WAVE PROPAGATION IN PERIODIC STRUCTURES

Electric Filters and Crystal Lattices

L. BRILLOUIN

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Dedicated to My Wife

WHOSE FAITH AND LOVE HAVE NEVER FAILED
THROUGH HARDSHIP AND SORROW

PREFACE

Some readers may be surprised or even disturbed at the mixture of problems assembled in this book. These problems actually extend from electrical engineering to electromagnetism and wave mechanics of the spinning electron, but the link connecting this variety of problems will soon be discovered in their common mathematical background.

Waves always behave in a similar way, whether they are longitudinal or transverse, elastic or electric. Scientists of the last century always kept this idea in mind. When Lord Kelvin built up his model for a dispersive medium or when Lord Rayleigh discovered radiation pressure, they never failed to try the same methods again and again on all conceivable types of waves. This general philosophy of wave propagation, forgotten for a time, has been strongly revived in the last decade and represents the backbone of this book.

All problems discussed deal with periodic structures of various kinds, and they all lead to similar results: these structures, be they electric lines or crystal lattices, behave like band-pass filters. If energy dissipation is omitted, there is a sharp distinction between frequency bands exhibiting wave propagation without attenuation (passing bands) and those showing attenuation and no propagation (stopping bands). These general properties are defined for an infinite unbounded medium, but they bear a very close relation to *selective reflections* shown by a bounded medium. A wave striking from outside may be partly reflected from the surface, if the second medium is able to transmit the corresponding frequency. The amount of reflection depends upon how well the media are matched at their common boundary. But when the frequency falls inside a stopping band of the reflecting medium, there is no longer any matching problem; the wave cannot be transmitted, and hence it must be totally reflected. This same explanation applies to electric filters, rest rays, anomalous optical reflections, and selective reflection of X rays or electrons from a crystal. In the case of rest rays, the theory was developed

by M. Born and his school; for X rays, it corresponds to Bragg's reflections and P. P. Ewald's now classical investigations summarized in his book "Kristalle und Roentgen Strahlen" (Springer, 1923), and a paper in the *Annales de l'Institut Poincaré* (vol. 7, p. 79, 1938). Many practical examples of electric filters may be found in the treatises of K. S. Johnson and T. E. Shea, in the collection of books from the Bell Telephone Laboratories (van Nostrand). The general connection between stopping bands and selective reflection is exemplified in the definition of the *zones* for a crystal lattice, a theory first developed by the author in his original papers and in a book "Quantenstatistik" (Springer, 1931). A general discussion of the zone theory is found in the present book and will serve as an introduction to Mott and Jones, "Theory of Metals and Alloys" (Oxford, 1936), and to F. Seitz's "The Modern Theory of Solids" (McGraw-Hill, 1940), where the theory is applied to many practical discussions.

Apart from physical and engineering problems, the general theory developed in this book bears a close connection with many problems of applied mathematics, such as the Mathieu functions and Mathieu's and Hill's equations.

The author discussed these general problems in his lectures at the Collège de France (1937–1938) and at the University of Wisconsin (1942), when Mary Hewlett Payne very kindly proposed to write down her notes and to prepare them for publication. Circumstances resulted in great delays before this could be completed, and the author's present duties would never have permitted him to undertake such a work if Mrs. Payne had not made a really excellent record of his lectures, so that very few corrections and additions were necessary on her manuscript. Let her find here the author's very best thanks for her valuable collaboration.

LÉON BRILLOUIN.
Honorary Professor, Collège de France, Paris
Watson Laboratory, International Business Machines, New York

NEW YORK, N.Y.,
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CHAPTER I

ELASTIC WAVES IN A ONE-DIMENSIONAL LATTICE OF POINT MASSES: EARLY WORK AND INTRODUCTION

1. Historical Background; Eighteenth Century

The first work done on a one-dimensional lattice was that of Newton[1] in his attempt to derive a formula for the velocity of sound. Newton assumed that sound was propagated in air in the same manner in which an elastic wave would be propagated along a lattice of point masses. He assumed the simplest possible such lattice, *viz.*, one consisting of equal masses spaced

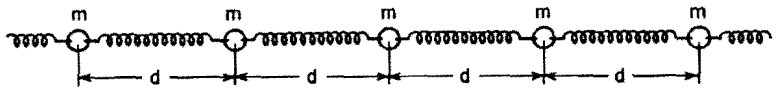


FIG. 1.1.

equally along the direction of propagation (Fig. 1.1). Neighboring masses were assumed to attract one another with an elastic force with constant e. Taking m to be the mass of each of the particles and d to be the distance between neighboring particles in the state of equilibrium, Newton obtained for the velocity V of propagation of an elastic wave

$$V = d\sqrt{\frac{e}{m}} = \sqrt{\frac{ed}{\rho}} \qquad \rho = \text{density} \qquad (1.1)$$

To compare this result with the experimental value of the velocity of sound in air, Newton took ρ to be the density of air and ed to be the isothermal bulk modulus of air. The theoretical value thus computed was smaller than the experimental value. In 1822 Laplace pointed out that the expansions and condensations

[1] NEWTON, "Principia," Book II, 1686.

associated with sound waves take place adiabatically and that, therefore, the adiabatic elastic constant should be used instead of the isothermal. A computation using the adiabatic constant in Newton's formula gave excellent agreement with experiment. It should be mentioned that Newton's formula holds only for wave lengths large compared with d.

The reason why Newton considered the one-dimensional lattice of Fig. 1.1 was that at that time a continuous structure represented an insoluble problem, and nothing was known about partial differential equations. Hence, a model had to be chosen that would lead to a number of simultaneous equations of motion of the usual type.

The work on one-dimensional lattices was continued in a series of letters, starting in 1727, between John Bernoulli in Basel and his son Daniel in St. Petersburg at that time. They showed that a system with n point masses has n independent modes of vibration, *i.e.*, n proper frequencies. Later (1753), Daniel Bernoulli formulated the principle of superposition, which states that the general motion of a vibrating system is given by a superposition of its proper vibrations. This investigation may be said to form the beginning of theoretical physics as distinct from mechanics, in the sense that it is the first attempt to formulate laws for the motion of a system of particles rather than for that of a single particle. The principle of superposition is important, as it is a special case of a Fourier series, and in time it was extended to become a statement of Fourier's theorem.

The laws of vibrating strings were first discovered empirically, and in 1713 Taylor started a theoretical investigation. Euler's treatment of the continuous string by means of partial differential equations (1748) was much more complete. He took the string to be along the x axis and to be vibrating in some plane perpendicular to this axis. The result he obtained was that the displacement of the string was given by an arbitrary function of $(x \pm vt)$, where v is the velocity of propagation of the wave and t is the time, provided that the function satisfied certain continuity conditions. Euler's result started a controversy lasting until 1807. If one takes Euler's result and the principle of superposition together, one must conclude that any arbitrary function of $(x \pm vt)$ may be described by a superposition of sine and cosine functions, since it is well known that the proper vibrations of a

string are given by sine and cosine functions. This is, of course, merely a statement of Fourier's theorem, but Fourier's theorem was not proved until 1807, and to Euler's mind the theorem was almost an absurdity. Since he could not doubt the validity of his solution to the problem of the vibrating continuous string, Euler refused to accept the principle of superposition.

The Bernoullis had given the problem of the one-dimensional lattice of point masses a fairly complete treatment. Euler had solved the problem of the vibrating continuous string. The task of treating the continuous string as a limiting case of the one-dimensional lattice of point masses still remained. This problem was solved by Lagrange in 1759.

Lagrange followed Euler in refusing to accept the principle of superposition. This is very strange, since Lagrange's paper practically contains the principle of the Fourier series. A number of examples of trigonometric series were already known at the time, but it was not believed that such expansions could be used to represent any arbitrary function. In a paper on celestial mechanics, Clairaut (1754) actually had the proof, but it remained unnoticed; and it was left for Fourier to give the general statement and to emphasize its great practical and theoretical importance.

All this work at the end of the eighteenth century is most interesting since it cleared the way for a number of modern problems in theoretical physics as well as for pure mathematics:

Proper functions, proper values; first discovered in connection with proper vibrations of strings, plates, etc.

Fourier expansion; expansion in series of proper functions.

Partial differential equations.

Wave propagation.

Atomic theory of solids and crystal structure.

Lagrange's paper was often quoted by the famous electrical engineer Pupin, who discovered in Lagrange's theory the solution of an important problem of electrical engineering, the loaded cable.

2. Historical Background; Nineteenth Century. Cauchy, Baden-Powell, and Kelvin

In 1830, Cauchy used Newton's model in an attempt to account for dispersion of optical waves. Cauchy assumed that

light waves were just elastic waves of very high frequency. He obtained the result that for waves with wave length large compared with the distances between the point masses in the one-dimensional lattice, the velocity was independent of wave length. For shorter wave lengths and hence for higher frequencies, however, he showed that the velocity of propagation was a function of wave length. The result is correct for elastic waves; however, it did not agree quantitatively with values obtained experimentally for light waves.

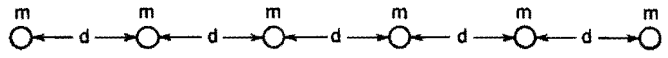


FIG. 2.1.

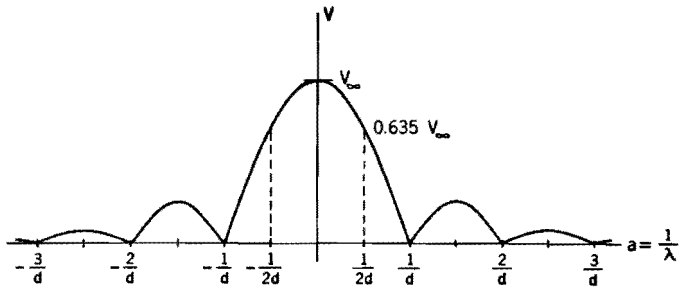


FIG. 2.2.—Wave velocity V as a function of a along the row of particles shown on Fig. 2.1.

In 1841, Baden-Powell computed the velocity of a wave propagating along one axis of a cubic lattice structure as a function of wave length. This is equivalent to considering a wave propagating along a one-dimensional lattice of point masses. Baden-Powell's lattice consisted of point masses of mass m spaced along a straight line at distance d from one another (see Fig. 2.1). Then he assumed each mass to be elastically bound to each of its neighbors with the restoring force the same for all masses. His equation for the propagation velocity V of the wave as a function of wave length is

$$V = V_\infty \frac{|\sin \pi d/\lambda|}{\pi d/\lambda} \tag{2.1}$$

where λ is the wave length and V_∞ is the velocity for infinite wave length. The curve of V plotted against reciprocal wave length is shown in Fig. 2.2. It is evident that if velocity is a function

of wave length, the frequency must also be a function of the wave length. However, Baden-Powell neglected to consider the frequency as a function of the wave length and thus missed a very important point. The curve of velocity as a function of reciprocal wave length appears to be perfectly normal at the point $\lambda = 2d$; not so, however, for the frequency vs. reciprocal-wave-length curve. This point was noted by Kelvin, who gave a detailed discussion in 1881.[1]

Kelvin assumed the same lattice that Baden-Powell treated (see Fig. 2.3). Let us number the particles in such a way that

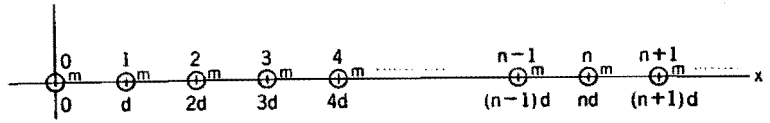


FIG. 2.3.

the x coordinate of the nth particle in its equilibrium position is given by

$$x_n = nd \tag{2.2}$$

In a sine wave, we obtain for y_n, the displacement of the nth particle,

$$y_n = A \cos 2\pi(\nu t - ax) = A \cos 2\pi(\nu t - and) \tag{2.3}$$

where ν is the frequency, a the wave number or reciprocal wave length, A an arbitrary constant, and t the time. Now in Eq. (2.3) we may replace a by

$$a' = a \pm \frac{m}{d} \qquad m \text{ an integer} \tag{2.4}$$

without changing the value of the displacement. This means that ν must be a periodic function of a with period $1/d$.

Now the phase velocity V, with which the waves propagate, is given by

$$V = \frac{\nu}{a} \tag{2.5}$$

Therefore, if we draw a curve of $\nu = \nu(a)$ as a function of a, the phase velocity for a given wave length will be given by the slope of the line drawn from the origin to the point on the $\nu(a)$ curve corresponding to the given wave length. The function $\nu(a)$ may

[1] "Popular Lectures," vol. I, p. 185.

be calculated and turns out to be

$$\nu(a) = B\,|\sin \pi a d| \tag{2.6}$$

where B is a constant that is a function of the constants of the lattice. From Eq. (2.6) we see that

$$V = \left|\frac{\nu(a)}{a}\right| = B\left|\frac{\sin \pi a d}{a}\right| = V_\infty \frac{|\sin \pi a d|}{|\pi a d|} \tag{2.7}$$

in agreement with Baden-Powell's equation (2.1), if we take

$$V_\infty = \pi\, dB \tag{2.8}$$

From Eq. (2.6) we see that $\nu(a)$ is a straight line for small values of a, *i.e.*, for large values of wave length. This means that the

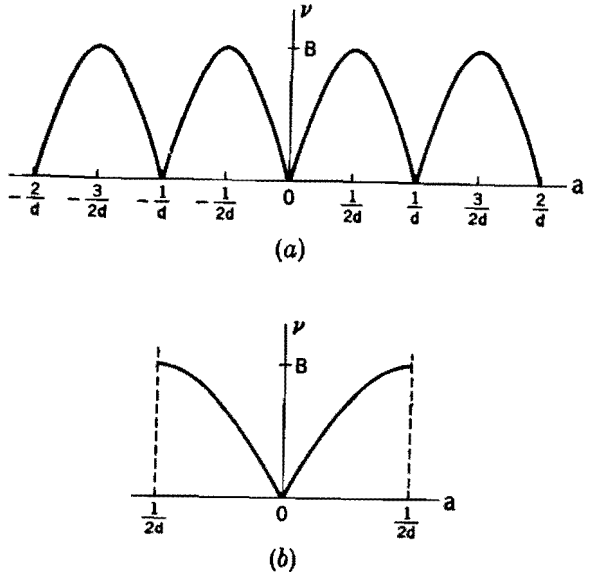


FIG. 2.4.—Frequency ν as a function of $a = 1/\lambda$ for the row of particles shown on Fig. 2.1.

velocity of propagation should be constant for large wave lengths, in agreement with the earlier calculations.

The curve of ν vs. a is shown in Fig. 2.4*a*. The periodicity of ν as a function of a means that for a given frequency the wave length is not completely determined. In fact, any a', where a' is defined by Eq. (2.4), will give the same ν. The ambiguity in wave length results in an ambiguity in the direction of propagation—an uncertainty both in magnitude and in direction. This is easily seen by referring to Eq. (2.7).

The physical meaning of the ambiguity in wave length may be seen from Fig. 2.5. The solid circles give the equilibrium positions of the point masses and the open circles the displaced positions at some instant. Through the displaced positions are drawn three possible sine waves. All three waves give equally good descriptions of the motion, as far as observation of the

FIG. 2.5.—Different sine curves passing through the position of the particles.

points is concerned. The solid line gives the wave form for the only value of a such that

$$-\frac{1}{2d} \leqq a \leqq \frac{1}{2d} \tag{2.9}$$

Changing a by $1/d$ will take a out of this interval, as is immediately obvious. The dashed curve corresponds to $a + (1/d)$, and the dotted curve to $a - (1/d)$. A glance at the diagram shows that the solid and the dashed curves must propagate in the same direction for a given motion of the particles, and the dotted curve propagates in the opposite direction.

From now on, we shall adopt the convention expressed by Eq. (2.9). All ambiguity in wave length and direction of motion is removed if we restrict a to this interval, except in the two special cases where

$$a = \pm \frac{1}{2d} \tag{2.10}$$

We shall discuss these special cases shortly. The convention is not so arbitrary as might appear at first sight. It allows any wave length such that

$$\infty \geqq \lambda \geqq 2d \tag{2.11}$$

to have either direction of propagation, and excludes only wave lengths that lie in the interval

$$0 \leqq \lambda \leqq 2d \tag{2.12}$$

If we had a continuous structure so that the motion of all points lying on a straight line could be observed, the wave lengths included in the interval (2.11) would be the only ones observed, since in this case $d = 0$. Thus there will be no inconsistency in what we mean by wave length when we go from a continuous to a

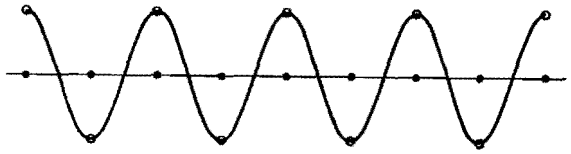


FIG. 2.6.—The limit $\lambda = 2d$.

