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Low-frequency dispersion of phonons in one-dimensional chains

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Abstract

The wave velocity of long-wavelength acoustic phonons is found in one-dimensional crystals with an arbitrary basis by an elementary argument founded upon the equality of kinetic and potential energies in a linear wave. This argument also extends to quasiperiodic crystals such as those based on the Fibonacci sequence. Inspired by recent experiments, these ideas are then applied to an artificial quasicrystalline transmission line made by coupling electromagnetic cavities in a Fibonacci sequence.

Keywords: phonons, sound velocity, quasicrystals, resonant cavities, Fibnacci sequence

(Some figures may appear in colour only in the online journal)

1. Introduction

The problem of the normal modes of a one-dimensional crystal with a two-atom basis is a classic one in the undergraduate and first-year graduate curricula. Typically, it is seen in the first course on solid state physics [1–4], but may be encountered as part of classical mechanics also. Several universal features emerge from this study, including optical and acoustic phonons separated by a gap at the band edge, and a linear dispersion relation for long-wavelength acoustic phonons:

$$\omega = \bar{v}k \qquad (k \to 0). \tag{1.1}$$

Here k and ω are the wavevector and angular frequency of the wave, and the ratio $\bar{v}$ is naturally identified as its (group and phase) velocity.

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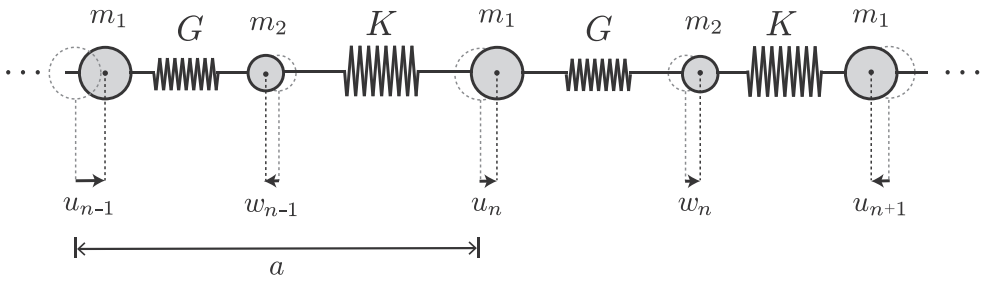

Figure 1. A one-dimensional lattice with a two-atom basis, showing two types of atoms (solid circles) connected by two types of springs. The equilibrium positions of the atoms are shown as dashed circles.

This note is concerned with this last aspect, i.e. the limited issue of the long-wavelength dispersion of acoustic phonons. The formula for $\bar{v}$ is readily found for the monatomic chain consisting of identical atoms connected by nearest neighbour springs, and many textbooks note that $\bar{v}$ is the same as the velocity of sound. It takes a little more effort to find $\bar{v}$ for the diatomic chain, but now the connection with the sound velocity is made only by some authors (see, e.g. [4]). This is as it should be, since phonons are central to a large number of phenomena in solids that are more deserving of the authors' attention. However, the quantity $\bar{v}$ is an important physical property. In addition to the speed of sound, it is also relevant to the low-temperature Debye specific heat and the lattice thermal conductivity. Any investigation of its general character is therefore worthwhile.

Our analysis surely cannot be new, but we present it for three reasons. First, we have been unable to find it in any of the common textbooks in current use, or the major journals of physics pedagogy. Second, it applies to a periodic crystal with any number of atoms in the basis, and also to quasiperiodic crystals such as a Fibonacci sequence. Finally, the argument based on equating the kinetic and potential energies in a linear wave is a powerful one, worth knowing. Feynman uses it to great effect, for example, to find the dispersion relation for plasma oscillations in a degenerate electron gas [5][2].

We present the (well-known) answer for the diatomic chain in section 2. The polyatomic chain is discussed in section 3, where we give our main physical argument. We apply this argument to the quasiperiodic Fibonacci chain in section 4. We also explain our interest in this problem stemming from a study of a Fibonacci sequence of electromagnetic cavities, and the connection between the cavity and phonon problems.

