$$k_n = \frac{\pi}{L} n = \frac{\pi}{(N+1)a} n, \quad n = 1, 2, 3, \dots, N. \quad (2)$$

If there is more than one bead per unit cell, some of these wave vectors are degenerate. If the number of beads in the unit cell is p , and if N is an integer multiple of p , the wave vectors within the first Brillouin zone are still given as in Eq. (2). The only change is that n has the upper limit N/p . For each wave vector there are p corresponding resonance frequencies.

The restriction of a uniformly loaded string is important in order to calculate the wave vectors. If disorder were present, there would be localized vibrational modes (Anderson localization).^{9,12,13} These localized modes cannot be modeled using simple normal modes. The wave profile is then a linear superposition of more than one normal mode, and the concept of one single wave vector per resonance frequency breaks down.

The three examples we will consider are the bare string, a monatomic lattice, and a diatomic lattice. For the bare string, the dispersion relation is given by

$$\omega(k) = \sqrt{\frac{T}{\mu}} k, \quad (3)$$

where μ is the mass per unit length of the string and T is the tension in the string.

For a string loaded uniformly with one type of beads (monatomic lattice), the dispersion relation is given by

$$\omega(k) = \sqrt{\frac{4T}{ma}} \left| \sin\left(\frac{1}{2} ka\right) \right|, \quad (4)$$

where m is the mass of the (identical) beads. In the limit of long wavelengths, the dispersion relation reduces to that of the simple string:

$$\lim_{k \rightarrow 0} \frac{d\omega(k)}{dk} = \sqrt{\frac{4T}{ma}} \frac{1}{2} a = \sqrt{\frac{T}{m/a}}. \quad (5)$$

If we assume that the string is massless, and if the mass density μ is identified with m/a , then the group speeds are identical for the bare string and the monoatomic lattice.

For the “diatomic lattice” (two different bead masses, string loaded uniformly), there are two solutions for the dispersion relation corresponding to the acoustic and the optical branch of the dispersion relation:

$$\omega^2(k) = \frac{2T}{a} \left(\frac{1}{m} + \frac{1}{M} \right) \left[1 \pm \sqrt{1 - \frac{4mM}{(M+m)^2} \sin^2(ka)} \right]. \quad (6)$$

In Eq. (6), M and m are the masses of the two beads (atoms). The two branches are separated by a gap, the size of which is determined by the square root of the ratio of the two masses.

There are two important properties that need to be discussed with students:

- (1) The word “linear” is used in two different contexts. The *interaction* is always linear, meaning that the displacement is proportional to the force. The *dispersion relation* can be linear (bare string) or nonlinear (loaded string).
- (2) The only reason for the change of the dispersion relation from linear to nonlinear is that the wavelength of the excitation becomes comparable to the periodicity of the experiment.

The dispersion relation of a simple string is linear, and the frequency is proportional to the wave vector. But as soon as the medium is discrete (for example, if beads are added) and the wavelength of the excitations is comparable to its periodicity, the dispersion relation becomes nonlinear and shows features such as band gaps or localization. However, the interaction between the beads is still linear. Band gaps and nonlinear dispersion relations are not only present for vibrational waves in crystals and on wires, but also for electrons in metals and semiconductors, electromagnetic waves in photonic crystals, and acoustic waves in sonic crystals. On the other hand, if the wavelength is much larger than the periodicity, the dispersion relation of the systems with and without beads is identical [see Eq. (5)].

There may be circumstances that require a more sophisticated theory, for example, when the string tension changes because of large oscillation amplitudes.⁹ The force is then no longer linearly dependent on the displacement. This nonlinearity of the response has nothing to do with the nonlinearity of the dispersion relation which occurs even for a linear interaction. An excellent overview of different ways to account for nonlinear interactions can be found in Ref. 9.