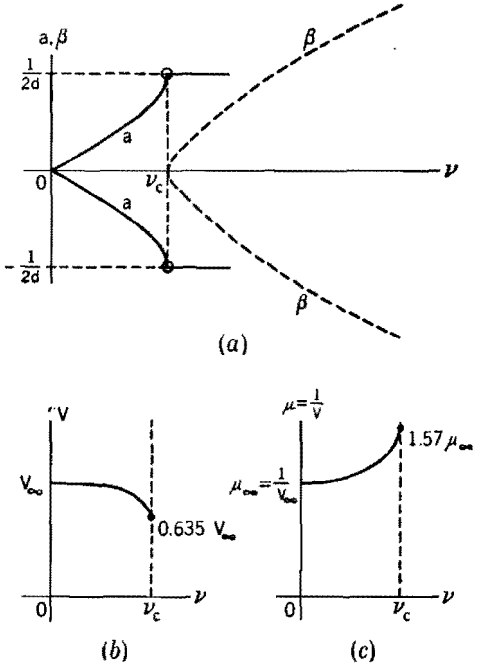


FIG. 2.7.

discontinuous structure, and vice versa. Furthermore, the allowed interval contains a complete period of $\nu(a)$, so that none of the frequencies that can be propagated are omitted.

The special case noted in Eq. (2.10) is shown in Fig. 2.6. Here there is no way of distinguishing between the two possible wave numbers allowed by our convention, or between the two

possible directions of propagation. In fact, the wave might even be considered as a standing wave, *i.e.*, a superposition of the two allowed wave numbers. The wave length is, of course, in both cases $2d$.

Engineers frequently find it convenient to use other curves giving essentially the same information as our ν vs. a curve. The one of greatest interest is the attenuation curve (Fig. 2.7*a*). The solid part of the curve is our ν vs. a curve rotated through 90 deg. The dotted, or β, part gives the attenuation β for frequencies higher than those that may be propagated. The attenuation will be discussed in detail in a later chapter. A lattice such as this, which allows propagation of all frequencies up to a maximum, or critical, frequency ν_c and damps all others, is called a *low-pass filter; i.e.*, it will pass low frequencies and stop higher frequencies. Figures 2.7*b* and 2.7*c* give V, the phase velocity, and μ, the index of refraction or reciprocal of phase velocity, as functions of frequency. Both curves terminate at the critical

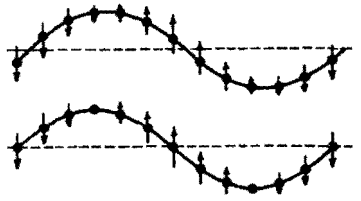


FIG. 2.8.—An example given by Lord Kelvin.

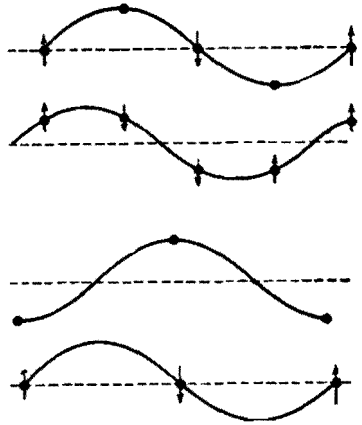


FIG. 2.9.—Other examples given by Lord Kelvin. The lower vibration corresponds to the limit $\lambda = 2d$.

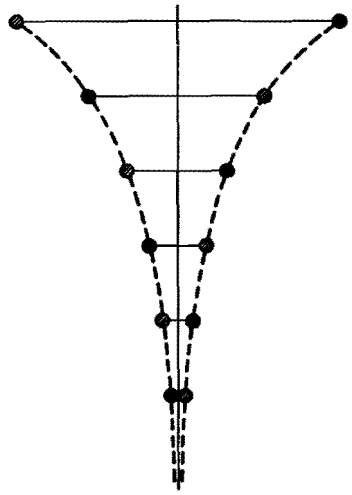


FIG. 2.10.—Attenuation of the wave for a frequency above cutoff (Lord Kelvin).

frequency, as phase velocity is not defined for attenuated waves. The curves shown in Figs. 2.7*a*, *b*, and *c* are very useful for some practical purposes. However, in general, we shall find the ν vs. a curve (Fig. 2.4*b*) most useful for our analytical discussions.

Lord Kelvin's discussion is of great significance, since it contains the discovery of the cutoff frequency. Figures 2.8 to 2.11 are reproductions of Kelvin's original drawings and show the variation of wave velocity as a function of $N = \lambda/d$, the number of atoms per wave length. Modes of vibration are shown for large N and for $N = 2$ (cutoff), together with the attenuated wave corresponding to a frequency above cutoff. All this shows how clearly Kelvin understood the problem.

N	W
2	63,64
4	90,03
8	97,45
12	98,86
16	99,36
20	99,59
∞	100,00

FIG. 2.11.

The paper was often overlooked, since its title, "The Size of Atoms," did not imply any discussion of wave propagation. The connection is found in Cauchy's theory of dispersion. The curve in Fig. 2.2 shows that a material change in the wave velocity can be expected only if the wave length is just larger than $2d$. Hence, Cauchy's theory leads to the conclusion that interatomic distances should be just smaller than $\lambda/2$, giving a distance d of about 2,000 angstroms. This, however, sounded impossible since there was, at Kelvin's time, plenty of experimental evidence that interatomic distances could not amount to more than a few angstrom units. The thickness of oil films on water, for instance, had been measured and was quite well known.

Kelvin's conception of the molecular structure of matter may be illustrated by the following quotation:

> I believe that by imagining each molecule to be loaded in a certain definite way by elastic connection with heavier matter . . . we shall have a rude mechanical explanation for refractive dispersion. . . . It is not seventeen hours since I saw the possibility of this explanation.[1]

This was a remarkable guess, which led Kelvin to the discovery of the modern refraction formula, usually known as the *Lorentz formula.*

3. Later Work on Models Similar to That Treated in Sec. 2

After analyzing Baden-Powell's work and discussing the critical wave length and frequency, Kelvin proceeded to devise a theory

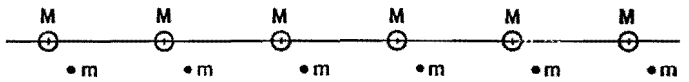


FIG. 3.1.—Kelvin's model for optical dispersion.

of dispersion based on a more complicated lattice than Baden-Powell's. He used the lattice shown in Fig. 3.1. Each of the masses in this model is supposed to have a small mass associated with it. The large masses are taken to have mass M and are the large circles in Fig. 3.1, while the small masses have mass m and are represented by dots. Each of the large masses interacts with the nearest large masses and with the small mass associated with it, so that there are two elastic constants in the system. Introducing two masses effectively doubles the number of degrees of freedom of the system, and hence one would expect to find twice as many proper vibrations as if there were only one mass. The curve of ν vs. a is shown in Fig. 3.2. The curve is restricted to values of a between $\pm 1/2d$. It is seen that for each a there are two modes of vibration of the system, so that we do indeed have twice the number of modes obtained by Baden-Powell for his model with one mass. Frequencies below ν_1 and between ν_2 and ν_3 are propagated by the lattice, and all others are stopped. This lattice is an example of a *band-pass* filter. The interval between ν_1 and ν_2 is known as a *stopping band*, while that between ν_2 and ν_3 is known as a *passing band.* The frequencies ν_1 and ν_2 are very near the proper frequency of oscillation of one iso-

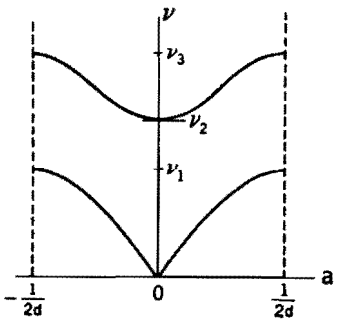


FIG. 3.2.

[1] *Op. cit.*, p. 194.

lated M-m molecule. This resonance frequency has nothing to do with the distance between molecules, and a material change in wave velocity is obtained when the resonance frequency lies in the near ultraviolet, just above the optical spectrum. Thus Kelvin explains refraction and escapes Cauchy's paradox.

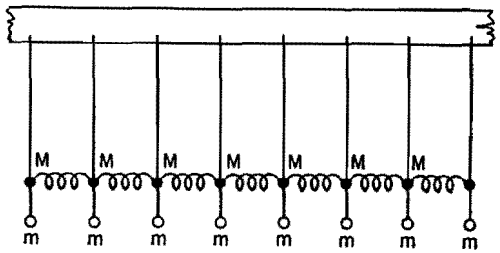


FIG. 3.3.—Vincent's model of the first mechanical filter.

Vincent[1] built a mechanical model to which Kelvin's theory was assumed to apply. The model is shown in Fig. 3.3. The large masses M are suspended from a beam on strings of equal length and connected to one another by springs. The small masses m are each suspended from one of the large masses. This model is evidently equivalent to Kelvin's more abstract scheme and was the *first mechanical filter* to be built. The motion of the system was observed for different frequencies. Vincent plotted curves of index of refraction μ against the frequency for comparison with standard dispersion curves. These curves are shown in Fig. 3.4. The solid curve is for negligible damping and the dotted curve for large damping. It is to be noted that the dotted curve is a typical anomalous dispersion curve. Vincent's curve of ν vs. a agreed with Kelvin's curve. The ratio $V = \nu/a$ can be measured on Fig. 3.2 and curve 3.4 obtained for $\mu = 1/V$ as a function of frequency ν.

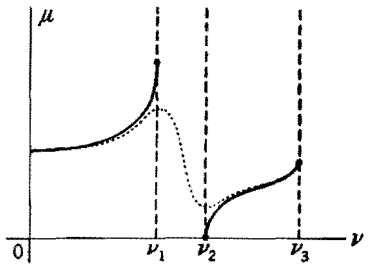


FIG. 3.4.—Index of refraction μ as a function of frequency ν for Vincent's model.

Kelvin's paper received little notice, and the analogy between the propagation of electromagnetic radiation and the propagation of elastic waves along a loaded string was forgotten.

[1] *Phil. Mag.*, **46**, 537 (1898).

In 1887, Heaviside noted that increasing the inductance per unit length of a cable should reduce the attenuation of waves propagating along the cable. However, he discussed no experimental details. Two years later, in 1889, Vaschy tried loading a very long cable with four inductances, an experiment much too crude to give any observable result. In 1900, Pupin developed the analogy between mechanical and electric lines and, referring to Lagrange's work on the discontinuous string, succeeded in building loaded lines and low-pass electric filters. The line is shown in Fig. 3.5*a*. The inductances L' were spaced so that

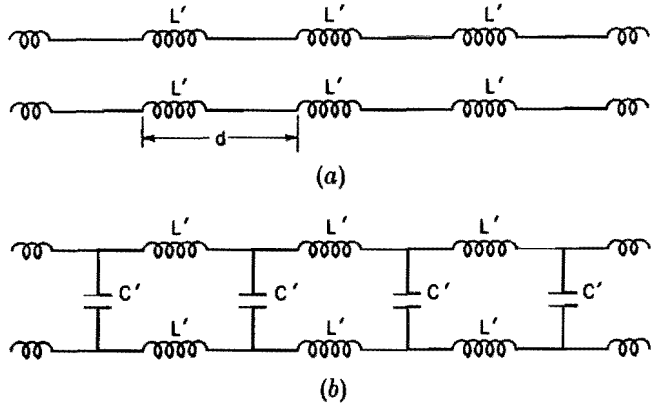


FIG. 3.5.—Low-pass electric filter and loaded line.

there were about ten inductances per wave length. Calling the capacitance per section d between the two halves of the line C', Pupin obtained a critical frequency of

$$\nu_m = \frac{1}{\pi\sqrt{2L'C'}} \tag{3.1}$$

Figure 3.5*b* shows an equivalent line with the capacitance of the line lumped and placed along the line as indicated.

The first high-pass electric filter (*i.e.*, a line passing all frequencies higher than a certain critical frequency and stopping all others) was built by Campbell in 1906. The line is shown in Fig. 3.6. Campbell followed up his high-pass filter by designing various band-pass filters. Figure 3.7 is the band-pass filter analogous to Vincent's mechanical band-pass filter.

It is somewhat easier than in the analogous mechanical lines

to see why the electric lines mentioned above should pass some frequencies and stop others. The impedance offered by an electric circuit to a current passing through it is proportional to νL and inversely proportional to νC where ν is the frequency, L is the inductance, and C is the capacitance. Thus in the low-pass filter shown in Fig. 3.5*b* the impedance offered by the coils L' increases with the frequency, while the impedance of the capacities

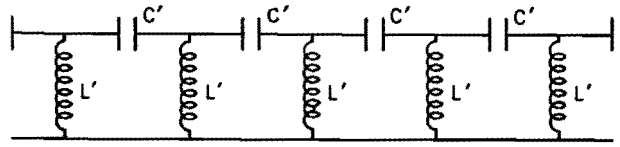


FIG. 3.6.—High-pass filter.

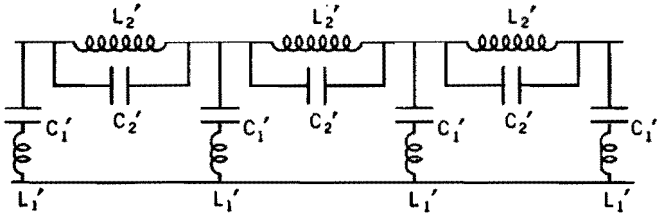


FIG. 3.7.—Band filter.

connected across the line decreases. The occurrence of a critical frequency is a result of the spacing and lumping of the inductances and capacities. In the high-pass filter the low frequencies will be shunted to the returning line through the inductances while the high frequencies will be passed. Again, the occurrence of a critical frequency is due to the discontinuous nature of the structure. These problems will be discussed in detail in a later section.

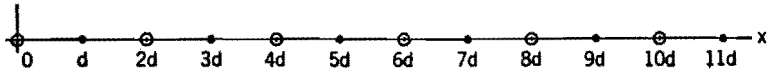


FIG. 3.8.—Born's model for sodium chloride.

In 1912, Born investigated the propagation of waves in crystals and rediscovered Kelvin's analysis. Using the model shown in Fig. 3.8, with large masses M and small masses m alternating at the points along the x axis defined by nd, where d is the distance between nearest neighbors, he obtained the curves shown in Figs. 3.9*a* and *b*. Figure 3.9*a* shows ν as a function of a. There are two branches to the curve because we have effectively

doubled the number of degrees of freedom of the system by adding another constant. The additional constant is, of course, the second value for mass. We shall find that in general the number of branches will equal the number of different masses occurring in the model; *i.e.*, the number of frequencies corresponding to a given wave number is equal to the number of degrees of freedom associated with each element or cell of the lattice. In this case the cell consists of a large mass and either of its neighboring small masses. If there were two different masses between

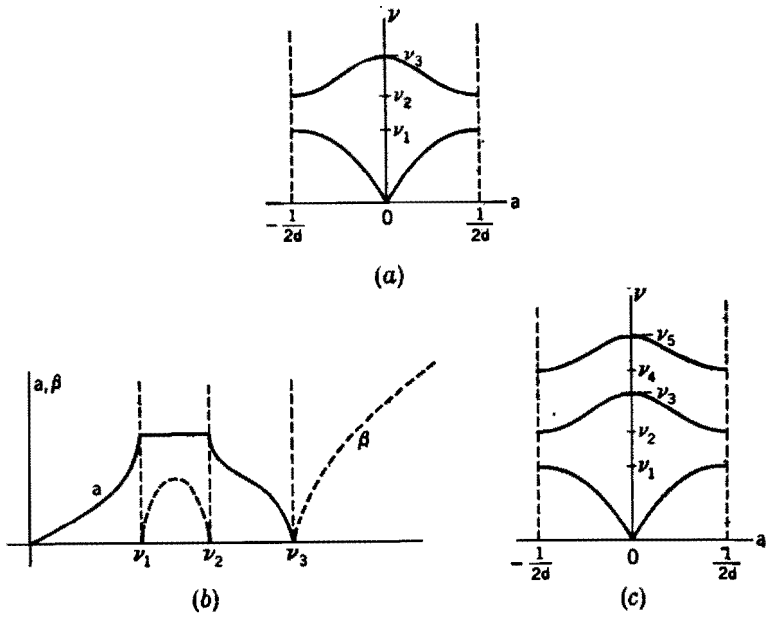


FIG. 3.9.

a given mass and the next one like it, and if this structure were repeated all along the lattice, each cell would have three degrees of freedom, and the ν vs. a curve would have one lower branch and two upper branches as in Fig. 3.9*c*. This property of discontinuous media will be discussed in greater detail later.

In general, the lower branch is called the *acoustical* branch. It corresponds to motion of the particles such that in each short section of the line all particles move in the same direction at a given instant. The upper branches are called *optical* branches and correspond to one or more types of particles moving in the

direction opposite to that of the others at any given instant. In Born's model, where we have only two types of particle, the optical branch corresponds to the motion of the large masses in one direction while the small masses move in the other.

Figure 3.9*b* is the attenuation curve for Born's model and represents the generalization of Fig. 2.7*a*. There are one stopping band and two passing bands associated with this model. The

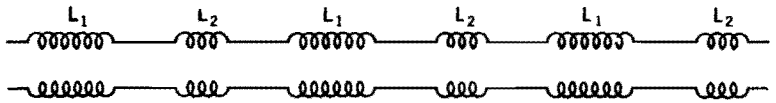


FIG. 3.10.—Electric filter corresponding to Born's sodium-chloride model.

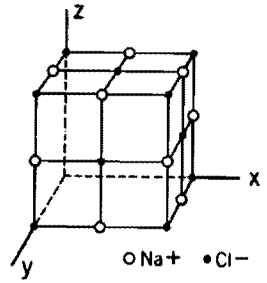


FIG. 3.11.—NaCl crystal lattice.

electrical analogue to Born's lattice is a line with small and large inductances alternating (Fig. 3.10).