2. Diatomic basis

We consider an infinite periodic chain of two types of atoms of mass m_1 and m_2, connected by springs with alternating spring constants K and G. The lattice constant is a (see figure 1). If the displacements of the atoms are taken as shown in the figure, the equations of motion are

[2] To avoid misunderstanding we note that Feynman's dynamical model is incorrect. He uses a simplified hydrodynamic approximation for the potential energy from pressure variations ignoring Fermi statistics, which is inconsistent because even the $k = 0$ plasma frequency is much greater than the characteristic long-wavelength response frequency of a degenerate electron gas. A proper calculation of this energy is much more difficult, and was first done by Bohm and Pines [6]. Our point is only that equating the kinetic and potential energies in a linear wave is a nice methodological device, but of course one must be able to find these two energies in the first place. How well or easily that can be done depends on the problem at hand, and does not invalidate the device.

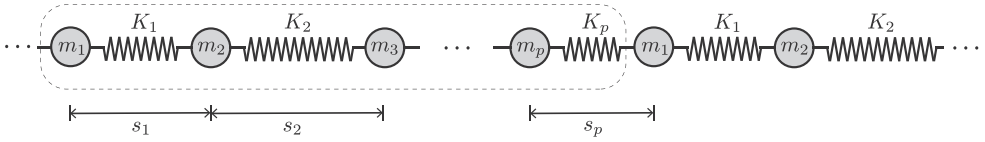

Figure 2. A one-dimensional lattice with a polyatomic basis. We show the atoms and the springs connecting them in their equilibrium positions only.

$$\begin{aligned} m_1\ddot{u}_n(t) &= G(w_n - u_n) + K(w_{n-1} - u_n), \\ m_2\ddot{w}_n(t) &= K(u_{n+1} - w_n) + G(u_n - w_n). \end{aligned} \tag{2.1}$$

These equations have wave solutions which may be conveniently sought using the complex exponential form

$$\begin{pmatrix} u_n(t) \\ w_n(t) \end{pmatrix} = \mathrm{Re}\begin{pmatrix} u \\ w \end{pmatrix} \mathrm{e}^{\mathrm{i}(kna - \omega t)}. \tag{2.2}$$

The subsequent analysis is standard, and yields the dispersion relation

$$\omega^2 = \frac{(m_1 + m_2)(G + K)}{2m_1m_2} \pm \frac{\left[(m_1 + m_2)^2(G + K)^2 - 16GKm_1m_2 \sin^2 \frac{1}{2}ka\right]^{1/2}}{2m_1m_2}. \tag{2.3}$$

The upper and lower signs give the optical and acoustic branches. For the latter, we find

$$\omega^2 \approx \frac{1}{(m_1 + m_2)(G^{-1} + K^{-1})}(ka)^2 \qquad (k \to 0), \tag{2.4}$$

from which $\bar{v}$ can be read off.

In addition to [1–4], special cases of the diatomic lattice are discussed in [7–9][3], containing proposals of undergraduate laboratory experiments to study analogs of phonons using either masses and springs, torsional oscillators, or electrical circuits.

3. Polyatomic basis

Next, we consider an infinite polyatomic chain, and label the atoms by a single index, n. The mass of the nth atom is m_n, and it is coupled to atom $n + 1$ by a spring of spring constant K_n and a relaxed length s_n. All these quantities repeat after a period p, i.e. $m_{n+p} = m_n$, etc (see figure 2).

It is useful to define the averages of the inverse spring constants, masses, and interatomic distances as

$$\langle K^{-1} \rangle = \frac{1}{p}\sum_{n=1}^{p} K_n^{-1}, \quad \langle m \rangle = \frac{1}{p}\sum_{n=1}^{p} m_n, \quad \langle s \rangle = \frac{1}{p}\sum_{n=1}^{p} s_n. \tag{3.1}$$

The lattice constant is thus $a = p\,\langle s \rangle$.