III. EXPERIMENTAL SETUP

There are many experiments that demonstrate the phonon properties of solids. Most demonstrations focus on one dimension,^{6,8,9} but there also are experiments for two-dimensional systems.⁷ In these experiments, either the assumption of a linear interaction between adjacent “atoms” cannot be demonstrated, or the assumed linear dispersion relation shows nonlinear behavior.⁹ When using such a demonstration as a teaching tool, the discussion becomes difficult if students ask questions such as: “If there already is a discrepancy between the theory and the demonstration for the

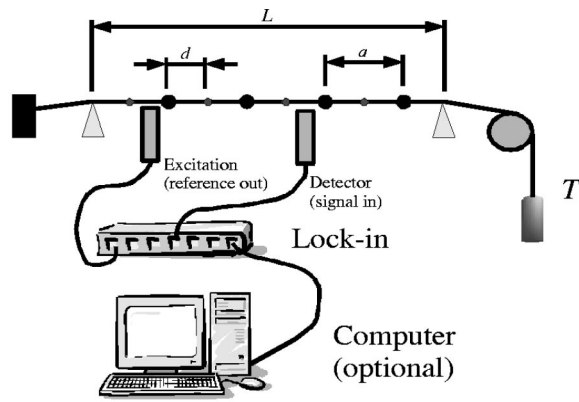


Fig. 1. Schematic of the experimental setup. A wire is stretched over two knife-edges with a well-defined tension. This force is achieved through a mass that is attached to the wire via a pulley. At the core of the experiment is a lock-in amplifier that provides both the frequency for the magnetic driver and the signal detection with a low noise level. Computer control of the experiment is possible but not necessary.

simple case, how can we be certain that the experimental results for the more complex case are meaningful?"

Our experimental approach displays quantitative agreement between theory and experiment for both the simple and the complex cases. This agreement makes it easier to understand the results of the demonstration and allows one to focus on the challenge of understanding why the lattice vibrations have their specific properties.

To study the vibrations of a wire, we stretch the wire over two knife-edges using a hanging mass (Fig. 1). The distance between the two knife-edges is the effective length of the wire L and determines the possible vibrational normal modes of the wire through the boundary conditions. This wire can be loaded with additional masses, for which we use split shots. The spot beads are fishing accessories that can be bought in different sizes from a sporting good store.

To excite and detect the vibrations of the wire, we use a pair of magnetic transducers (PASCO, WA-9613 driver and detector). A lock-in amplifier (Stanford Research SR-830) is not only used to obtain a reliable signal with very little noise, but also to provide the time varying voltage for the excitation via the internal oscillator output. The use of the lock-in amplifier for the signal detection allows the use of small amplitude oscillations to minimize nonlinearities.

The use of the magnetic transducers requires additional thought about the excitation and the detection of the vibrations of the wire. If the driver is supplied with a sinusoidal voltage, it attracts the wire for positive as well as for negative voltages. Hence, the wire is not excited at the frequency f_1 of the driving voltage, but at $2f_1$. Accordingly, the detection frequency of the lock-in amplifier needs to be set to the second harmonic of the frequency of the internal oscillator.

The setup can be operated at several levels of automation. The easiest use of the setup involves nothing else but manually changing the frequency and adjusting the sensitivity of the lock-in amplifier, and reading and writing down the resonance frequencies based on the observed amplitudes. In this way, students can see the dramatic effect of a resonance and can obtain a good feeling for the signal-to-noise ratio. This procedure is most useful for studying the eigenfrequencies of the individual modes.

In a more sophisticated setup, we use a computer to control the lock-in amplifier via a serial interface, allowing us to

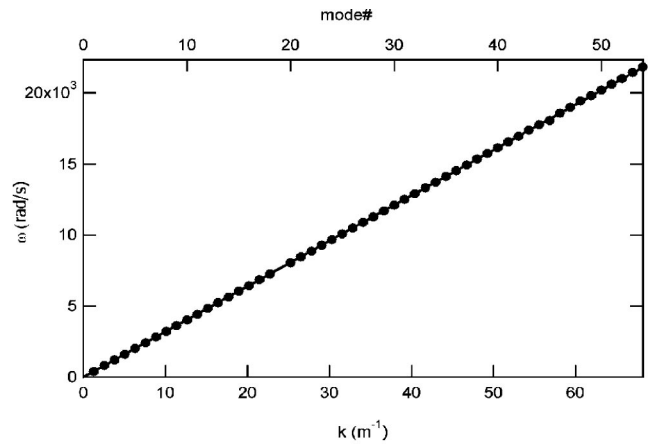


Fig. 2. Plot of the dispersion relation for a simple stretched wire. The proportionality between the wave number and the angular frequency agrees with theory. This linear relation might hold for frequencies higher than what are shown, but no measurements were taken for higher frequencies.

automate the entire experiment. We are able to scan a specifiable frequency range and record the amplitude and phase of the oscillation while averaging several measurements. This procedure also allows us to obtain their respective uncertainties. Also the line shape of the resonance curves can be studied, and the phase shift at the resonance can be analyzed.