Born's problem is usually referred to as the NaCl crystal lattice problem, since a very similar situation is found in the NaCl crystal structure: it is a cubic lattice with Na^+ and Cl^- ions alternately located at the lattice points, as shown in Fig. 3.11. Along one axis, the x axis, for instance, the structure is exactly the same as that in Fig. 3.8.

CHAPTER II

PROPAGATION OF WAVES ALONG ONE-DIMENSIONAL LATTICES. GENERAL RESULTS AND QUALITATIVE DISCUSSION

4. General Remarks

Before proceeding to the mathematical treatment of waves propagating along a one-dimensional lattice, we shall make some general remarks about the problem and discuss some particular cases qualitatively. The simplest example of a one-dimensional lattice is Baden-Powell's model with equal masses spaced uniformly in a line. If we take the masses along the x axis, the x coordinate of the nth mass will be given by

$$x = nd + \psi_n \tag{4.1}$$

where ψ_n is the displacement of the nth particle from its equilibrium position. ψ_n may be taken to represent transverse or longitudinal displacement, or any other quantity whose value may be defined at the points occupied by the masses but not elsewhere (electric polarization, for instance); *i.e.*, we may regard ψ_n as a property associated with point mass n. This property is propagated as a wave if the physical problem admits a solution of the type

$$\left.\begin{aligned} \psi_n &= Ae^{2\pi i(\nu t - and)} = Ae^{i(\omega t - kn)} \\ a &= \frac{1}{\lambda}, \qquad k = 2\pi ad, \qquad \omega = 2\pi\nu \end{aligned}\right\} \tag{4.2}$$

where ν is the frequency, t the time, a the wave number, λ the wave length, d the period of the lattice, ω the angular frequency, k the product of the wave number and the period of the lattice multiplied by 2π, and A a constant amplitude. The quantity k is the change in phase in passing from a point n to its right-hand neighbor $n + 1$:

$$\psi_{n+1} = \psi_n e^{-ik} \tag{4.3}$$

Thus k is essentially defined as an angle and can be known only as *modulus* 2π. The *same solution* of the problem is obtained for

$$k \quad \text{or} \quad k' = k + 2m\pi \tag{4.4}$$

when m is a positive or negative integer. Equations of the physical problem must yield the same value of ω or ν for every equivalent k or k', which means that the frequency ν is a periodic function of k or a:

$$\left.\begin{aligned} \omega &= f(k) \qquad \text{period } 2\pi \text{ in } k = 2\pi a d \\ \nu &= F(a) \qquad \text{period } \frac{1}{d} \text{ in } a \end{aligned}\right\} \tag{4.5}$$

This is a general and direct consequence of the periodic and discontinuous structure of the one-dimensional line. It was explained in Chap. I in Eq. (2.4) by saying that if ψ could be measured between particles, the uncertainty in k or a would be eliminated, but since ψ is measured only at the discrete points nd, the condition (4.5) is unavoidable.

On account of the periodic properties of the line, it is sufficient to discuss the properties of the functions f or F inside one period of k or a. The most convenient choice is

$$\left.\begin{aligned} -\pi \leqq k &\leqq \pi \\ -\frac{1}{2d} \leqq a &\leqq \frac{1}{2d} \end{aligned}\right\} \tag{4.6}$$

since a wave always propagates in the same way to the right and to the left. This means that the functions f and F have the additional property of being *even* functions. Positive k means a wave propagating to the right; negative k a wave propagating to the left. If k_0 is a positive number in the fundamental interval (4.6), it represents a wave going to the right, and so does $k_0 + 2\pi$; but $k_0 - 2\pi$ is negative and represents a wave going to the left (Fig. 2.5). Hence, the uncertainty is not only in the magnitude of a or k but also in the direction of propagation.

The limitation (4.6) means

$$\lambda = \frac{1}{|a|} \geqq 2d \tag{4.7}$$

The shortest wave length is thus equal to twice the distance between particles and corresponds to a certain *critical frequency* or *cutoff frequency* ν_m that is characteristic of the structure. In many important cases ν_m is the maximum frequency, and the system works as a *low-pass filter* for all frequencies

$$\nu \leqq \nu_m \tag{4.8}$$

Frequencies above ν_m are strongly attenuated. Condition (4.8) is, however, not the only possible one, and other situations may arise when ν_m would be a minimum. The system as a whole is always a filter, but it can be of the low-pass, high-pass, or band-pass type.

These general results, plus a direct discussion of the waves corresponding to the limiting cases, $\lambda = \infty$, $a = 0$, and $\lambda = 2d$, a maximum, may in a number of instances give enough information to enable one to describe, at least qualitatively, the general properties of the structure. In the next few sections we shall apply this discussion to specific examples of one-dimensional lattices.

5. A Lattice of Free Particles

By a lattice of free particles we mean particles in a one-dimensional lattice with no forces present except those due to interactions of the particles among themselves For purposes of this discussion we shall limit the interactions to nearest neighbors. An example of this is a loaded elastic cord with the masses distributed uniformly, where the elasticity of the cord remains constant along its length and plays the part of the interaction forces.

Let us first consider longitudinal displacements. The case $a = 0$ corresponds to infinite wave length. In this case the lattice as a whole is displaced, and no change in the distance between masses occurs. Thus no force is brought into play. The frequency is zero. For $a \neq 0$, but still very small, the wave length is large compared with the distance between masses, and hence the waves are propagated as if the lattice were a continuous string. The velocity of propagation of waves along a continuous string is constant for all wave lengths; *i.e.*, for long wave lengths, the frequency is proportional to $|a|$. A rigorous treatment shows that the velocity decreases for wave lengths comparable with the distance between masses. Now if a wave is to be propagated at all, the frequency must be a periodic function of a. Further-

more, the curve of ν vs. a must be symmetrical about the origin. If it were not, the frequencies for a given wave length propagating in opposite directions would be different, a fact that would be in contradiction with the symmetry of the structure. If ν is to be both periodic and symmetrical about the origin, there must be a maximum in the value of ν at $1/2d$, since the period of ν is $1/d$. Thus we obtain a curve of the general shape of that in Fig. 2.4*a*. We shall, of course, justify the exact shape mathematically in a later section.

The remarks made on the longitudinal vibrations also apply to transverse vibrations. Qualitatively, they may be treated in just the same way. Quantitatively, however, there is a difference. The velocities of propagation for large wave length are

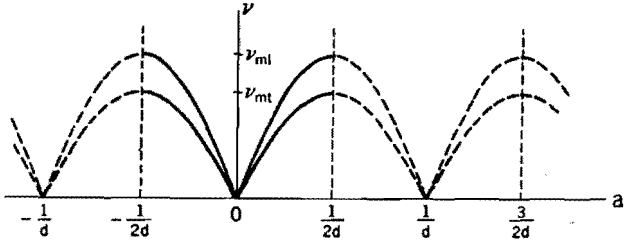


FIG. 5.1.—Longitudinal and transverse vibration along the row of particles shown on Fig. 2.1.

different in the longitudinal and transverse cases, and the maximum frequencies are also different. A typical curve for a one-dimensional lattice with particles with two degrees of freedom is shown in Fig. 5.1. The subscripts t and l on the maximum frequencies refer to transverse and longitudinal vibrations, respectively. The lower curve, representing transverse vibrations, should properly be considered a superposition of two branches of the same frequency, since there are two independent directions perpendicular to the lattice in which the masses might move. If there were an asymmetry in the elastic cord (*e.g.*, if it were of elliptical cross section), the lower branch would split into two distinct branches to give the extra frequencies demanded by the added degree of freedom. The solid curve corresponds to the interval (4.6), and its periodic continuation is shown as a dashed curve.

The transverse branches will usually be below the longitudinal branch in a loaded string, since the force required for a given displacement is smaller in the transverse than in the longitudinal direction. The frequency of displacement is proportional to the square root of the elastic constant, which will be smaller in the case of transverse displacements.

6. Longitudinal Vibration in a Row of Equidistant Coupled Oscillators

A particle attracted to some equilibrium position by an elastic restoring force acts as a harmonic oscillator. It has one proper frequency ν_0 that depends on the elastic restoring force and the mass of the particle. If its elastic restoring force is different in the x, y, and z directions, we have what is called an *anisotropic oscillator*. An anisotropic oscillator has three proper frequencies,

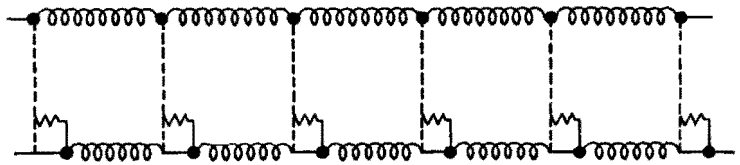


FIG. 6.1.—A row of harmonic oscillators coupled together.

ν_{0x}, ν_{0y}, and ν_{0z}, corresponding to vibrations in the x, y, and z directions, respectively.

Let us consider a row of similar harmonic oscillators (isotropic) spaced at distance d from one another along the x axis and allow interactions between nearest neighbors (Fig. 6.1). We wish to study the longitudinal modes of vibration of this system. For infinite wave length, $a = 0$. Infinite wave length means that all the particles are displaced simultaneously by the same amount. Since the distances between the particles do not change, the forces of interaction do not enter into the problem. Each particle is attracted to its equilibrium position with the same elastic force, and the system will oscillate with frequency ν_0. For a slightly smaller wave length the particles will be displaced relatively to one another, and the forces of interaction will play a part in the motion of the system. The frequency associated with this wave length will be slightly different from ν_0. Whether the frequency increases or decreases will depend on whether the resulting forces (elastic plus interaction) are larger or smaller than the restoring force tending to return each particle to its equilibrium position.

It may be shown that for large wave lengths ν is given by

$$\nu = \nu_0 + ba^2 \tag{6.1}$$

The sign of b depends on the constants of the system and determines whether ν shall increase or decrease as $|a|$ increases. As the wave length becomes comparable with $2d$, the considerations of the previous sections on one-dimensional lattices apply, and ν approaches an extremum. Thus we will have two limiting frequencies, ν_0 and ν_m (where m stands for maximum or minimum as the case may be). Frequencies between ν_0 and ν_m will propagate along the system, and other frequencies will be damped out. The system therefore forms a band-pass filter. The solid curve

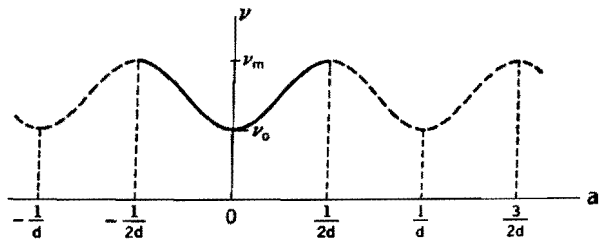


FIG. 6.2.—Frequency ν as a function of $a = 1/\lambda$ for the row of harmonic oscillators.

in Fig. 6.2 shows the curve ν vs. a in the fundamental interval (4.6) for the case $b > 0$. If each particle represented an anisotropic oscillator instead of an isotropic oscillator, there would be three curves, one for longitudinal and two for transverse vibrations. These curves might overlap and would not necessarily all rise as $|a|$ increases from zero.

7. Longitudinal Vibrations in a Row of Diatomic Molecules

The scheme described in the last section is somewhat artificial. It is rather difficult to imagine a particle in nature being tied to an equilibrium position by a little spring. A more realistic picture is obtained by considering diatomic molecules. This is a more complicated problem, since we must introduce a second type of particle that may interact with the first type as well as with its own type.

A lattice of diatomic molecules is shown in Fig. 7.1. The open circles are to have mass M, and the dots are to have mass m. An isolated molecule will have a certain proper frequency of vibration that we call ν_0. This frequency corresponds to an oscillation of the two masses along the x axis in opposite directions in such a way that their center of mass remains at rest.

Let us consider the motion of a row of diatomic molecules spaced at distance d from one another along the x axis. We assume, of course, that the molecules interact, but we limit the interaction to nearest neighbors. There will now be *two* wave functions, both imaginary exponential, one describing the motion of the masses M and the other describing the motion of the masses m. These two functions may be written

$$\psi_M = A_M e^{2\pi i(\nu t - ax)} \quad \text{and} \quad \psi_m = A_m e^{2\pi i(\nu t - ax)} \tag{7.1}$$

The frequencies and wave numbers will be the same, but the amplitudes may be different. The frequency ν may be found as

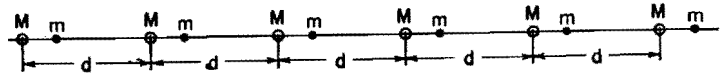


FIG. 7.1.—A row of diatomic molecules.

a function of the constants of the system and of a. It turns out to be double valued in ν, as will be shown in the rigorous theory, corresponding to the doubly infinite set of degrees of freedom of the system.

For infinite wave length, the atoms all oscillate in phase, and we may take

$$A_M = A_m \tag{7.2}$$

This corresponds to a translation of the lattice as a whole without alteration of the distance between particles, and hence the frequency is zero. Another frequency for infinite wave length is obtained if we take the small and large masses moving in opposite directions in such a way that the centers of gravity of the molecules remain at rest. This frequency would be ν_0 if there were no interaction between molecules. The presence of interactions would change this frequency. If the wave length is decreased, the lower branch of the ν vs. a curve will rise. This branch is just what would be obtained if we took each molecule to be a single particle. The upper branch will increase or decrease from its frequency at $a = 0$, depending on the relative values of the constants involved. Figure 7.2 shows the frequency curves. The limit to the frequency of the upper branch is ν'_0 for $a = 0$. Either, but not both, of the two upper branches shown may

occur. Figure 3.2 (Vincent) and Fig. 3.9 (Born) represent two typical examples with different upper curves. The size of ν_0 relative to the maximum frequency of the lower branch depends on the constants of the system, as does also the width of the

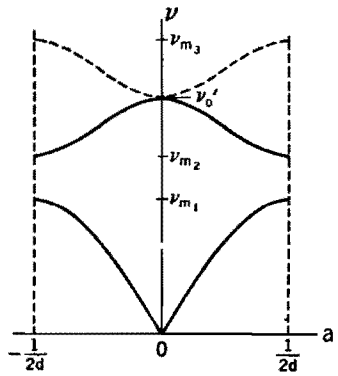


FIG. 7.2.—Frequency ν as a function of $a = 1/\lambda$ for a row of diatomic molecules.

upper branch. Frequencies located in the stopping bands may be shown to decay exponentially, as in the other models we have discussed. The a corresponding to these frequencies are complex with imaginary part β. β is therefore the attenuation constant for a given frequency. The attenuation curves are shown

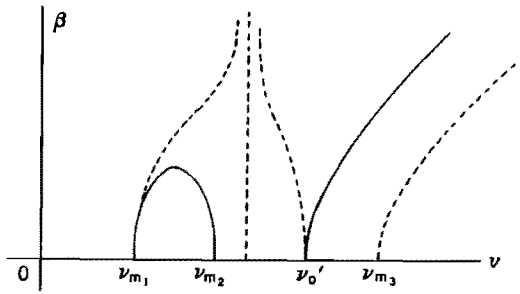


FIG. 7.3.—Attenuation as a function of frequency for a row of diatomic molecules.

in Fig. 7.3. The solid curve is for the solid upper branch and the dashed curve for the dashed upper branch of Fig. 7.2.

In these examples, the following features can be recognized that will be proved in the detailed analysis of later chapters:

1. Periodicity of ν as a function of k or a (4.5).

2. The possibility of a reduction of k or a inside the fundamental interval (4.6).

3. If the elementary cell of the one-dimensional lattice contains a system with N degrees of freedom, there will be N different waves corresponding to each k value, with N different frequencies. Examples with $N = 1, 2, 3$ were given in Secs. 5, 6, and 7.

4. Hence, the number of degrees of freedom inside an elementary cell equals the number of branches in the curve $\nu = F(a)$ and the number of passing bands of the structure (with possible overlapping of the passing bands).

5. Frequencies outside the passing bands are not propagated but decay exponentially along the line.

These are the general properties of one-dimensional periodic structures that will be investigated mathematically in the following sections.

A careful discussion of Vincent's model (p. 12, Fig. 3.3) is recommended as a typical problem, and leads to curves of the type represented on Figs. 7.2 and 7.3 as dashed lines.