Let the displacement of the nth atom from its equilibrium position be denoted by u_n and let us consider a small-amplitude right-moving wave of wavevector k and frequency ω. In

[3] It should be noted that [9] does not discuss experiments with real inductors and capacitors, but only how such circuits may be simulated on a computer.

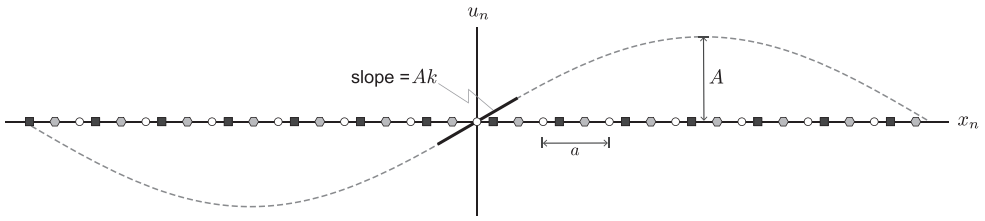

Figure 3. How the slope at the node of the waveform is related to the amplitude of oscillation for long wavelengths. The figure shows a snapshot of the envelope of the displacements u_n at some time, as a function of the equilibrium position x_n of the nth atom, measured from an arbitrary origin; for example, $x_n = \sum_{j=0}^{n} s_j$ with the origin at atom 0. A schematic of a three-atom basis crystal in its equilibrium state is shown on the x axis.

such a wave, all the u_n's vary harmonically at ω, and the equation of motion reduces to

$$-\omega^2 m_n u_n = K_n(u_{n+1} - u_n) - K_{n-1}(u_n - u_{n-1}). \tag{3.2}$$

We consider only long wavelengths, where $k \ll a^{-1}$. The limit $k = 0$ describes a rigid displacement of the entire chain in which all the springs stay relaxed, so there are no restoring forces and $\omega = 0$. It is then natural to expect that $\omega \to 0$ continuously as $k \to 0$, so we may plausibly assume, and will verify self-consistently[4], that $\omega \propto k$. With this assumption, let us examine how both sides of equation (3.2) must behave when expanded in powers of k. Since the left-hand side is $O(\omega^2) = O(k^2)$, the $O(k^0)$ and $O(k^1)$ terms on the right-hand side must separately add to zero. The $O(k^0)$ terms describe the rigid displacement discussed above, for which the relative displacement of neighbouring atoms, $u_{n+1}(t) - u_n(t)$, vanishes for all n, and the combination on the right vanishes automatically. This leaves the terms of $O(k)$. These will add to zero only if the relative displacements are inversely proportional to the spring constants K_n. Incorporating the harmonic time dependence, we thus find that, to $O(k)$

$$\begin{aligned} u_{n+1} - u_n &= \frac{Bk}{K_n}\cos\omega t, \\ u_n - u_{n-1} &= \frac{Bk}{K_{n-1}}\cos\omega t, \end{aligned} \tag{3.3}$$

where B is an arbitrary constant. (We stick to real forms for u_n from here on.) Setting $t = 0$ and adding together these compressions over an entire unit cell, we obtain

$$u_{n+p} - u_n = B\ k\ p\ \langle K^{-1}\rangle. \tag{3.4}$$

We now relate the constant B to the amplitude of motion of the atoms. As already discussed, to zeroth order in k, all the relative near-neighbour displacements, $u_{n+1} - u_n$, vanish. Thus, the amplitude of motion of all atoms is the same. If this amplitude is denoted by A, then using the physical meaning of the wavevector as the rate of advance of the phase with distance, the spatial slope of the waveform near a node is given by Ak in magnitude. This is illustrated in figure 3. Let us consider a unit cell centered on such a node with positive slope. Since $k \ll a^{-1}$, the displacement of the atoms varies linearly across the sites in this unit cell,

[4] If we assume other forms of the dispersion, $\omega \propto k^\alpha$ with $\alpha > 0$ but $\alpha \neq 1$, we get an inconsistency. If $0 < \alpha < 1$, the combination Bk in equations (3.3) and (3.4) must be replaced by $B'k^\alpha$, equation (3.5) stays as is, and we get an inconsistency at equation (3.6). If $\alpha > 1$, the argument goes through up to equation (3.9), and we get an inconsistency when we equate $\langle V\rangle$ and $\langle T\rangle$.