For the automation, we use the software package DDDA from Stanford Research. The data collection program was written in the programming language provided by this software. The source code and programming tips are available on the authors' website.¹⁵

IV. SAMPLE RESULTS AND ANALYSIS

As mentioned, the crucial point we want to show is that the results for the bare string are in agreement with theoretical predictions, that is, the vibrational frequency ω_k and the wave number k are proportional. This relation can be expressed in terms of the mode number n :

$$\omega_n = \frac{\pi}{L} \sqrt{\frac{T}{\mu}} n. \quad (7)$$

The tension was chosen to be $T = 58.8 \text{ N}$, the length of the wire was measured to be $L = 2.486 \text{ m}$, and the mass per unit length, μ , was determined by a fit to the data (Fig. 2). We found $\mu = (5.7573 \pm 0.0014) \times 10^{-4} \text{ kg/m}$. For the steel wire that we used in the setup (diameter $0.30 \pm 0.01 \text{ mm}$) this value corresponds to a density $\rho = (8100 \pm 500) \text{ kg/m}^3$, which agrees quantitatively with tabulated values¹⁶ (between $\rho = 7700 \text{ kg/m}^3$ for chromium steel and $\rho = 8130 \text{ kg/m}^3$ for nickel steel).

From Fig. 2 it is clear that the proportionality between ω and k is strictly maintained up to an angular frequency $\omega \approx 1.8 \times 10^4 \text{ rad/s}$, the largest frequency we measured. The mode number is as high as $n = 53$, which corresponds to a wavelength $\lambda < 10 \text{ cm}$. This wavelength is less than half of the distance between two adjacent beads in the other experiments we will show. It is therefore sufficient to show that the interaction is linear for all wavelengths that will be used later.

The uncertainty of the linear fit parameter $\sqrt{(T/\mu)}$ is $(319.58 \pm 0.08) \text{ rad/s}$ is a mere 0.025%. This result is very

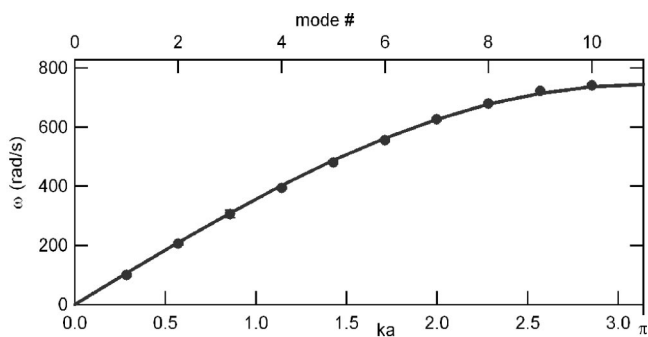


Fig. 3. Measured data for the resonance frequencies vs the calculated wave vectors of the normal modes for a monoatomic chain with 10 beads. The continuous line is the result of a fit using Eq. (9).

different from the one reported in Ref. 9, where a significant curvature of the dispersion relation of the bare string was found because of a change in the tension T . This change in the tension is due to the large amplitudes at which the string had to be driven to obtain reliable results. Here, using a lock-in amplifier, we were able to avoid this effect because the detection technique permits us to use very small vibrational amplitudes and still obtain a good signal-to-noise ratio.

We next loaded the string with the split shot beads. We studied both mono- and diatomic lattices (Figs. 3 and 4, respectively). From these graphs it is obvious that the data can no longer be fit by a linear function. It should be pointed out to students that this difference is due only to the periodicity that is imposed by the beads: nothing else about the experiment has changed.