CHAPTER III

MATHEMATICAL TREATMENT OF A ONE-DIMENSIONAL LATTICE OF IDENTICAL PARTICLES

8. Equation of Motion of a One-dimensional Lattice of Identical Particles

In this and the following sections we shall derive rigorously the results discussed qualitatively in the first two chapters. We shall assume an infinite lattice of identical particles of mass M. The particles in equilibrium are separated by a distance d along the x axis, and we shall take the oscillations of the particles to be longitudinal. We number the particles by calling the particle at the origin 0, the next particle to the right 1, etc. The displacement of the nth particle is denoted by y_n, so that x_n, the coordinate of particle n, will be given by

$$x_n = nd + y_n \tag{8.1}$$

We shall assume interactions between all particles, and for this we require the expression for the distance between two particles n and $n + m$. This distance is

$$r_{n,n+m} = x_{n+m} - x_n = md + y_{n+m} - y_n \tag{8.2}$$

This expression may be either positive or negative, depending on whether m is positive or negative. The energy of interaction between two particles will be expressed as a potential function that will be assumed to depend only on the distance between the two particles:

$$U(r) = U(|x_{n+m} - x_n|) \tag{8.3}$$

The total potential energy of the lattice will then be given by

$$U = \sum_n \sum_{m>0} U(|x_{n+m} - x_n|) \tag{8.4}$$

m must be restricted to positive values so that the interaction between a given pair of particles will be counted only once. We

might take the sum over all values of m and divide by two to compensate for counting each pair of particles twice. However, we prefer to restrict m to positive values, since this enables us to drop the absolute-value sign in the argument of U. If we assume that the displacements y_n are small compared with d, we may expand U in a Taylor series. Thus

$$U(x_{n+m} - x_n) = U(md) + (y_{n+m} - y_n)U'(md) + \tfrac{1}{2}(y_{n+m} - y_n)^2U''(md) + \cdots,$$

where $U'(md)$ and $U''(md)$ are the derivatives $\partial U/\partial r$ and $\partial^2 U/\partial r^2$ evaluated at md. Substituting the Taylor expansion in Eq. (8.4), and neglecting powers of $(y_{n+m} - y_n)$ higher than the second, we obtain for the potential energy of the lattice

$$U = \sum_n \sum_{m>0} \left[U(md) + (y_{n+m} - y_n)U'(md) + \frac{1}{2}(y_{n+m} - y_n)^2U''(md) \right],$$

or

$$U = \text{const.} + \sum_n \sum_{m>0} \left[(y_{n+m} - y_n)U'(md) + \frac{1}{2}(y_{n+m} - y_n)^2U''(md) \right], \tag{8.5}$$

where the constant is given by

$$\text{Const.} = \sum_n \sum_{m>0} U(md) = n \sum_{m>0} U(md)$$

The force F_p acting on the pth particle is obtained by taking the negative derivative of the potential energy with respect to the displacement of this particle. Before performing the differentiation it should be noted that only two terms from the sum over all values of n will remain, the others dropping out because they do not contain the variable y_p. The two remaining terms will be those for which $n = p$ and $n + m = p$. m is to be positive, so the terms for which $n = p$ will give the force on particle p due to particles to the right, while terms for which $n + m = p$ give the force on particle p due to particles on the left. Therefore,

$$F_p = -\frac{\partial U}{\partial y_p} = -\frac{\partial}{\partial y_p}\sum_n \sum_{m>0} \left[(y_{n+m} - y_n)U'(md) + \frac{1}{2}(y_{n+m} - y_n)^2 U''(md)\right]$$

$$= -\frac{\partial}{\partial y_p}\sum_{m>0}\left[(y_{p+m} - y_p)U'(md) + \frac{1}{2}(y_{p+m} - y_p)^2 U''(md) + (y_p - y_{p-m})U'(md) + \frac{1}{2}(y_p - y_{p-m})^2 U''(md)\right]$$

$$= -\sum_{m>0}[-U'(md) - (y_{p+m} - y_p)U''(md) + U'(md) + (y_p - y_{p-m})U''(md)] \quad (8.6a)$$

or, writing U''_m instead of $U''(md)$,

$$F_p = \sum_{m>0} U''_m(y_{p+m} + y_{p-m} - 2y_p) \quad (8.6b)$$

These formulas require some discussion and explanation. In Eq. (8.6a), for instance, we find in the first row a term $-U'(md)$ representing the force of atom $(p + m)$ on atom p. In an

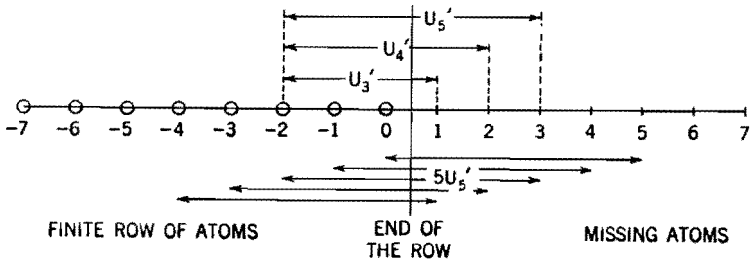


FIG. 8.1.

infinite lattice this term is compensated by an opposite force $+U'(md)$ found in the second row of Eq. (8.6a) and representing the force of atom $(p - m)$ on atom p.

The situation is different in a *finite* lattice (Fig. 8.1). Let us assume the row of atoms to extend from $n = -\infty$ to $n = 0$, with all atoms $n = 1, 2, 3, \ldots$ missing, and let us discuss the forces to be added in order to keep the structure undisturbed near the end of the row. External forces that would make up exactly for the forces that the missing atoms would produce on

the end of the row must be provided for. For instance, we must add the forces

$$U'_3, U'_4, U'_5, \ldots$$

on atom $n = -2$. This means a very complicated set of forces acting on the last atoms of the row, if the row is to be kept unperturbed with the constant distance d up to the last atom. The *total force* required on all the last atoms of the row is

$$F_t = U'_1 + 2U'_2 + 3U'_3 \cdots = \sum_{m=1}^{\infty} mU'_m \quad (8.7)$$

since there are m pairs of atoms interacting at distances md across the border. The sketch in Fig. 8.1 visualizes the situation for $m = 5$. In order to obtain a one-dimensional lattice with distance d between neighboring particles, it is *necessary* that the *total force* acting upon the end of the lattice be F_t, but the condition is not sufficient.

If this total force F_t, is differently distributed between the particles at the end of the row, two things may happen:

1. It is possible that a local perturbation of the row is produced near the end, but that at large distances from the end the equidistance d is obtained. This is usually the case, with forces decreasing rapidly when the distance is increased, such as the ones encountered in most physical problems of crystal lattices. If the forces extend only to a distance Ld, the sum in Eq. (8.7) must be taken from $m = 1$ to $m = L$, and the distance upon which the perturbation of the lattice occurs is of the order of Ld.

2. The perturbation may extend throughout the lattice and offer a periodic character as a function of the distance, thus resulting in a sort of superlattice or periodic structure with a distance $D > d$. There may also be different values $d_1, d_2, \ldots$ corresponding to the same total end force F_t.

For instance, a free row of particles is one terminating freely with no external forces added. This means that no perturbation will occur only if all terms $U'_1 = U'_2 = \ldots = U'_L = 0$, and in this case the lattice will keep the interval d up to its end. If all U'_m are not zero, a perturbation appears near the end of the lattice (case 1) or even along the whole lattice (case 2).

This one-dimensional example corresponds to the problem of

surface structure and *surface tension* for solids or liquids. In the three-dimensional problems of physics, the interaction between particles decreases very rapidly for increasing distances, and case 1 above is practically always obtained. The last L atoms of each row build a surface layer Ld deep, which surrounds the solid or liquid structure. The perturbation of the lattice inside this surface layer results in additional forces, the resultant of which is known as surface tension.

The type of perturbation in the lattice and the extent of this perturbation will be discussed later on (see Sec. 10), but we should immediately emphasize the *great complexity of the boundary conditions* for structures including *particles interacting at large distances*. The situation at the boundary cannot be defined by a set of forces acting on the last particles, but the whole distribution of these forces on the different particles at the end of the row must be specified. The usual mathematical statements about forces on the boundary are completely inadequate. A similar situation will be found in connection with problems of wave propagation across the junction of two lattices, or reflection of waves at the boundary of a lattice (see Sec. 24), where a minute description of the type of junction extending all through a boundary layer of order of thickness Ld would be required.

As for Eq. (8.6*b*) and vibrations inside an infinite lattice, the force F_p will be balanced by the inertial force so that the equation of motion for the system will be

$$F_p = M\frac{d^2y_p}{dt^2} = \sum_{m>0} U''_m(y_{p+m} + y_{p-m} - 2y_p) \tag{8.8}$$

Let us assume a wave solution for Eq. (8.8).

$$y_p = Ae^{2\pi i(\nu t - ax_p)} = Ae^{2\pi i(\nu t - apd)} \qquad a = \frac{1}{\lambda} \tag{8.9}$$

ν is, of course, the frequency and a the wave number. This gives

$$\begin{aligned} y_{p+m} + y_{p-m} - 2y_p &= Ae^{2\pi i(\nu t - apd)}(e^{-2\pi imda} + e^{2\pi imda} - 2) \\ &= -2y_p(1 - \cos 2\pi amd) = -4y_p \sin^2 \pi amd \end{aligned}$$

Therefore, Eq. (8.9) will be a solution of Eq. (8.8) if the following relation between ν and a is satisfied:

$$\begin{aligned} \frac{M\omega^2}{4} = M\pi^2\nu^2 &= \sum_{m>0} U''_m \sin^2 \pi amd \\ &= \frac{1}{2}\sum_{m>0} U''_m(1 - \cos 2\pi amd) \end{aligned} \tag{8.10}$$

with $U''_m = U''(md)$. From Eq. (8.10) we may verify at once that ν is a periodic function of a and has period $1/d$, since

$$\nu^2\left(a + \frac{1}{d}\right) = \nu^2(a)$$

and ν must be positive.

9. Rigorous Discussion for the Case of Interactions between Nearest Neighbors Only

If we assume that the interactions among the particles are negligible except for nearest neighbors, Eq. (8.10) reduces to

$$M\pi^2\nu^2 = U'' \sin^2 \pi ad \qquad U'' = U''_1 \tag{9.1}$$

This is the equation on which the qualitative discussions in the first two chapters were based. We may compute the velocity of propagation of the wave.

$$V = \frac{|\nu|}{a} = \sqrt{\frac{U''}{M}}\frac{|\sin \pi ad|}{|\pi a|} = d\sqrt{\frac{U''}{M}}\frac{|\sin \pi\, ad|}{|\pi ad|} \tag{9.2}$$

The velocity for infinite wave length V_∞ is therefore

$$V_\infty = d\sqrt{\frac{U''}{M}} \qquad \lambda \to \infty, \qquad a \to 0 \tag{9.2a}$$

and Eq. (9.2) checks with Baden-Powell's equation (2.1).

In order to set up the connection between these results and Newton's calculation for the velocity of sound in air, we must define a modulus for our discontinuous system; and this must be done in such a way that in the limit of dense spacing of our particles (*i.e.*, a continuous structure) the modulus will go over into the ordinary extension modulus, defined as tension divided by strain. In our discontinuous structure, we can define the tension between two particles as simply the force between them, and this will be equal, for the pth and $(p + 1)$st particles, to

$$U''(d)(y_{p+1} - y_p)$$

since the resultant force on the pth particle, due to both particles $(p+1)$ and $(p-1)$, is

$$U''(d)(y_{p+1} + y_{p-1} - 2y_p)$$

Furthermore, we can define the strain between particles p and $(p+1)$ as $(y_{p+1} - y_p)/d$. The modulus will, accordingly, be

$$\epsilon = dU''(d) \tag{9.3}$$

and it is evident that in the limiting case of dense spacing all our definitions will go over into the usual definitions.

If we call our modulus ϵ and the average linear density of our system ρ (*i.e.*, $\rho = M/d$), Eq. (9.2*a*) becomes

$$V_\infty = \sqrt{\frac{\epsilon}{\rho}} \tag{9.3a}$$

which is Newton's formula [Eq. (1.1)] with ϵ in place of Newton's bulk modulus ed. We can identify our U'' with Newton's elastic constant e.

For the wave length large compared with d, *i.e.*, if the lattice may be regarded as a continuous medium, the velocity is V_∞ and is independent of the wave length. As the wave length decreases, the velocity decreases and approaches $2V_\infty/\pi$, or 0.635 times V_∞, the value for infinite wave length (see Fig. 2.2). This velocity is reached at the wave length $\lambda = 2d$. For $\lambda = 2d$, there is an ambiguity in the velocity of propagation, as pointed out in an earlier section, since the wave may be propagating in either direction with velocity $0.635V_\infty$ or may be a standing wave. The cutoff frequency ν_m is obtained from Eq. (9.1) by setting $ad = \frac{1}{2}$.

$$\nu_m = \frac{1}{\pi}\sqrt{\frac{U''}{M}} \tag{9.4}$$

For frequencies lower than the limiting frequency ν_m we obtain real solutions for a. For higher frequencies a is complex, since

$$\pi^2\nu^2 M = U'' \sin^2 \pi ad \tag{9.1}$$

If we set

$$\left.\begin{aligned} a &= \pm\frac{1}{2d} \pm i\beta, \qquad k = 2\pi ad = \pm\pi \pm i2\pi\beta d \\ \sin \pi ad &= \pm \sin\frac{\pi}{2} \cos i\pi\beta d = \pm \cosh \pi\beta d \end{aligned}\right\} \tag{9.5}$$

then

$$\pi^2\nu^2 M = U'' \cosh^2 \pi\beta d \tag{9.6}$$

or

$$|\nu| = \frac{1}{\pi}\sqrt{\frac{U''}{M}}\,|\cosh \pi\beta d| \tag{9.7}$$

β is called the *attenuation coefficient*, and in the attenuation curves the magnitude of β is plotted as a function of ν. Curves representing the real and imaginary parts of $a = \alpha + i\beta$ as functions of the frequency ν have been drawn in Fig. 2.7 (Sec. 2). Between 0 and ν_m, a is real, and above ν_m the real part of a keeps a constant value $\pm 1/2d$ while the imaginary part β increases very rapidly. This means that for frequencies above the cutoff ν_m the vibration decays exponentially along the string (β term) while successive atoms oscillate in opposite directions (real part $1/2d$). This is easily seen in Fig. 2.10, which is a reproduction of one of Kelvin's original drawings. It shows that Kelvin had actually grasped all the details of this problem.

10. Discussion of the Distance of Interaction

In the case of interactions between nearest neighbors only, we find that there is a single frequency corresponding to a given wave length and that there is only one wave length larger than $2d$ for each frequency. Now if the interactions extend to the Lth neighbor, *i.e.*, to a distance of Ld, we obtain the following expression relating frequency and wave number [Eq. (8.10)]:

$$\begin{aligned} \pi^2\nu^2 M &= \sum_{0<m<L} U'''_m \sin^2 \pi amd \\ &= \frac{1}{2}\sum_{0<m<L} U''_m(1 - \cos 2\pi amd) \end{aligned} \tag{10.1}$$

For very large wave lengths

$$V_\infty{}^2 = \frac{\nu^2}{a^2} = \frac{1}{\pi^2 M}\sum_{0<m<L} U''_m \frac{\sin^2 \pi amd}{a^2} = \frac{d^2}{M}\sum_{0<m<L} U''_m m^2 \tag{10.2}$$

Thus V_∞ is still a constant whose value depends on the constants of the system. As the wave length decreases, the velocity of

propagation varies. The frequency corresponding to the limiting wave length $\lambda = 2d$, $a = 1/2d$, may be computed.

$$\nu^2 = \frac{1}{\pi^2 M} \sum_{0<m<L} U''_m \sin^2 \frac{\pi m}{2} = \frac{1}{\pi^2 M} \sum_{\substack{0<m<L \\ m \text{ odd}}} U''(md) \qquad (10.3)$$

since

$$\sin \frac{\pi m}{2} = \begin{cases} 0 & m \text{ even} \\ \pm 1 & m \text{ odd} \end{cases} \qquad (10.4)$$

so that the even terms in the sum drop out.

Returning to the general equation for ν [Eq. (10.1)], we note that to each value of a there will correspond a single frequency regardless of the extent of the interactions. Now $\cos 2\pi amd$ may be expanded as a polynomial of degree m in $\cos 2\pi ad$. Thus the frequency will be expressed as a polynomial of degree L in $\cos 2\pi ad$. This means that for a given frequency there will be L solutions for $\cos 2\pi ad$ and hence L solutions for a in the interval $-1/2d$ to $+1/2d$. The result of these remarks is that ν is a single-valued function of a, but a is not a single-valued function of ν, as shown in Fig. 10.1. It is not necessary in this case that the maximum value of the frequency appear at the ends of the interval $-1/2d \leqq a \leqq +1/2d$, but the curve must end with a horizontal tangent in any case.

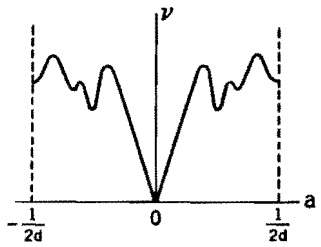


FIG. 10.1.

The L solutions for a for a given frequency need not all be real; some may be imaginary or complex. Such solutions are to be interpreted as meaning that the wave decays exponentially along the lattice. This is of special importance in the case of a finite lattice such as the one already discussed in Sec. 8 with Fig. 8.1. If we assume a sinusoidal motion of frequency ν imposed on the last particle of the lattice, the different waves corresponding to this frequency will be excited in various proportions. Those for which a is real will propagate along the lattice, and those for which a is imaginary or complex will decay exponentially from the point of excitation. If we wish to excite only one of the waves on a semiinfinite row of particles, we must impose on the

first L particles the motion characteristic of this special wave. In the case of interactions between nearest neighbors only, the boundary conditions were simple: we had only to specify the motion of the first particle. However, added interactions complicate the procedure, and the boundary conditions must be specified over a length Ld of the lattice.

The problem of the lattice at rest corresponds to the case $\nu = 0$. In drawing the curve in Fig. 10.1, it was assumed that the forces between the particles were such as to give only one real solution a for low ν values. The remaining $(L - 1)$ solutions must then be complex and result in a perturbation of the lattice that would decay exponentially from the border. The whole distance over which these exponential perturbations extend (at the limit $\nu = 0$) represents the thickness of the border in the one-dimensional case or of the surface layer in the three-dimensional problem. This assumption corresponds to case 1 discussed in Sec. 8 after Eq. (8.7). Another possibility would correspond to a curve going down to $\nu = 0$ for some $\pm a_1$ value of a, such as the curve of Fig. 10.2. Under such circumstances a steady periodic perturbation of wave length $\lambda_1 = 1/a_1$ may obtain throughout the lattice and realize a superlattice structure of period

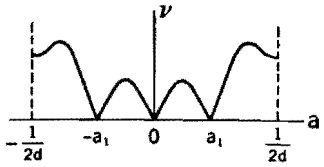


FIG. 10.2.

$$\lambda_1/d = 1/a_1 d_1$$

as anticipated in Sec. 8, case 2.