and the total compression over the cell is

$$Ak\sum_{n=1}^{p} s_n = Akp\langle s\rangle. \tag{3.5}$$

Equating this to (3.4), we get

$$B = \frac{\langle s\rangle}{\langle K^{-1}\rangle}A. \tag{3.6}$$

The final step is to consider the kinetic and potential energies in the wave. The instantaneous elastic energy in the spring between atoms n and $n+1$ is

$$\frac{1}{2}K_n(u_{n+1}-u_n)^2 = \frac{1}{2}\frac{B^2k^2}{K_n}\cos^2\omega t. \tag{3.7}$$

Likewise, the instantaneous kinetic energy of the nth atom is

$$\frac{1}{2}m_nA^2\omega^2\sin^2\omega t. \tag{3.8}$$

The time averages of these energies over one time period, per atom, are given by

$$\langle V\rangle = \tfrac{1}{4}B^2k^2\langle K^{-1}\rangle, \quad \langle T\rangle = \tfrac{1}{4}A^2\omega^2\langle m\rangle. \tag{3.9}$$

In a linear wave these must be equal. Using equation (3.6), we thus obtain

$$\omega^2 = \frac{\langle s\rangle^2}{\langle m\rangle\langle K^{-1}\rangle}k^2. \tag{3.10}$$

We have shown, as promised, that $\omega \propto k$, and found the wave speed as

$$\bar{v} = \frac{\langle s\rangle}{\sqrt{\langle m\rangle\langle K^{-1}\rangle}}. \tag{3.11}$$

Equation (3.11) reduces to equation (2.4) in the diatomic case [10][5] .It relates to the speed of sound as follows. In a three-dimensional elastic solid with compressibility κ and mass density ρ, longitudinal sound (or pressure) waves travel at speed

$$v_l = (\kappa\rho)^{-1/2}. \tag{3.12}$$

The density ρ is naturally associated with $\langle m\rangle/\langle s\rangle$ in our one-dimensional crystal. Likewise, a simple statics argument based on balance of forces shows that κ is associated with $\langle K^{-1}\rangle/\langle s\rangle$. These associations are valid even though our lattice is one-dimensional, since the one-dimensional argument can be adapted to three-dimensional crystals by taking all the atoms in a crystal plane perpendicular to the wavevector to move in sync with one another [2, 3].

4. The Fibonacci chain

In this section we consider a Fibonacci sequence of atomic masses and springs. (We do not consider general quasiperiodic sequences based on irrational numbers other than the golden

[5] These authors consider a triatomic chain, but give specific solutions only at $k = 0$ and the Brillouin zone edge. However, it is simple to find $\bar{v}$ from their general eigenvalue condition, equation (4). If we let $k \to 0$ and $\omega \to 0$, we obtain

$$(C_1C_2 + C_2C_3 + C_3C_1)(M_1 + M_2 + M_3)\omega^2 = C_1C_2C_3k^2a^2,$$

where the C_i's are near-neighbour spring constants, M_i are the atomic masses, and a is the lattice constant. (Note that the frequency ω is denoted W there.) This equation is easily seen to be the same as equation (3.11).

mean as the discussion adds little more physics.) What is the nature of vibrational waves in such a system? This, along with other model systems in which wave phenomena are expected to occur, is relevant to the phonon and electronic spectra of quasicrystals [11–13] and (perhaps surprisingly and not obviously) the faceting and roughening of their surfaces [14, 15]. Such problems were of great interest in the 1980s when quasicrystals were a novelty. Our own interest was sparked by recent experiments by Houck and coworkers at Princeton University [16]. They have fabricated superconducting microwave cavities in the form of coplanar two-dimensional waveguide segments that are connected in (small portions of) a Fibonacci sequence, making a nonuniform transmission line analogous to a coaxial cable. There are two types of cavities, with inductances, capacitances, and lengths L_a, C_a, and s_a, $a = \mathrm{L}, \mathrm{S}$, where the letters L and S stand for Long and Short. It should be noted that the names Long and Short are historical, and do not necessarily correspond to the actual lengths of the cavities. The distinguishing characteristic is that cavities of type L are more numerous, and in the infinite sequence would occur with a frequency τ^{-1} versus τ^{-2} for those of type S, where τ is the golden ratio