For the monoatomic and diatomic lattices, the cut-off wave number $k_a = \pi/a$ of the first Brillouin zone is finite. Here, the lattice constants are $a = 22.6$ and 45.2 cm, respectively. They are the smallest lengths over which a spatial periodicity is observed. For the bare string, k_a is virtually infinite in comparison with the monoatomic and diatomic lattices because the lattice constant of the atoms in the wire

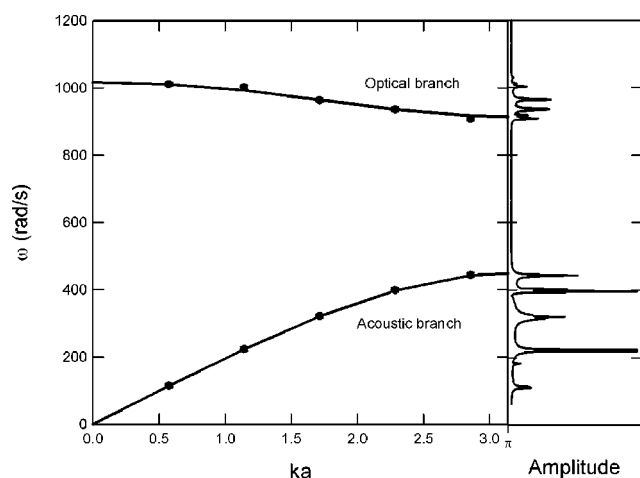


Fig. 4. Left: Measured data for the resonance frequencies vs the calculated wave vectors of the normal modes for a diatomic chain with 5 bead pairs. The continuous curve is the result of a fit using Eq. (10). The fitted curve represents the data well. To find the fit, only two parameters were varied, and the fitting was done for both branches of the dispersion relation simultaneously. Right: The measured amplitude of the oscillation at one detector location as a function of the angular frequency. The band gap can be observed between 400 and 900 rad/s, where the oscillation amplitude is zero.

is about seven orders of magnitude smaller. The curvature of the dispersion relation toward a horizontal slope due to Bragg reflection occurs at the edges of the Brillouin zone. That is, the deviation from linear dispersion is noticeable only when the wavelength is comparable to the lattice constant. Because the measured wavelengths are much larger than the interatomic distance, we could not observe any evidence of this curvature in our data for the bare string; however, we could observe this curvature for the loaded string.

To demonstrate a monoatomic chain, we used 10 beads with an average mass $\bar{m} = (1.860 \pm 0.003)$ g, lattice constant $a = 22.6$ cm, and tension $T = 58.8$ N. We fit the measured dispersion relations using the function

$$\omega = A \sin\left(\frac{\pi}{2} \frac{n}{11}\right), \quad n = 1, 2, \dots, 10. \quad (8)$$

We found that $A = (744.6 \pm 2.5)$ rad/s, which is in reasonable agreement with the expected value $\sqrt{4T/ma} = (748.0 \pm 0.5)$ rad/s. The slight difference between the two values can be explained by taking into account that the wire is not massless. The quality of the fit to the experimental data can be confirmed in Fig. 3. There is no notable discrepancy between theory and experiment.

For the diatomic chain, the beads had average masses $\bar{M} = (2.53 \pm 0.02)$ g and $\bar{m} = (0.553 \pm 0.002)$ g. Five beads of each kind were used to obtain a lattice constant of $a = 45.2$ cm, which was chosen to maintain the same bead positions as in the monoatomic setup. The tension also was kept constant.

As fitting functions for the optical and acoustic branch of the dispersion relation, we used

$$\omega_{a/o} = \sqrt{A \left[1 \pm \sqrt{1 - B \sin^2\left(\frac{\pi}{2} \frac{n}{5.5}\right)} \right]}, \quad n = 1, 2, \dots, 5, \quad (9)$$

which corresponds to Eq. (6). We fitted the optical and acoustic branches simultaneously because the fit parameters A and B are identical for both branches. We found $A = (5.175 \pm 0.023) \times 10^5 \text{ rad}^2 \text{ s}^{-2}$ and $B = (0.626 \pm 0.007)$. The error for both A and B is 1% or less. The quantitative agreement between the data and the fit is very good, and we conclude that Eq. (4) represents the measured data well (see also Fig. 4). In the inset of Fig. 4 we show a sample measurement of the amplitudes versus the angular frequency. The meaning of the term “forbidden gap” is clear here because the amplitude trace is flat between about 400 and 900 rad/s.