Equation (10.1) gives ν^2 as a finite Fourier expansion in a. We may use Fourier's theorem to obtain the interactions among the various particles if we assume $\nu = F(a)$ is a known function.

$$U''(md) = -4\pi^2 M d \int_{-1/2d}^{1/2d} F^2(a) \, (\cos 2\pi amd) da \qquad (10.5)$$

As an example, let us seek the interactions that would give a constant velocity of propagation W throughout the passing band. Then

$$\nu = W|a|, \qquad \nu^2 = F^2(a) = W^2 a^2$$

a is, of course, to be taken in the usual interval. Curves corresponding to this problem are shown in Fig. (10.3). Then

$$U''_m = -4\pi^2 M d W^2 \int_{-1/2d}^{1/2d} a^2(\cos 2\pi amd)da$$

$$= (-1)^{m-1}2M\frac{W^2}{m^2d^2} \quad (10.6)$$

Now U''_m is the second derivative of the interaction energy of the two particles separated by md and appears as a function defined at discrete points at intervals of d along the x axis. We may take the continuous function

$$U''(x) = -2\frac{MW^2}{x^2}\cos\frac{\pi x}{d} \quad (10.7)$$

to represent the discontinuous function. The function (10.7) has the same values as $U''(md)$ at the points where $U''(md)$ is

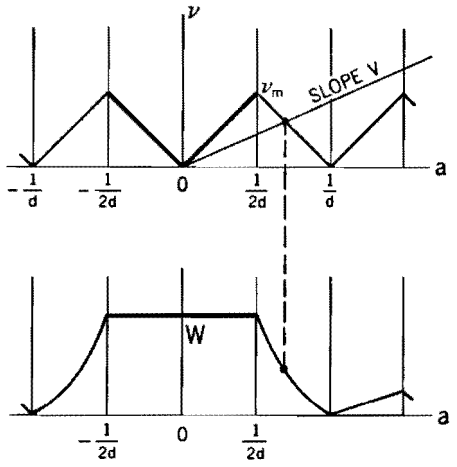


FIG. 10.3.

defined, but it is continuous, and hence we may integrate twice to find the interaction energy. The integration must be done by tables in this case. Once the function $U''(x)$ is known, however, one may construct a discontinuous line with the proper elastic forces between the elements to obtain a low-pass mechanical filter having a constant velocity of propagation for all frequencies in the passing band. The same method may be applied to a high-pass filter or to more complicated filters having one or more passing bands. For this simple example we may easily obtain ω^2, where ω is the angular frequency, 2π times the frequency ν, as a Fourier series.

$$\omega^2 = 4\pi^2\nu^2 = 4\sum_m \frac{U''_m}{2M}(1 - \cos 2\pi amd)$$

$$= \sum_m \frac{4(-1)^{m-1}W^2}{m^2d^2}(1 - \cos 2\pi amd)$$

$$= \frac{4W^2}{d^2}\left[(1 - \cos 2\pi ad) - \frac{1}{4}(1 - \cos 4\pi ad)\right.$$

$$\left. + \frac{1}{9}(1 - \cos 6\pi ad) - \frac{1}{16}(1 - \cos 8\pi ad) + \cdots\right]$$

$$= \frac{4W^2}{d^2}\left[\left(1 - \frac{1}{4} + \frac{1}{9} - \frac{1}{16} + \cdots\right) - \cos 2\pi ad\right.$$

$$\left. + \frac{1}{4}\cos 4\pi ad - \frac{1}{9}\cos 6\pi ad + \frac{1}{16}\cos 8\pi ad - \cdots\right]$$

$$= \frac{4W^2}{d^2}\left[\frac{\pi^2}{12} - \cos 2\pi ad + \frac{1}{4}\cos 4\pi ad\right.$$

$$\left. - \frac{1}{9}\cos 6\pi ad + \frac{1}{16}\cos 8\pi ad \cdots\right] \quad (10.8)$$

since

$$\frac{\pi^2}{12} = 1 - \frac{1}{4} + \frac{1}{9} - \frac{1}{16} + \cdots \quad (10.9)$$

Let us replace $2\pi ad$ by k and recall that $a = \nu/W$ to obtain

$$k^2 = 4\pi^2a^2d^2 = \frac{4\pi^2\nu^2d^2}{W^2}$$

$$= 4\left(\frac{\pi^2}{12} - \cos k + \frac{1}{4}\cos 2k - \frac{1}{9}\cos 3k + \cdots\right) \quad (10.10)$$

Thus we have k^2 as a well-known Fourier expansion in k in the interval $-\pi$, $+\pi$.

11. The Low-pass Electric Filter

The electric filter shown in Fig. 11.1 is a low-pass electric filter. The equal self-inductances L alternate with equal capacities C. The capacities shunt out the high frequencies, and the low frequencies are allowed to pass. To obtain the equations of this line, we call Q_n and V_n the charge and potential, respectively, on condenser n, while i_n will be the current flowing between condensers $(n-1)$ and n. Then

$$L\frac{di_n}{dt} = V_{n-1} - V_n = \frac{Q_{n-1}}{C} - \frac{Q_n}{C}$$

and

$$i_n - i_{n+1} = \frac{dQ_n}{dt} \tag{11.1}$$

since

$$V_n = \frac{Q_n}{C} \tag{11.2}$$

Differentiating Eq. (11.1), we obtain

$$L\frac{d^2i_n}{dt^2} = \frac{1}{C}\left(\frac{dQ_{n-1}}{dt} - \frac{dQ_n}{dt}\right) = \frac{1}{C}(i_{n-1} + i_{n+1} - 2i_n) \tag{11.3}$$

The solution of Eq. (11.3) gives the flow of current in the line, and from this the potential differences and charges on the condenser plates may be found. Equation (11.3) is identical with

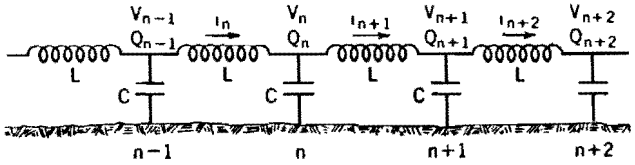


FIG. 11.1.

the equation of motion of a one-dimensional mechanical lattice [Eq. (8.8)] with interaction between nearest neighbors only (Chap. I, Sec. 2, or Chap. III, Sec. 9).

$$M\frac{d^2y_n}{dt^2} = U''_1(y_{n-1} + y_{n+1} - 2y_n) \tag{11.4}$$

U''/M is replaced by $1/LC$, and y_n is replaced by i_n. Thus all the results obtained for the low-pass mechanical filter apply automatically. The velocity of propagation for very long waves is $d/\sqrt{LC}$ where d is the distance between condensers; there is a cutoff frequency ν_m, and all frequencies higher than ν_m decay exponentially; ν is a periodic function of the wave number. From Eq. (9.4) we may compute the cutoff frequency.

$$\nu_m = \frac{1}{\pi\sqrt{LC}} \tag{11.5}$$

The low-pass electric filter shown in Fig. 11.1, to which Eq. (11.3) applies, contains no resistance. Introduction of resistance changes the properties of the line slightly. There will be a slight attenuation of frequencies in the passing band due to energy losses in the resistance, and the cutoff frequency will be less

abrupt; *i.e.*, there will be a region of rapidly increasing attenuation for increasing frequency near ν_m. This problem will be discussed in detail in Chap IX. The curves in Fig. 2.7 will be changed into those in Fig. 11.2.

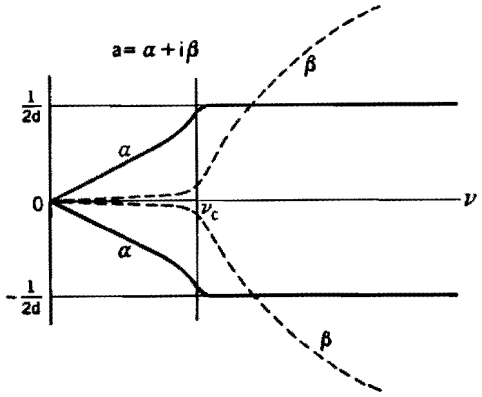


FIG. 11.2.

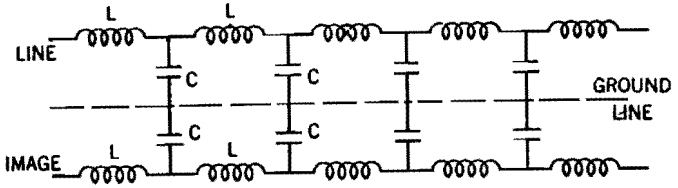


FIG. 11.3.

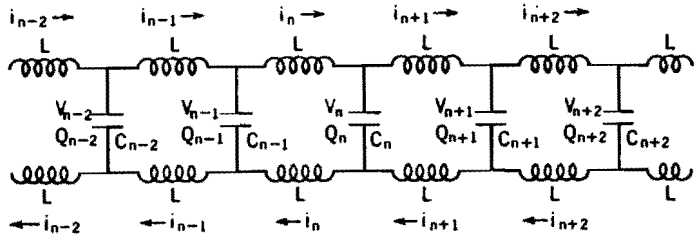


FIG. 11.4.

The single-line structure of Fig. 11.1 is equivalent to a double line (Fig. 11.3) constructed from the original line of Fig. 11.1 and its image. This can be simplified in the scheme of Fig. 11.4 with the same L values as in the single line but with capacities $\frac{1}{2}C$.

$$L' = L, \qquad C' = \frac{C}{2} \tag{11.6}$$

Hence, the double line of Fig. 11.4 has exactly the same properties as the single line, with the values

$$V_\infty = \frac{d}{\sqrt{LC}} = \frac{d}{\sqrt{2L'C'}} \qquad (11.7)$$
$$\nu_m = \frac{1}{\pi\sqrt{LC}} = \frac{1}{\pi\sqrt{2L'C'}}$$

as announced in Eq. (3.1).

12. Analogies between Electrical and Mechanical Systems

In the last section we saw that the equation for the propagation of electric waves along a low-pass electric line was of exactly the same form as that for the propagation of elastic waves along a low-pass mechanical lattice. This suggests the possibility of making an analogy between electrical and mechanical lines that will hold generally. The detailed discussion of electrical lines will be reserved for Chap. IX. However, we shall examine the problem in sufficient detail here to form a basis for an analogy with mechanical lattices.

In the last section we found that the quantity $\sqrt{1/LC}$ played the part for electrical lines that $\sqrt{U''/M}$ plays for mechanical lattices. The classical method for drawing an analogy between electromagnetic and mechanical effects is to associate electromagnetic energy with kinetic energy and electrostatic energy with potential energy. This leads to associating

$$\frac{1}{C} \text{ with } U'' \qquad \text{and} \qquad L \text{ with } M \qquad (12.1)$$

However, this method is not the only one that can be used, and we shall find another method more convenient for some purposes. The design of the system under consideration will, in general, determine the analogy to be used.

Another way in which we could make the analogy would be to take

$$U''_p \sim \frac{1}{L_p} \qquad \text{and} \qquad M \sim C \qquad (12.2)$$

For instance, this is the proper analogy to use if we wish to construct an electrical line with the same propagation properties as a lattice with equally spaced particles of equal mass and interactions between all particles. This can best be shown by constructing such a line according to Eq. (12.2) and verifying that the line equations of the two systems are exactly the same. The line is shown in Fig. 12.1. Each condenser has capacity C and is connected to its nearest neighbors through an inductance L_1. The condensers are connected to next nearest neighbors by inductances L_2 and to the pth neighbors by inductances L_p. Only L_1 and L_2 are shown in the diagram in order not to complicate it too much. The condensers are numbered as before. The current flowing through L_1 will be $i_{n-1,n}$, $i_{n,n+1}$, $i_{n+1,n+2}$, and, in general, that flowing through L_p will be $i_{n-p,n}$, $i_{n-p+1,n+1}$, $\cdots$,

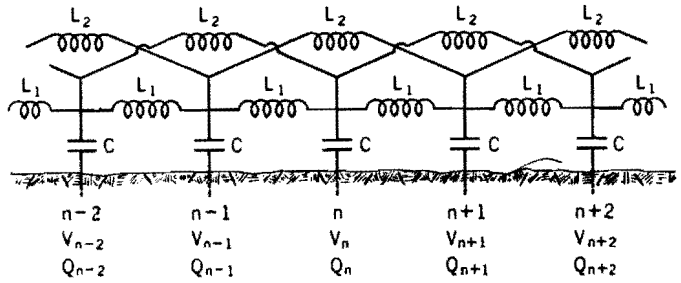


FIG. 12.1.

$i_{n-1,n+p-1}$, $i_{n,n+p}$. The second subscript on the current indicates the condenser into which the current flows, and the first subscript indicates the condenser from which the current started. The charge Q_n on condenser n will be given by

$$\frac{dQ_n}{dt} = i_{n-p,n} + i_{n-p+1,n} + \cdots + i_{n-1,n} - (i_{n,n+1} + i_{n,n+2} + \cdots + i_{n,n+p})$$
$$= \sum_p (i_{n-p,n} - i_{n,n+p}) \qquad (12.3)$$

We have the following equations for the current in the various branches of the circuit denoted by L_p, if we take the potential of condenser n to be V_n:

$$\left.\begin{aligned} L_1 \frac{d}{dt} i_{n-1,n} &= V_{n-1} - V_n = \frac{Q_{n-1} - Q_n}{C} \\ L_2 \frac{d}{dt} i_{n-2,n} &= V_{n-2} - V_n = \frac{Q_{n-2} - Q_n}{C} \\ L_p \frac{d}{dt} i_{n-p,n} &= V_{n-p} - V_n = \frac{Q_{n-p} - Q_n}{C} \end{aligned}\right\} \qquad (12.4)$$

Differentiating Eq. (12.3) and combining with Eq. (12.4), we obtain

$$C\frac{d^2Q_n}{dt^2} = C\sum_p\left(\frac{di_{n-p,n}}{dt} - \frac{di_{n,n+p}}{dt}\right)$$

$$= \sum_p \frac{Q_{n-p} + Q_{n+p} - 2Q_n}{L_p} \qquad (12.5)$$

Equation (12.5) is indeed identical with that for a row of particles, each having mass M, with interactions allowed among all neighbors [Eq. (8.8)], if we make the correlation.

$$M \sim C \qquad \text{and} \qquad U''_p \sim \frac{1}{L_p} \qquad (12.2)$$

The line shown in Fig. 12.1 will thus have the same propagation properties as the lattice of like particles with unlimited interactions (Chap. III, Sec. 8).

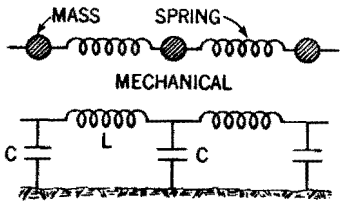


FIG. 12.2.

A geometrical argument leading to Eq. (12.2) may be given. The mechanical low-pass filter consists of point masses joined by elastic elements that we might visualize as springs. The elastic elements (Fig. 12.2) each have two ends, one connected to one mass and one to another mass, while the masses are represented by single points. An electric line having all its condensers shunting the high frequencies may be regarded as a single line with the condensers connected between the line and ground at regular intervals. Then the inductances appear as having two ends connected to different condensers, and the condensers are essentially points in the structure. Another way of looking at the problem is to regard the elastic forces as coupling forces in the lattice and the inductances as coupling forces in the electric line, while the masses and condensers are thought of as supplying inertial forces to their respective systems.

In the case of a high-pass filter, the electric circuit would have inductances leading to ground with condensers incorporated in the line and separating the inductances. In this case the inductances would have to be regarded as the points of the system and

the condensers as the parts having two ends, so that the classical analogy [Eq. (12.1)] would again hold. For a band-pass filter with a low-pass band and higher bands in addition, the inductances would have to be shunted by condensers that would be regarded as masses, since one plate of each condenser could still be taken as grounded. However, a closer analysis of the system would be necessary to decide which analogy to use, since there might be condensers elsewhere in the circuit.

There is a limit to which these analogies may be carried. It is not possible, for instance, to construct an electrical line by Eq. (12.5), giving an arbitrary relation between a and ν, as it is for a mechanical lattice (discussed in Sec. 10). The reason is that it is sometimes necessary to allow U''_p to take on negative values. This is easy to realize mechanically, but it would not be possible to obtain a negative self-inductance for the analogous electrical line.

The electrical problem offers different possibilities, if mutual inductances between the coils are used. This was first discussed by G. W. Pierce and carefully investigated by L. Brillouin (Proc. of a Symposium on Large-Scale Digital Calculating Machinery, Harvard Univ. Press, 1948, p. 110) with a discussion of the possibility of obtaining a constant velocity of propagation, as plotted on Fig. 10.3.