$$\tau = \frac{1}{2}(\sqrt{5} + 1). \tag{4.1}$$

The natural question is how electromagnetic waves propagate in such a system [17].

In a uniform coaxial or two-wire transmission line with inductance per unit length L' and capacitance per unit length C', the current $I(x, t)$ obeys the *telegrapher's equation* [18, 19]

$$\frac{\partial^2 I}{\partial x^2} - L'C'\frac{\partial^2 I}{\partial t^2} = 0, \tag{4.2}$$

which is a wave equation with speed $(L'C')^{-1/2}$. (We are considering an ideal line with no resistance or leakage conductance.) The voltage $V(x, t)$ obeys the same equation and is related to the current by

$$\frac{\partial V}{\partial x} = -L'\frac{\partial I}{\partial t}. \tag{4.3}$$

To study the Fibonacci chain, we apply equation (4.2) to each resonator, and demand continuity of I and V at every junction. The resulting piecewise-connected wave equation has no upper bound to the spectrum in contrast to the phonon problem. As $\omega \to 0$, however, the transmission line is equivalent to an infinite ladder of lumped circuit inductances and capacitances, L_a and C_a, which are now in a Fibonacci sequence instead of the more familiar periodic structure [20]. We obtain an exact mapping onto a phonon problem with the masses and spring constants replaced by the capacitances and inverse inductances, C_a and L_a^{-1} (or the other way around depending on whether one takes the current or the voltage to correspond to the atomic displacement) [9, 21]. This is the problem to which we now turn.

The argument of section 3 is immediately extendable to the above phonon problem. The main new point is that k must be defined more carefully now. Instead of a wavevector, it is better viewed as a *rotation number*, defined as $2\pi/L$ times the number of sign changes of the displacement in a large distance $L \gg \langle s \rangle$. Equivalently, we consider the integrated density of states, $H(\omega)$, defined as the number of normal modes with a frequency less than ω per unit length. Then, since the density of modes in an interval $\mathrm{d}k$ in k-space is always $\mathrm{d}k/2\pi$, and since there is a left-moving and a right-moving wave for any ω,

$$H(\omega) = \int_{-k(\omega)}^{k(\omega)} \frac{\mathrm{d}k}{2\pi} = \frac{1}{\pi}k(\omega). \tag{4.4}$$

This is also a good place to note that a Fibonacci sequence is more precisely defined by its hull or indicator function, χ_n. Let $x_n = \{n\tau^{-1} + \beta\}$ be the fractional part ($0 \leqslant x_n < 1$) of $n\tau^{-1} + \beta$, where β is an arbitrary number. Then

$$\chi_n = \begin{cases} 1, & 0 \leqslant x_n < \tau^{-1}, \\ 0, & \tau^{-1} \leqslant x_n < 1. \end{cases} \tag{4.5}$$

The values 1 and 0 correspond to L and S. The most common choice is to take $\beta = 0$ so that $x_0 = 0$, but by changing β, we can begin the sequence at an arbitrary point.