Even though the shape of the fit function allows one to model the data with great precision, there is a slight discrepancy between the fitted parameters A and B , and their equivalents that can be calculated from known parameters (tension, bead masses, and lattice constant). This discrepancy is summarized in Table I. However, the discrepancy can be lifted if the assumption of a massless string is not made. The masses of the beads in Eq. (6) can be replaced by effective bead masses. These effective masses can be calculated from the fit parameters A and B and can be compared with a corrected bead mass. The lower limit for the corrected bead mass is its measured mass, and the upper limit is the sum of the bead mass and the mass of the string between two adjacent beads (here, $\mu a/2 = 0.13$ g). The results of this analysis are summarized in Table I and show that there is quantitative agreement

Table I. From the masses of the beads on the string (second and third columns), the characteristic parameters of the dispersion relation (last two columns) can be calculated and vice versa [the conversion is $A = (2T/a) \times (1/M + 1/m)$ and $B = (2T/a)(1/M + 1/m)$], with the experimentally given parameters $T = 58.8$ N and $a = 45.2$ cm. The measured/fitted parameters are in *italic*, while the calculated ones are not *italic*. This comparison provides an important diagnostic tool for the comparison of experiment and theory: although the fitted curve can represent the data well, there still does not have to be quantitative agreement between the measured bead masses and the ones calculated from the fit parameters. Only if we consider that the string has a mass of 0.13 g between two adjacent beads and allow for this additional mass in the calculation is there quantitative agreement between the fit parameters and the theoretical prediction (compare the lower two rows).

	M (g)	m (g)	A (from the fit) ($10^5 \text{ rad}^2 \text{ s}^{-2}$)	B (from the fit)
Measured bead masses	<i>2.53 ± 0.02</i>	<i>0.553 ± 0.002</i>	<i>5.733 ± 0.025</i>	<i>0.589 ± 0.002</i>
Fit	2.59 ± 0.03	0.624 ± 0.005	5.175 ± 0.023	0.626 ± 0.007
Bead and wire mass	2.60 ± 0.09	0.62 ± 0.07	5.2 ± 0.4	0.62 ± 0.05

between the effective bead masses and the corrected ones. This agreement is important because the same assumption (linear interaction) was used in the theory and the experiment and leads to quantitative agreement. This agreement confirms that also the second assumption of the theory (next-neighbor interaction) is valid.

One point still needs to be addressed: the comparison of the vibrational patterns of the atoms between theory and experiment. Because the amplitudes of the vibrations are intentionally very small, we cannot observe the oscillations visually. But the lock-in amplifier can record the *phase* of the signal in addition to the amplitude. The phase can be used to determine the vibrational profile of the string if the detector is placed close to each of the beads along the string.

To illustrate how we can find the vibrational pattern of the beads from a measurement of the phase of the oscillation relative to the driving frequency, we use the simple example of just two beads on the string. The expected vibrational patterns are easy to sketch (see Fig. 5). The two beads will either vibrate in phase (low frequency and longer wavelength) or out of phase (higher frequency and shorter wavelength).

Figure 6 shows the measured response of the phase and amplitude versus frequency for both beads. At the lower frequency, ω_1 , it can be clearly seen that both beads oscillate in phase and behave identically. They also oscillate in the way that is expected for any mechanical system close to a resonance: at the resonance frequency, there is a phase shift of 180° .

Near the frequency ω_2 , the two beads have a phase difference of 180° , which means that the beads are always on opposite sides of the equilibrium position. From Fig. 5 we can see that for higher frequencies (shorter wavelengths), this change in the relative phase could have been expected.