CHAPTER IV

MATHEMATICAL TREATMENT OF MORE COMPLICATED ONE-DIMENSIONAL LATTICES

13. Equations of Motion for the One-dimensional NaCl Lattice

The one-dimensional NaCl lattice is a special case of the one-dimensional diatomic lattice that was discussed qualitatively in Secs. 3 and 7. The general lattice is shown in Fig. 13.1. There are two masses M_1 and M_2 alternating. A given mass M_1 will have its right-hand neighbor a distance d_1 away and its left-hand

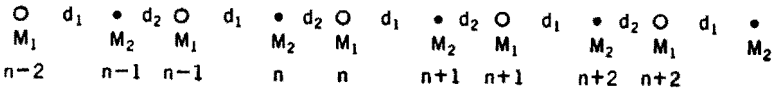


FIG. 13.1.—A row of diatomic molecules.

neighbor a distance d_2 on the other side. The period of the lattice is then

$$d = d_1 + d_2 \tag{13.1}$$

In Sec. 7 we assumed one mass, say M_2, much smaller than the other. Then M_1 was supposed to interact with the small mass nearest to it and with each of the two large masses nearest to it. The small masses were supposed to interact only with the nearest large mass. In other words, we allowed molecules as a whole to interact and then included the internal degree of freedom in our discussion.

In this section we shall discuss a slightly different lattice. The two will have the same type of curve, however, since we shall change only the rules of interaction. The *interactions* shall take place *between nearest neighbors only*, without reference to the size of the masses. This implies, of course, that we are dealing with particles that are comparable. If we limit the problem to one in which the distances are equal and the interactions of a particle with its two nearest neighbors are equal, we obtain the one-dimensional analogue of the NaCl lattice used by Born in his

theory of specific heats. The lattice is shown in Fig. 13.2. The solid dots represent particles of mass M_2 and the open circles those of mass M_1. The particles can be numbered in two different ways as shown in Figs. 13.1 and 13.2. We use the second one, where we have assigned even numbers to solid dots and odd numbers to the open circles. This means that the equilibrium coordinates of the particles with mass M_1 are $(2n + 1)d/2$, while the equilibrium coordinates of particles with mass M_2 are $2nd/2 = nd$.

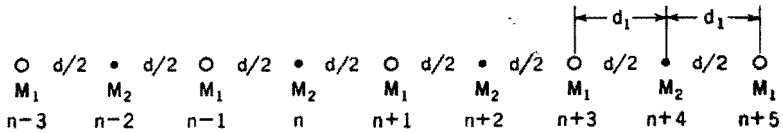


FIG. 13.2.—M. Born's model for sodium chloride.

The equations of motion of the two types of particles are different because of their different masses. If we denote the force on the mth particle by F_m, which is computed exactly as in Sec. 8, Eq. (8.6) or Eq. (11.4), we obtain for the equations of motion

$$\left.\begin{aligned} F_{2n} &= U''_1(y_{2n-1} + y_{2n+1} - 2y_{2n}) = M_2 \frac{d^2y_{2n}}{dt^2} \\ F_{2n+1} &= U''_1(y_{2n} + y_{2n+2} - 2y_{2n+1}) = M_1 \frac{d^2y_{2n+1}}{dt^2} \end{aligned}\right\} \tag{13.2}$$

where y_k is the displacement of the kth particle from its equilibrium position. Let us assume a wave solution to these equations of the following form:

$$\left.\begin{aligned} y_{2n} &= A_2 e^{i(\omega t - 2nk_1)} \\ y_{2n+1} &= A_1 e^{i(\omega t - (2n+1)k_1)} \end{aligned}\right\} \tag{13.3}$$

where

$$\begin{aligned} k &= 2\pi a d \\ k_1 &= 2\pi a \frac{d}{2} = \pi a d = \frac{1}{2}k \\ \omega &= 2\pi\nu \\ a &= \frac{1}{\lambda} \end{aligned}$$

It should be noted that the first of Eqs. (13.3) represents a wave propagating only through the particles of mass M_2, while the second represents a wave propagating only through those of

mass M_1. The wave lengths and frequencies for a given disturbance must be equal. The amplitudes of the two waves, on the other hand, are not necessarily equal. They may differ in magnitude as well as in phase.

In order that Eq. (13.3) may satisfy Eq. (13.2), certain relations must be imposed on the constants in the solution. These relations are obtained by substituting the assumed solution (13.3) in Eq. (13.2). The substitution yields

$$\begin{aligned} M_2(-A_2\omega^2) &= U''_1(A_1e^{ik_1} + A_1e^{-ik_1} - 2A_2) \\ M_1(-A_1\omega^2) &= U''_1(A_2e^{ik_1} + A_2e^{-ik_1} - 2A_1) \end{aligned}$$

The exponential term $e^{i(\omega t-2nk_1)}$ divides out of the first equation, while $e^{i[\omega t-(2n+1)k_1]}$ divides out of the second. Making use of the relation

$$e^{ik_1} + e^{-ik_1} = 2\cos k_1$$

and rearranging terms, we obtain two linear equations in A_1 and A_2.

$$\left.\begin{aligned} A_2(M_2\omega^2 - 2U''_1) + 2A_1U''_1\cos k_1 &= 0 \\ A_1(M_1\omega^2 - 2U''_1) + 2A_2U''_1\cos k_1 &= 0 \end{aligned}\right\} \tag{13.4}$$

The condition that these equations give nontrivial solutions for A_1 and A_2 is that the determinant of the coefficients of A_1 and A_2 shall vanish. This condition gives us a relation between ω and k_1 in terms of the constants of the lattice: M_1, M_2, and U''_1. Thus

$$(M_1\omega^2 - 2U''_1)(M_2\omega^2 - 2U''_1) = 4U''^2_1\cos^2 k_1$$

or, expanding,

$$\omega^4 - 2U''_1\left(\frac{1}{M_1} + \frac{1}{M_2}\right)\omega^2 + 4\frac{U''^2_1}{M_1M_2}\sin^2 k_1 = 0 \tag{13.5}$$

This equation possesses two solutions for ω^2 and hence two solutions for ω, since the frequency is always taken to be positive; *i.e.*, for each value of k_1 there will be two values of the frequency, so that the ω vs. k_1 curve will have two branches.

$$\omega^2 = U''_1\left[\left(\frac{1}{M_1} + \frac{1}{M_2}\right) \pm \sqrt{\left(\frac{1}{M_1} + \frac{1}{M_2}\right)^2 - 4\frac{\sin^2 k_1}{M_1M_2}}\right] \tag{13.6}$$

Substitution of Eq. (13.6) into Eq. (13.4) yields two equations for A_1 and A_2. These two equations are, however, not linearly independent and hence may be used only to determine the ratio A_1/A_2, which is real. The magnitudes and actual phases of the amplitudes for the two waves will depend on the initial conditions.

14. Electrical Analogue of the One-dimensional Diatomic Lattice

To construct the electrical line analogous to the one-dimensional diatomic lattice, we must use the classical method of association [Eq. (12.1)]. This means that since we have two masses in the mechanical model, we must have two inductances in the electrical model. We could generalize the problem treated in the preceding section and allow different coupling between the two masses or, what amounts to the same thing, allow the distance between M_1 and M_2 to be different on the two sides of the particle.

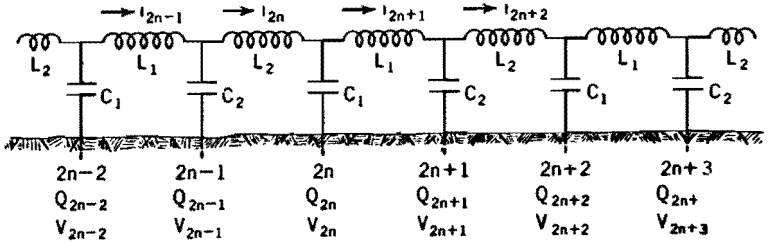


FIG. 14.1.—Electric line corresponding to the sodium-chloride model.

This would give an electric line with condensers C_1 and C_2 alternating. The condenser C_1 to the right of a given condenser C_2 would be joined to it by an inductance L_2, while the condenser C_1 to the left would be joined by an inductance L_1. This arrangement would, in general, be analogous to the mechanical model described in Sec. 7.

The electric line is shown in Fig. 14.1. As before, i_m represents current flowing from condenser $(m-1)$ to condenser m as in the case of Fig. 11.3. The fundamental equations are

$$i_{2n} - i_{2n+1} = \frac{dQ_{2n}}{dt}; \qquad i_{2n+1} - i_{2n+2} = \frac{dQ_{2n+1}}{dt} \tag{14.1}$$

$$\left.\begin{aligned} L_1\frac{di_{2n+1}}{dt} &= V_{2n} - V_{2n+1} = \frac{Q_{2n}}{C_1} - \frac{Q_{2n+1}}{C_2} \\ L_2\frac{di_{2n}}{dt} &= V_{2n-1} - V_{2n} = \frac{Q_{2n-1}}{C_2} - \frac{Q_{2n}}{C_1} \end{aligned}\right\} \tag{14.2}$$

Differentiating Eq. (14.2) and combining with Eq. (14.1) will yield

$$\left.\begin{aligned} L_1\frac{d^2i_{2n+1}}{dt^2} &= \frac{i_{2n}-i_{2n+1}}{C_1}-\frac{i_{2n+1}-i_{2n+2}}{C_2} \\ L_2\frac{d^2i_{2n}}{dt^2} &= \frac{i_{2n-1}-i_{2n}}{C_2}-\frac{i_{2n}-i_{2n+1}}{C_1} \end{aligned}\right\} \tag{14.3}$$

These two equations would be identical with Eq. (13.2) for the diatomic lattice treated in the last section if $C_1 = C_2$ and we replaced capacitance by the elastic constant and inductance by mass.

The solution of Eq. (14.3) is carried out in exactly the same way as that of Eq. (13.2). We assume wave solutions for i_{2n} and i_{2n+1} with the same frequency and wave number but with different amplitudes, as in Eq. (13.3).

$$i_{2n} = A_2 e^{i(\omega t - 2nk_1)}, \qquad i_{2n+1} = A_1 e^{i[\omega t-(2n+1)k_1]} \tag{14.4}$$

Substitution in Eq. (14.3) gives two equations linear in the amplitudes

$$\left.\begin{aligned} \left(-L_1\omega^2+\frac{1}{C_1}+\frac{1}{C_2}\right)A_1-\left(\frac{1}{C_1}e^{ik_1}+\frac{1}{C_2}e^{-ik_1}\right)A_2 &= 0 \\ \left(-L_2\omega^2+\frac{1}{C_1}+\frac{1}{C_2}\right)A_2-\left(\frac{1}{C_2}e^{ik_1}+\frac{1}{C_1}e^{-ik_1}\right)A_1 &= 0 \end{aligned}\right\} \tag{14.5}$$

These simultaneous linear equations in A_1 and A_2 have a nontrivial solution if their determinant vanishes.

$$\left(-L_1\omega^2+\frac{1}{C_1}+\frac{1}{C_2}\right)\left(-L_2\omega^2+\frac{1}{C_1}+\frac{1}{C_2}\right) - \left(\frac{1}{C_1}e^{ik_1}+\frac{1}{C_2}e^{-ik_1}\right)\left(\frac{1}{C_2}e^{ik_1}+\frac{1}{C_1}e^{-ik_1}\right) = 0 \tag{14.6}$$

which reduces to

$$\omega^4-\omega^2\left(\frac{1}{L_1}+\frac{1}{L_2}\right)\left(\frac{1}{C_1}+\frac{1}{C_2}\right)+4\frac{\sin^2 k_1}{L_1L_2C_1C_2}=0 \tag{14.7}$$

the solution of which is

$$\omega^2 = \frac{1}{2}\left(\frac{1}{L_1}+\frac{1}{L_2}\right)\left(\frac{1}{C_1}+\frac{1}{C_2}\right) \pm \sqrt{\frac{1}{4}\left(\frac{1}{L_1}+\frac{1}{L_2}\right)^2\left(\frac{1}{C_1}+\frac{1}{C_2}\right)^2-\frac{4\sin^2 k_1}{L_1L_2C_1C_2}} \tag{14.8}$$

This reduces to the expression (13.6) obtained for the mechanical case if $L_1 = M_2$, $L_2 = M_1$, and $1/U''_1 = C_1 = C_2$. There will be two branches to the ω vs. k_1 curve whether $L_1 \neq L_2$ or not, but taking $C_1 \neq C_2$ would distort the shape of the curves.

This problem was discussed by electrical engineers[1] who did not notice the similarity with the one-dimensional NaCl lattice discussed by Born. The problem originated from an attempt to join an aerial telephonic line with a city cable, as shown in

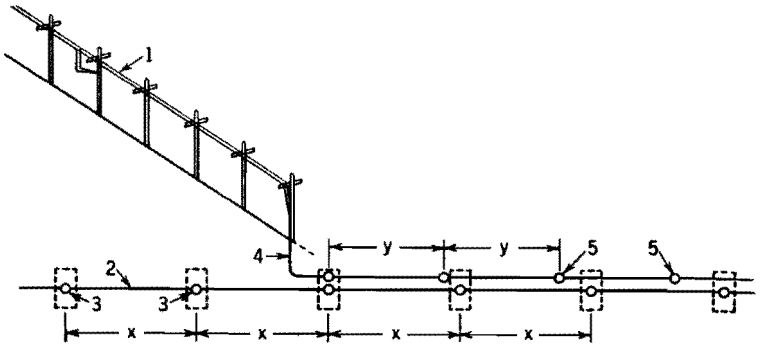


FIG. 14.2.—Junction of an aerial line with an underground cable.

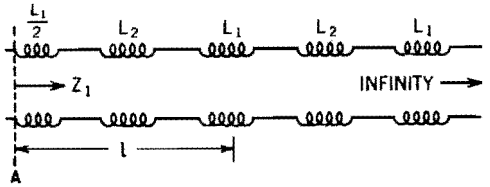


FIG. 14.3.

Fig. 14.2. In order to obtain a correct junction at 4, where the line is connected with the cable, it would be necessary to load the cable with equal coils at a distance y, y, ... This results from two conditions that must be satisfied in order to match the line and the cable at their junction: (1) to have the same passing bands, and (2) to have the same characteristic impedances (see Chap. V). The difficulty was that the underground city cable was already built to receive its loading coils at given distances x, x, ... The solution proposed consists in using alternately two types of coils L_1 and L_2 (Fig. 14.3), resulting in a structure

[1] FRENCH, N. R., U.S. patent 1,741,926, Dec. 31, 1929; S. P. MEAD and N. R. FRENCH, U.S. patent 1,769,959, July 8, 1930.

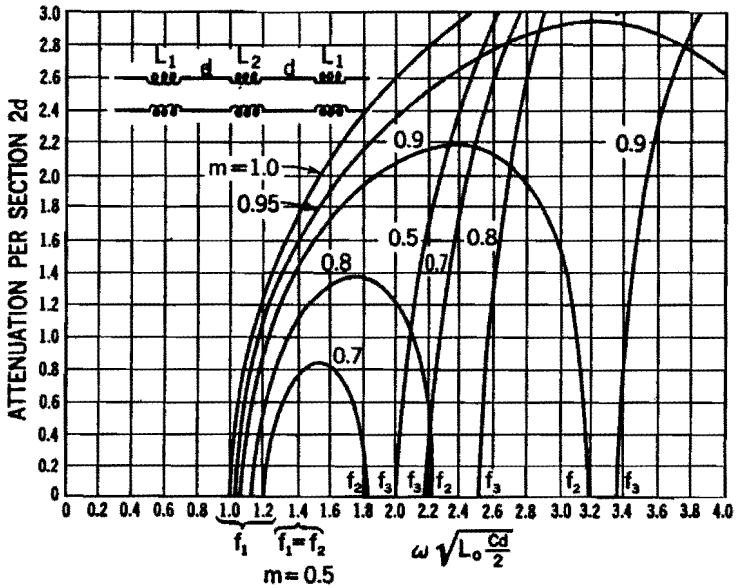


FIG. 14.4.—Curves computed by Mead and French. Compare with Fig. 7.3 or 3.9*b*.

practically identical with the one of Fig. 14.1. Attenuation curves for different values of m [$L_1 = mL_0$, $L_2 = (1 - m)L_0$, L_0 a constant] were computed and are shown in Fig. 14.4. They are identical with the attenuation curves β shown in Fig. 3.9*b*, which were obtained by Born for the NaCl structure, the theory of which will now be discussed.

15. Discussion of the One-dimensional NaCl Lattice

In this section we shall discuss the motion given by the two branches of the ω vs. $k_1 = k/2$ curve with particular attention to the case $k_1 = 0$ and $k_1 = \pm\pi/2$. The relation between ω and k_1 is given by Eq. (13.6).

$$\omega^2 = U''_1\left[\left(\frac{1}{M_1} + \frac{1}{M_2}\right) \pm \sqrt{\left(\frac{1}{M_1} + \frac{1}{M_2}\right)^2 - \frac{4\sin^2 k_1}{M_1M_2}}\right] \tag{13.6}$$

or, rearranging terms,

$$\omega^2 = \frac{U''_1}{M_1M_2}(M_1 + M_2 \pm \sqrt{M_1^2 + M_2^2 + 2M_1M_2\cos 2k_1}) \tag{15.1}$$

Equation (15.1) is completely symmetrical in M_1 and M_2, and we may therefore assume M_1 the larger of the two masses without loss of generality.

$$M_1 > M_2$$

The ratio of the amplitudes of the waves may be obtained from either of Eqs. (13.4). Both give the same result in terms of k_1. Using the first,

$$\frac{A_1}{A_2} = \frac{2U''_1 - M_2\omega^2}{2U''_1\cos k_1} \tag{15.2}$$

and, substituting Eq. (15.1) for ω^2, we obtain

$$\frac{A_1}{A_2} = \frac{M_1 - M_2 \mp \sqrt{M_1^2 + M_2^2 + 2M_1M_2\cos 2k_1}}{2M_1\cos k_1} \tag{15.3}$$

The minus sign in Eq. (15.3) corresponds to the plus sign in Eq. (15.1) or the upper branch of the ω vs. k_1 curve, while the plus sign of Eq. (15.3) corresponds to the minus sign of Eq. (15.1) or the lower branch. It should be noted that the amplitude ratio is always real; therefore, the waves may have only two phase relations: phase difference zero if $A_1/A_2 > 0$, and phase difference π if $A_1/A_2 < 0$. This is typical of a system without any resistance and with no damping.