The infinite Fibonacci sequence can be understood by considering successively larger periodic approximants with F_n atoms, where F_n are the Fibonacci numbers defined by $F_n = F_{n-1} + F_{n-2}$ with $F_0 = F_1 = 1$. The phonon spectrum of the nth approximant has F_n branches (of which just one is acoustic), with $F_n - 1$ gaps. Instead of restricting k to the first Brillouin zone, it is better to define it in the extended-zone scheme, for then its interpretation as the integrated density of states, equation (4.4), continues to hold unchanged. This interpretation is meaningful even in the gaps: the graph of k versus ω is a horizontal segment in every gap. In the $n \to \infty$ limit one then has gaps at every frequency scale, however small. The spectrum is like a Cantor set, and $k(\omega)$ is a monotone increasing function whose derivative vanishes almost everywhere. The k versus ω graph is also known as a *devil's staircase* [22]: any time one attempts to ascend the staircase, one encounters a horizontal step. Still, for low ω the graph is visually indistinguishable from a straight line with slope $1/\bar{v}$ given by equation (3.11). If we consider equal masses and interatomic spacings, with two types of spring constants K_L and K_S with relative frequencies τ^{-1} and τ^{-2}, then the only quantity requiring explanation is $\langle K^{-1}\rangle$, and this is given by

$$\langle K^{-1}\rangle = \tau^{-1}K_\mathrm{L}^{-1} + \tau^{-2}K_\mathrm{S}^{-1}. \tag{4.6}$$

It is straightforward to apply equation (3.11) to the general case, where the masses are unequal in a Fibonacci sequence, separated by three types of nearest neighbour bonds, with different spring constants and interatomic spacings. Translated into the language of the electromagnetic problem, this equation says that the wave speed is given by

$$\bar{v} = \frac{\langle s\rangle}{\sqrt{\langle L\rangle\langle C\rangle}} \tag{4.7}$$

with

$$\langle L\rangle = \tau^{-1}L_\mathrm{L} + \tau^{-2}L_\mathrm{S}, \quad \langle C\rangle = \tau^{-1}C_\mathrm{L} + \tau^{-2}C_\mathrm{S}. \tag{4.8}$$

The kinetic and potential energies now have direct meaning as the electric and magnetic energies in the transmission line.

In figure 4 we show the spectrum of an 89-resonator approximant ($89 = F_{10}$) to the infinite sequence. The devil's staircase structure is clearly visible. The figure was obtained by exploiting the trace map of Kohmoto, Kadanoff, and Tang [11], with capacitances, inductances, and cavity lengths: $L_\mathrm{L} = 1$, $L_\mathrm{S} = 0.15$, $C_\mathrm{L} = 1$, $C_\mathrm{S} = 2.4$, $s_\mathrm{L} = 1$, and $s_\mathrm{S} = 0.3$ in arbitrary dimensionless units. Also shown on the graph is the low-ω, straight-line dispersion $k = \omega/\bar{v}$, with $\bar{v}$ given by equation (4.7) in the same units.

We conclude the paper with a caveat. Equation (3.11) does not apply to a random sequence of masses and springs. In such a chain, a subtle argument shows that all the normal modes are localized [23–25], and there cannot be a propagating wave. Thus the argument based on periodic approximants is important in establishing the idea of a rotation number for the Fibonacci sequence.

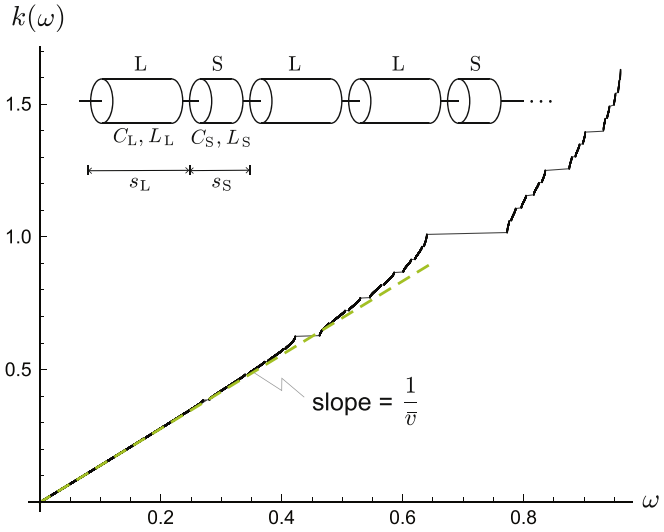

Figure 4. The k versus ω spectrum of a string of 89 ($=F_{10}$) cavities in a portion of the Fibonacci sequence. See text for explanation.

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