With more beads, the phase shift for all the beads can still be predicted easily from the sketches of the vibrational pattern of the string for all eigenfrequencies of the string. As preparation before using this demonstration, students could be asked to draw these sketches and predict the phase shifts for all beads relative to one reference bead (which in the experiment would be the one closest to the excitation and therefore always in phase). If in the experiment the phase

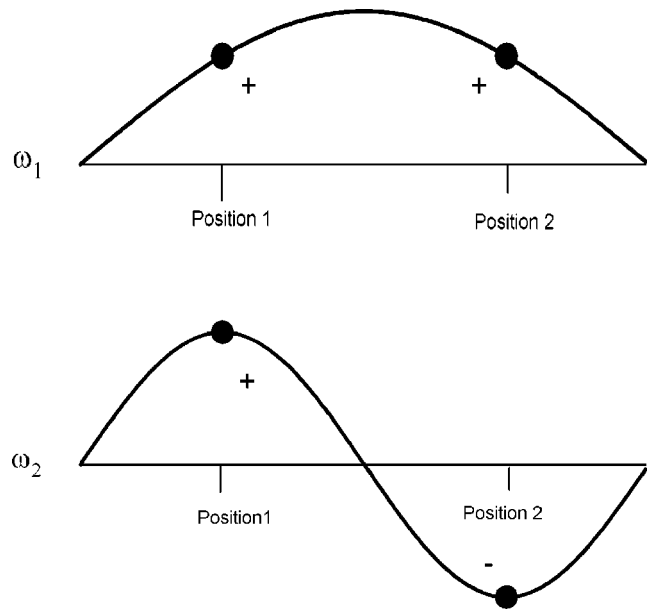


Fig. 5. Sketches of the modes on a string with 2 beads. With the positions of the beads marked on the profile of the string, it can be easily seen for different wavelengths if the beads are oscillating in or out of phase.

shifts are in agreement with the sketches, we can be certain that we have observed the normal modes of a perfectly ordered system. If, however, there were a slight disorder in the bead positions, the normal modes can be distinguished from localized ones because the amplitude and phase characteristics of the waveform are different, and sketches like Fig. 5 (using sinusoidal waveforms) are representations of the normal modes only.

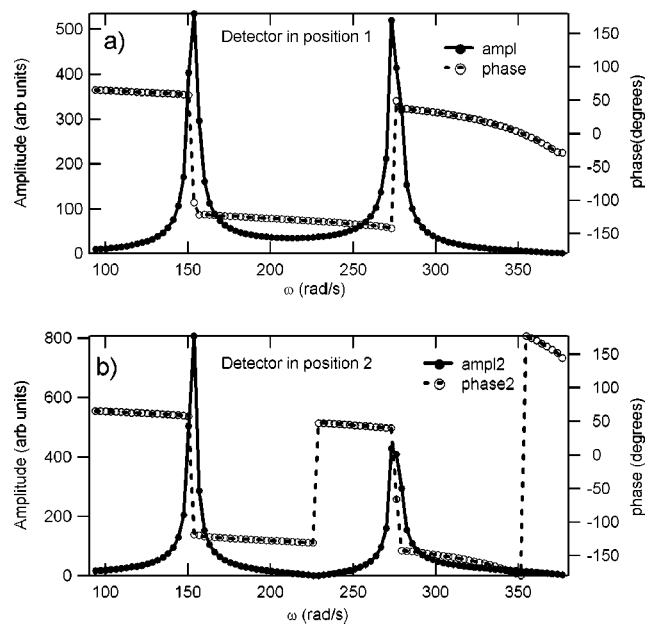


Fig. 6. Data corresponding to the loaded string shown in Fig. 5. (a) The detector is placed at the position of bead 1; (b) the results of the detector at position 2. It can be seen that for the lower frequency the oscillation is in phase and is out of phase for the higher frequency.

V. CONCLUSION

We have discussed an experiment that is useful for teaching undergraduate students the concepts of band gaps and nonlinear dispersion relations. The novel feature of our demonstration is that the assumption of Hooke's law can be experimentally validated. The demonstration can be set up with relative ease because of its simplicity. The experiment can be used to emphasize that band structures with nonlinear dispersion relations and band gaps are not unique features of vibrations in crystals, but can occur whenever the wavelength of an excitation becomes comparable to the length scale of a discrete periodicity in the medium in which the wave travels.

It has not been discussed here, but the setup also can be used to show Anderson localization in weakly disordered media, the influence of stacking faults in an otherwise perfect crystal, and the phenomenon known from superlattices and quantum wells that "confined" optical phonons are not really confined in their respective layer, but penetrate into the barriers.

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