For large wave lengths λ, $k_1 \to 0$ as does k. For this case we may set

$$\cos 2k_1 \approx 1 - 2k_1^2 = 1 - \tfrac{1}{2}k^2 \approx \cos k$$

where

$$k_1 = 2\pi a d_1 = \pi a d = \tfrac{1}{2}k$$

and the radical in Eq. (15.1) becomes

$$\begin{aligned}\sqrt{M_1^2 + M_2^2 + 2M_1M_2\left(1 - \frac{k^2}{2}\right)} &= (M_1 + M_2)\sqrt{1 - \frac{k^2M_1M_2}{(M_1 + M_2)^2}} \\ &\approx (M_1 + M_2)\left(1 - \frac{1}{2}\frac{k^2M_1M_2}{(M_1 + M_2)^2}\right)\end{aligned} \tag{15.4}$$

and Eq. (15.1) reduces to

$$\left.\begin{aligned}\omega_-^2 &= \frac{k^2U''_1}{2(M_1 + M_2)} && \text{lower branch} \\ \omega_+^2 &= 2U''_1\left[\frac{1}{M_1} + \frac{1}{M_2} - \frac{k^2}{4(M_1 + M_2)}\right] && \text{upper branch}\end{aligned}\right\} \tag{15.5}$$

The subscripts + and − denote the sign used before the radical. Thus ω_- is linear in k near the origin as in the case of like particles; ω_+ has a maximum at the origin and decreases parabolically as $|k|$ increases.

To interpret properly the meaning of a second frequency for infinite wave length, we must compute the amplitude ratio for small k_1. Substitution of Eq. (15.4) into Eq. (15.3) yields the following relations for small k (powers of k higher than the second are neglected):

$$\left.\begin{aligned}\left(\frac{A_1}{A_2}\right)_+ &= 1 + \frac{k^2}{8}\frac{M_1 - M_2}{M_1 + M_2} && \text{lower branch}\\ \left(\frac{A_1}{A_2}\right)_- &= -\frac{M_2}{M_1}\left(1 - \frac{k^2}{8}\frac{M_1 - M_2}{M_1 + M_2}\right) && \text{upper branch}\end{aligned}\right\} \tag{15.6}$$

Thus the lower branch increases parabolically at the origin as $|k|$ increases from zero. At $k = 0$

$$\left(\frac{A_1}{A_2}\right)_+ = 1, \qquad \left(\frac{A_1}{A_2}\right)_- = -\frac{M_2}{M_1}; \qquad |k| << 1 \tag{15.7}$$

The waves corresponding to the lower branch have equal amplitudes and phase difference zero; thus all the particles are displaced by the same amount and in the same direction. The wave length of each of the waves is infinite, and the lattice is displaced as a whole. There is thus no restoring force, and the frequency is zero. On the other hand, the waves for the upper branch are exactly out of phase; *i.e.*, the displacement of particles of mass M_1 is opposite to that of the neighboring particles M_2. Evidently the center of mass of two neighboring particles is stationary, but restoring forces enter in so that the frequencies of the waves are no longer zero. The lengths of the waves are still infinite since each wave is regarded as propagating through just one type of particle.

The values for k on the limits of the interval to which k is restricted are $\pm\pi$. The two limits will be symmetrical, and we consider only the case

$$k = \pi - \epsilon = 2k_1 \qquad \epsilon \text{ small}$$

Then

$$\cos k = \cos(\pi - \epsilon) = -\cos\epsilon \approx -1 + \frac{\epsilon^2}{2}$$

and the radical in Eq. (15.1) becomes

$$\sqrt{\cdots} = (M_1 - M_2)\left[1 + \frac{\epsilon^2 M_1 M_2}{2(M_1 - M_2)^2}\right]$$

if $(M_1 - M_2)$ is not too small. Substitution in Eq. (15.1) yields

$$\left.\begin{aligned}\omega_+^2 &= \frac{2U''_1}{M_2} + \frac{U''_1\epsilon^2}{2(M_1 - M_2)}\\ \omega_-^2 &= \frac{2U''_1}{M_1} - \frac{U''_1\epsilon^2}{2(M_1 - M_2)}\end{aligned}\right\} \tag{15.8}$$

so that the upper branch increases parabolically from

$$\omega = \sqrt{\frac{2U''_1}{M_2}}$$

while the lower branch decreases parabolically from

$$\omega = \sqrt{\frac{2U''_1}{M_1}}$$

as $|\epsilon|$ increases from zero. It should be noted that $\omega_+ > \omega_-$ at the limits of the interval since $M_1 > M_2$, and between these limiting values of ω we have a stopping band to be discussed later.

The amplitude ratio at the ends of the interval is easily obtained. We have

$$\cos k_1 = \cos\left(\frac{\pi}{2} - \frac{\epsilon}{2}\right) \approx \frac{\epsilon}{2}$$

(since $k = 2k_1$), and therefore from Eq. (15.3)

$$\left(\frac{A_1}{A_2}\right)_- = \frac{M_1 - M_2 - (M_1 - M_2)\left[1 + \epsilon^2\dfrac{M_1 M_2}{2(M_1 - M_2)^2}\right]}{\epsilon M_1} = \frac{-\epsilon M_1 M_2}{2M_1(M_1 - M_2)} \to 0 \tag{15.9a}$$

$$\left(\frac{A_1}{A_2}\right)_+ = \frac{M_1 - M_2 + (M_1 - M_2)\left[1 + \dfrac{\epsilon^2 M_1 M_2}{2(M_1 - M_2)^2}\right]}{\epsilon M_1} = \frac{2(M_1 - M_2) + \dfrac{\epsilon^2 M_1 M_2}{2(M_1 - M_2)}}{\epsilon M_1} \to \infty \tag{15.9b}$$

as $\epsilon \to 0$. The interpretation of these ratios is not very difficult. We have already seen that for the upper branch $[(A_1/A_2)_-, \omega_+]$

the amplitude ratio is negative and different from zero at and near the origin. Equation (15.9a) shows that it is negative near the ends of the interval $|k| \leqq \pi$ and zero at the ends. Then for infinite wave length the particles oscillate in opposite directions, the lighter particles with larger amplitude. As the wave length decreases, the amplitude of the heavy particles decreases, and for the limiting wave length the light particles oscillate while the heavy particles remain at rest.

For the lower branch $[(A_1/A_2)_+, \omega_-]$, on the other hand, the particles start out all in phase and with equal amplitudes for infinite wave length. As the wave length decreases, the amplitude of the light particles decreases, and they remain at rest for

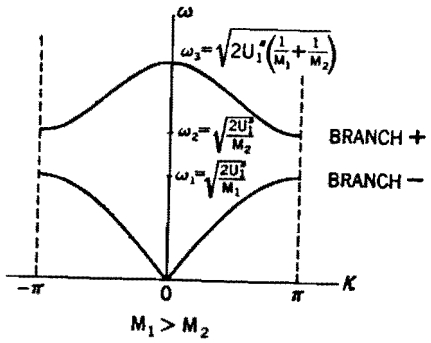


FIG. 15.1.

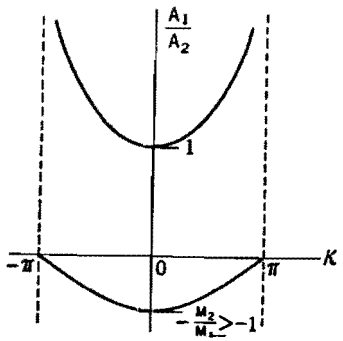


FIG. 15.2.

the limiting wave length while the heavy particles are still oscillating.

These results are summarized in Figs. 15.1 through 15.3. Figure 15.1 shows ω as a function of k for $M_1 > M_2$. Figure 15.2 shows the variation of the amplitude ratio for the two branches, and Fig. 15.3 gives the motion of the particles for the various cases discussed. The arrows in Fig. 15.3 indicate the amplitudes with which the two types of particles oscillate. Figure 15.3 shows clearly that the motions obtained for ν_1 and ν_2 are very similar: for ν_1 the particles M_2 are all at rest, and particles M_1 move in alternate directions. For ν_2, M_1 is at rest and M_2 moving. The forces involved are the same in both cases, since changes in the distances between particles are the same; hence, the frequency ratio must be proportional to the square root of the inverse ratio of the masses.

$$\frac{\nu_1}{\nu_2} = \sqrt{\frac{M_2}{M_1}}$$

as is actually obtained.

The lower branch is frequently called the *acoustical* branch. This name comes from the fact that the frequencies in it are of the same order of magnitude as acoustical or supersonic vibrations. The upper branch is frequently called the *optical* branch, because of the fact that its frequencies are of the order of magnitude of infrared frequencies. Further, if we think of the lattice

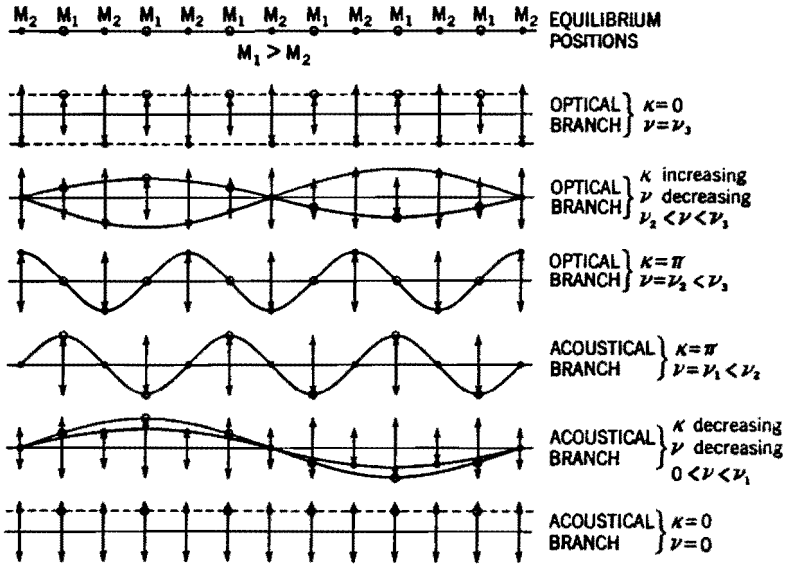


FIG. 15.3.

as being composed of ions having alternate signs, *e.g.*, Na^+ ions alternating with Cl^- ions, an alternating electric field could not excite the acoustical type of wave in which two neighboring particles are in phase, but it could excite the optical type and displace neighboring particles in opposite directions.

So far we have discussed only the passing bands of our lattice. We now consider the stopping bands. These occur for frequencies between ω_1 and ω_2 and for frequencies above ω_3. We return to Eq. (13.5).

$$-\left(\frac{\omega^2}{2U''_1}\right)^2 M_1M_2 + \frac{\omega^2}{2U''_1}(M_1 + M_2) = \sin^2 k_1 = \sin^2 \frac{k}{2}$$

We may rewrite this in the form

$$\omega^2\left(\frac{M_1+M_2}{2U''_1}-\frac{\omega^2M_1M_2}{4U''_1{}^2}\right)=\sin^2\frac{k}{2} \tag{15.10}$$

We have seen that as ω increases from zero to $\omega_1 = 2\pi\nu_1$, the expression on the right increases from zero to one. If ω increases still further, the expression on the right becomes greater than one, and $k/2$ must become complex. Let

$$k=\alpha+i\beta \tag{15.11}$$

Then

$$\sin\frac{k}{2}=\sin\frac{\alpha}{2}\cosh\frac{\beta}{2}+i\cos\frac{\alpha}{2}\sinh\frac{\beta}{2} \tag{15.12}$$

and since this expression must be real, we have the condition that

$$\cos\frac{\alpha}{2}\sinh\frac{\beta}{2}=0 \qquad \text{or} \qquad \frac{\alpha}{2}=\frac{\pi}{2} \tag{15.13}$$

That is, R.P. $k = \pi = 2\pi ad$ so that R.P. $a = 1/2d$ throughout the stopping band $\omega_1 < \omega < \omega_2$. R.P. means "the real part of." Somewhere between ω_1 and ω_2 the expression on the right of Eq. (15.10) reaches a maximum and starts to decrease. It equals one at ω_2 and is positive and less than one between ω_2 and ω_3. At ω_3 it is zero, and as ω increases still further, it becomes negative. In other words, Eq. (15.12) becomes pure imaginary and therefore

$$\sin\frac{\alpha}{2}\cosh\frac{\beta}{2}=0 \qquad \text{or} \qquad \frac{\alpha}{2}=0 \tag{15.14}$$

This means that

$$k=i\beta=2\pi ad$$

Hence

$$\text{R.P. } a=0 \qquad\qquad \omega>\omega_3$$

Since the real part of k is constant throughout both stopping bands and only the imaginary part varies, we have attenuation of the waves. In the first case $\omega_1 < \omega < \omega_2$ at the low frequency end ω_1 of the stopping band, the light particles are at rest and the heavy particles are in motion, neighboring heavy particles being just out of phase; and at the other end ω_2 the heavy particles are at rest with the light particles vibrating out of phase. The motion is attenuated along the lattice (*i.e.*, the amplitude of the vibrations decreases from particle to particle) with an attenuation constant that first increases with the frequency. Somewhere in the stopping band the motion changes from acoustical type to optical type, and as ω increases the attenuation decreases until $\omega = \omega_2$, where it becomes zero.

In the other stopping band $\omega > \omega_3$ the particles are vibrating in opposite phase with the limiting wave length. This motion is attenuated with an attenuation coefficient that increases as ω increases.

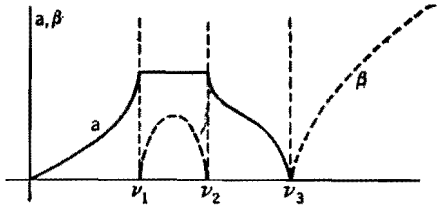


FIG. 15.4.

Curves of wave number a and of attenuation coefficient β against frequency are shown in Fig. 15.4. (Compare with Fig. 14.4.)

16. Transition from a Diatomic to a Monatomic Lattice

The diatomic lattice discussed in the last section is exactly like the monatomic lattice discussed previously except that two masses appear instead of only one; *i.e.*, the distances between neighboring particles are all the same and the interactions are restricted to nearest neighbors. The diatomic lattice may be reduced to a monatomic lattice in three ways:

1. Let $M_2 \to 0$.
2. Let $M_1 \to \infty$.
3. Let $M_1 \to M_2$.

The first two methods leave the period d of the lattice unchanged, while the last halves the period and results in a lattice $d/2 = d_1$. We shall discuss the three methods in the order given above.

1. *Let* $M_2 \to 0$.—In this case $\omega_1 = \sqrt{2U''_1/M_1}$ is unchanged, while $\omega_2 = \sqrt{2U''_1/M_2}$ and $\omega_3 = \sqrt{\omega_1^2+\omega_2^2}$ both go to infinity. The width of the upper passing band goes to zero; for

$$\omega_3-\omega_2=\sqrt{\omega_1^2+\omega_2^2}-\omega_2=\omega_2\left(\sqrt{\frac{\omega_1^2}{\omega_2^2}+1}-1\right)$$
$$\to\omega_2\frac{1}{2}\left(\frac{\omega_1}{\omega_2}\right)^2\to 0 \tag{16.1}$$

Thus the upper band rises and becomes narrower, finally disappearing entirely. The lower branch remains, and we have a low-pass filter with period $d = 2d_1$ left.

2. *Let* $M_1 \to \infty$.—Here $\omega_1 = \sqrt{2U''_1/M_1}$ goes to zero. ω_2 remains unchanged and $\omega_3 \to \omega_2$. Thus in the limiting case there is only a single frequency $\omega_2 = \sqrt{2U''_1/M_2}$, and this frequency does not really propagate. Each of the light particles oscillates separately with frequency ω_2. This corresponds to the case of a row of harmonic oscillators with no interaction. The heavy masses are responsible for the restoring force on the oscillators but take no part in the motion themselves. The amplitude

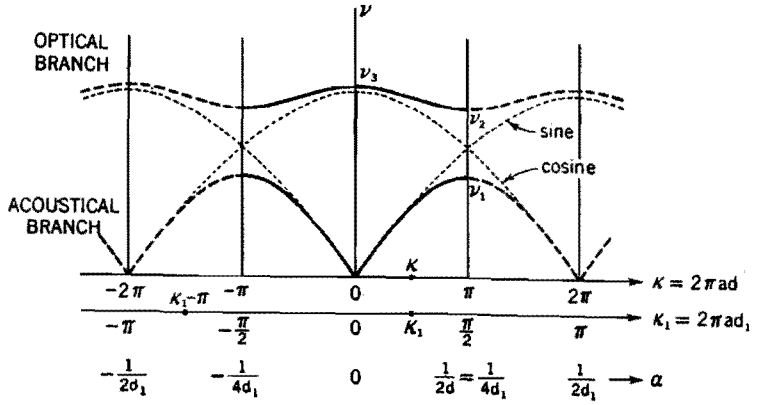


FIG. 16.1.

of the vibration is, of course, restricted to values less than d_1; the light particles must not go through the heavy particles.

Had we allowed interactions between second neighbors as well as nearest neighbors, we would have obtained in the limiting case a lattice of coupled harmonic oscillators that would lead to a band-pass filter. The single frequency present for independent oscillators would spread out into a band; the lower branch present in the diatomic lattice would still be missing.

3. *Let* $M_1 \to M_2$.—This process is considerably more complicated than the previous two because a sudden change in the periodicity of the lattice is involved. The original structure, with $M_1 > M_2$, repeats itself after a distance d, but when $M_1 = M_2$, the period suddenly drops to $d_1 = d/2$. Let us first discuss the relation between frequency and wave number $a = 1/\lambda$. This relation was shown in Fig. 15.1, which must be

understood as representing only one section of a periodic curve, as drawn in Fig. 16.1. The central section (Fig. 15.1) corresponds to $-\pi < k < \pi$ where $k = 2\pi ad$ as usual, and the complete curve is obtained when k takes any arbitrary value.

When $M_1 = M_2$, two changes must be made:

a. The change in periodicity results in a sudden extension of the fundamental interval. For a lattice with period d, the wave number a has period $1/d$, and its fundamental interval extends from $-1/2d$ to $+1/2d$. When the lattice period changes to $d_1 = d/2$, the wave-number period becomes $1/d_1 = 2/d$, and the fundamental interval is $\pm 1/2d_1 = \pm 1/d$.

The following table summarizes the changes in a, k, and k_1:

	Period for				Fundamental interval	
	Lattice	a	k	k_1	k	k_1
$M_1 > M_2$	d	$\frac{1}{d}$	2π	π	$\pm\pi$	$\pm\frac{\pi}{2}$
$M_1 = M_2$	$d_1 = \frac{d}{2}$	$\frac{1}{d_1} = \frac{2}{d}$	4π	2π	$\pm 2\pi$	$\pm\pi$

(16.2)

where $k = 2\pi ad$ and $k_1 = 2\pi ad_1 = k/2$.

b. Another change in the curve is that it must become a single curve as in Fig. 2.4 instead of the double curve of Fig. 15.1. The single curve is drawn as a dotted line in Fig. 16.1, assuming that $M_1, M_2 \to M = 2\sqrt{M_1M_2/(M_1 + M_2)}$ simultaneously.

All this can be obtained from Eq. (13.6), giving the frequency as a function of k_1. If we take $M_1 = M_2 = M$, the formula reduces to

$$\frac{M\omega_2}{2U''_1} = 1 \pm \sqrt{1 - \sin^2 k_1} = 1 \pm \cos k_1 = \begin{cases} 2\sin^2\frac{k_1}{2} \\ 2\cos^2\frac{k_1}{2} \end{cases} \tag{16.3}$$

Selecting the sine function, we obtain

$$\omega = 2\sqrt{\frac{U''_1}{M}}\left|\sin\frac{k_1}{2}\right| \tag{16.4}$$

which is identical with Eq. (9.1) for the monatomic structure (Fig. 2.4). The cosine curve duplicates the results and in its

middle part represents the upper curve of Fig. 16.1. The sine and cosine curves intersect at a point that is the common limit of ω_1 and ω_2.

$$\omega_1 \to \omega_2 \to \sqrt{\frac{2U''_1}{M}} \qquad M_1 \to M_2 \to M$$

and the stopping band disappears.

Another aspect of this transformation refers to the description of the wave and of the motion of the particles of the lattice. Referring to Eq. (13.3),

$$\left.\begin{aligned} y_{2n} &= A_2 e^{i(\omega t - 2nk_1)} \\ y_{2n+1} &= A_1 e^{i[\omega t - (2n+1)k_1]} \end{aligned}\right\} \tag{13.3}$$

we see that the solution for the lattice (with $M_1 > M_2$) is represented as two waves, one propagating along particles of mass M_2 and the other propagating along particles of mass M_1. The wave number k_1 is therefore to be restricted to values between $-\pi/2$ and $+\pi/2$. For the discussion of this section, it will be convenient to *change* our conventions and obtain the solution (13.3) as a *wave propagating through all of the particles.* This means that we must allow k_1 to take on values in the larger interval from $-\pi$ to π. To achieve this we introduce two new quantities C and D, defined by

$$\left.\begin{aligned} A_1 &= C - D = C + De^{i(2n+1)\pi} \\ A_2 &= C + D = C + De^{i(2n\pi)} \end{aligned}\right\} \tag{16.5}$$

From Eq. (16.5) it follows that

$$\frac{D}{C} = \frac{A_2 - A_1}{A_2 + A_1}$$

Equation (13.3) may now be written

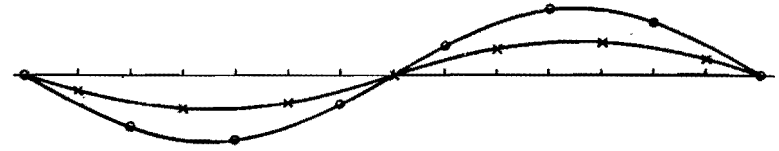
$$\begin{aligned} y_{2n} &= Ce^{i(\omega t - 2nk_1)} + De^{i[\omega t - 2n(k_1 - \pi)]} \\ y_{2n+1} &= Ce^{i[\omega t - (2n+1)k_1]} + De^{i[\omega t - (2n+1)(k_1 - \pi)]} \end{aligned}$$

and the sum of the two waves

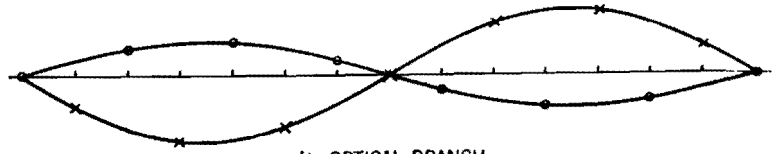
$$y_m = Ce^{i(\omega t - mk_1)} + De^{i[\omega t - m(k_1 - \pi)]} \tag{16.6}$$

gives a single wave propagating through all (both M_1 and M_2) particles. The two methods of representing the wave are shown in Figs. 16.2*a* to 16.3*b*. Figure 16.2 shows the representation

with two waves, one passing through each set of particles. The *a* part is for the acoustical and the *b* part for the optical branch. Figure 16.3 shows the k_1 and $k_1 - \pi$ waves and their sums for the acoustical and optical branches in *a* and *b*, respectively. It

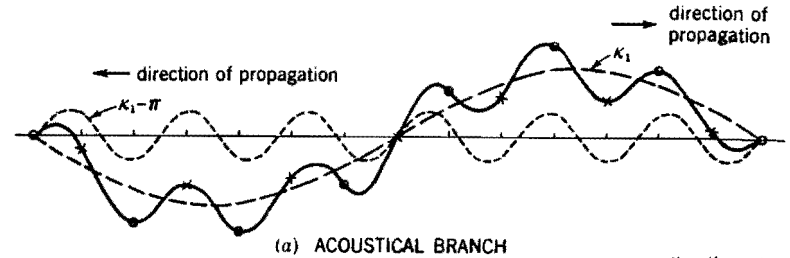


(*a*) ACOUSTICAL BRANCH

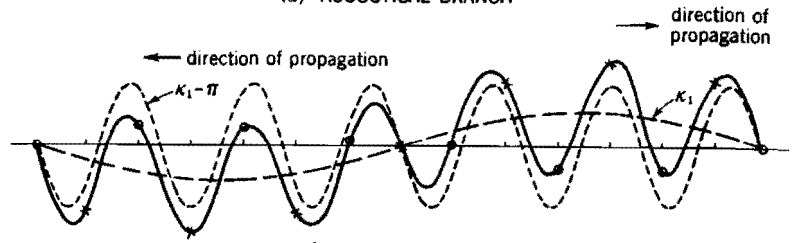


(*b*) OPTICAL BRANCH

FIG. 16.2.



(*a*) ACOUSTICAL BRANCH



(*b*) OPTICAL BRANCH

FIG. 16.3.

should be noted that the k_1 and k_1-π waves propagate in opposite directions, so that one may think of the wave propagating to the right as being partially reflected as it traverses each particle, thus giving rise to a disturbance that consists of a transmitted and a reflected wave.

In order to see clearly how the transition from the diatomic to the monatomic lattice takes place, we must refer to Table (16.2), which shows the interval of variation for k_1 in both cases. The original k_1 was restricted to values between $-\pi/2$ and $\pi/2$, which means that $k_1 - \pi$ varies between $-\pi$ and $-\pi/2$ for $k_1 > 0$ or $\pi/2$ and π for $k_1 < 0$, since k_1 and $k_1 + 2\pi$ are equivalent. This

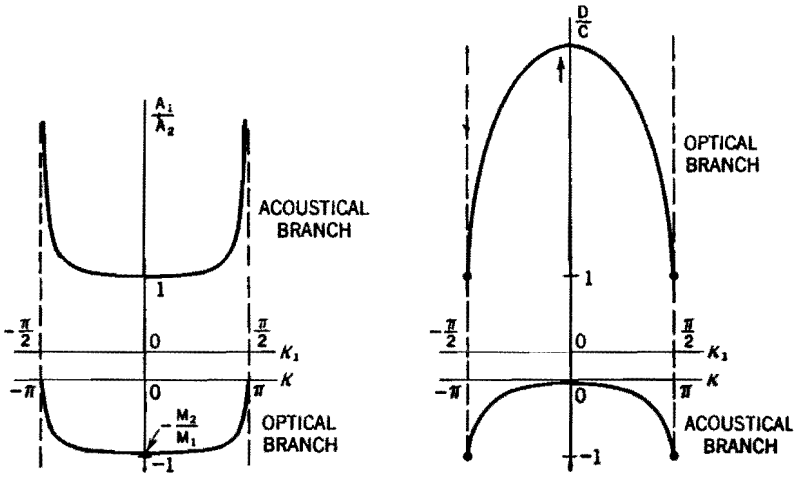
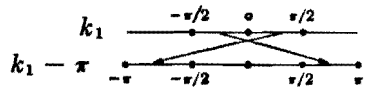


FIG. 16.4.

extends the interval to $-\pi$, π as shown in Table (16.2). The following scheme summarizes this transformation:



$$(k_1 - \pi + 2\pi = k_1 + \pi) \qquad (16.7)$$

This explains the correspondence between the different branches of the curves in Fig. 16.1.

We have previously discussed the variation of the ratio A_1/A_2 for the different types of waves [Eq. (15.3) and Fig. 15.2]. These same curves were drawn again in Fig. 16.4*a* under the assumption of a very small difference between the masses.

$$M_2 = M_1(1 - \epsilon) \qquad \epsilon << 1$$

In this case Eq. (15.3) reduces to

$$\frac{A_1}{A_2} = \frac{1 - \frac{M_2}{M_1} \mp \sqrt{1 + \left(\frac{M_2}{M_1}\right)^2 + 2\frac{M_2}{M_1}\cos 2k_1}}{2\cos k_1}$$

$$= \frac{\epsilon \mp \sqrt{2 + 2(1-\epsilon)\cos 2k_1 - 2\epsilon + \epsilon^2}}{2\cos k_1}$$

$$= \frac{\frac{\epsilon}{2} \mp \sqrt{\cos^2 k_1(1-\epsilon) + \left(\frac{\epsilon}{2}\right)^2}}{\cos k_1} \approx \frac{\epsilon}{2\cos k_1} \mp \left(1 - \frac{\epsilon}{2}\right) \qquad (16.8)$$

$$\cos k_1 >> \epsilon \qquad -\frac{\pi}{2} \leqq k_1 \leqq \frac{\pi}{2}$$

since $\frac{1}{2}(1 + \cos 2k_1) = \cos^2 k_1$.

The plus sign gives the acoustical branch, and the minus sign corresponds to the optical branch. The curves remain very near the horizontals ± 1 except at the ends of the interval.

These results can be expressed in terms of the ratio D/C of our new waves [Eq. (16.5)].

Acoustical branch:

$$\frac{D}{C} = \frac{1 - \frac{A_1}{A_2}}{1 + \frac{A_1}{A_2}} = \frac{-\frac{\epsilon}{2\cos k_1} + \frac{\epsilon}{2}}{2 + \frac{\epsilon}{2\cos k_1} - \frac{\epsilon}{2}} \approx \frac{\epsilon}{4}\left(1 - \frac{1}{\cos k_1}\right) \qquad (16.9)$$

The C wave is dominant with a very small D wave.

Optical branch:

$$\frac{D}{C} = \frac{2 - \frac{\epsilon}{2\cos k_1} - \frac{\epsilon}{2}}{\frac{\epsilon}{2\cos k_1} + \frac{\epsilon}{2}} \approx \frac{4}{\epsilon\left(1 + \frac{1}{\cos k_1}\right)} \qquad (16.10)$$

The D wave is dominant with a small C wave.

Here we see that in the limit $M_1 = M_2$ the description of the wave motion is much simpler with the C, D waves of Eq. (16.6) than with the A_1, A_2 waves previously used.

Let us allow k_1 to run from $-\pi$ to $+\pi$ as shown in the diagram 16.7. For the *acoustical branch*

$$-\frac{\pi}{2} < k_1 < \frac{\pi}{2} \qquad D \to 0 \qquad C \neq 0 \tag{16.11}$$

while for the *optical branch* we obtain

$$\left.\begin{array}{l} -\pi < k_1 < -\dfrac{\pi}{2} \\ \hline \dfrac{\pi}{2} < k_1 < \pi \end{array}\right\} \qquad C \to 0 \qquad D \neq 0 \tag{16.12}$$

There is only one wave left (either C or D) almost everywhere except in the immediate neighborhood of $k_1 = \pm\pi/2$, which are the branching points where the curves separate in case $M_1 > M_2$ and give place to a stopping band.

The example just discussed is very important, since it represents the first instance of a general type of problem very often

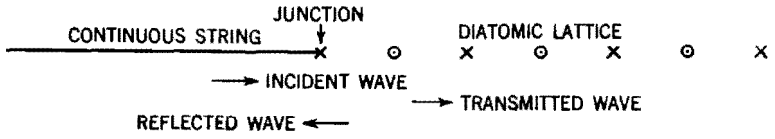


FIG. 16.5.

encountered on other occasions. Here it was possible to follow the transformation from the unperturbed case $M_1 = M_2 = M$ to the perturbed problem $M_1 \neq M_2$ in all details. This is not always possible, and the method followed in more complicated problems will be to start from the unperturbed C, D plane waves and to make linear combinations of them [as in Eq. (16.6)] before discussing the perturbation near the branching points. Such examples may be found in connection with electromagnetic waves (X rays) or with electronic De Broglie waves in crystals, when the periodic distribution of atoms in the crystal lattice can be treated as a small perturbation.

One more remark should be added to show the *connection* between *passing or stopping bands* and *reflection of waves*. If a continuous line capable of transmitting all frequencies is joined to the diatomic lattice (see Fig. 16.5), the coefficient of reflection at the junction will depend on the frequency incident from the continuous line. If the frequency is in one of the stopping bands of the lattice, total reflection will occur; *i.e.*,

$$R = \text{coefficient of reflection} = 1$$

while for a frequency in a passing band both a reflected and a transmitted wave will be excited. The coefficient of reflection will be less than one, and the actual value will depend on the characteristics of the lattice in this case.

17. The One-dimensional Lattice of Polyatomic Molecules

To treat a lattice of polyatomic molecules, we divide the lattice into cells. A cell contains one period of the lattice; *i.e.*, if we start out with atom 1, then the first cell consists of atom 1 to N, where atom $N + 1$ has the same relation to atom $N + 1 + m$ as atom 1 has to atom $1 + m$. Having defined what we mean by *cell* (in general, the same as molecule, unless the molecule itself possesses a periodic structure that is a period of the lattice), we

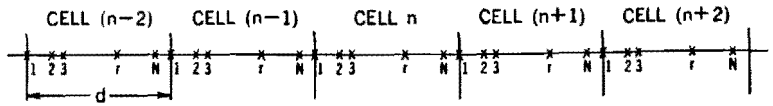


FIG. 17.1.—A row of polyatomic molecules.

change our notation slightly. We number the atoms in a given cell from 1 to N. The cells are also numbered, n being used to denote an arbitrary cell and $n + p$ being the number of the pth cell to the right of cell n. The notation is illustrated in Fig. 17.1. The crosses indicate the equilibrium positions of the atoms, and the vertical lines the positions of the first atom in each cell, *i.e.*, the boundaries of the cells. We take the length of a cell to be d.

We shall assume small displacements of the atoms when a wave propagates along the lattice and also shall assume that all interactions are elastic. We shall not limit the distance at which interactions occur. The force on atom r in cell n due to atom s in cell $n + p$ is therefore

$$f_{n,r;n+p,s} = C_{prs}(y_{n+p,s} - y_{n,r}) \tag{17.1}$$

where C_{prs} is the interaction constant and is independent of n.

It follows that the force on particle s in cell $n + p$ due to particle r in cell n is

$$f_{n+p,s;n,r} = C_{-psr}(y_{n,r} - y_{n+p,s}) \tag{17.2}$$

According to Newton's third law

$$f_{n,r;n+p,s} = -f_{n+p,s;n,r} \tag{17.3}$$

and substituting Eqs. (17.1) and (17.2) into Eq. (17.3), we obtain

$$C_{prs}(y_{n+p,s} - y_{n,r}) = -C_{-psr}(y_{n,r} - y_{n+p,s})$$

or

$$C_{prs} = C_{-psr} \tag{17.4}$$

We take

$$C_{0rr} = 0 \tag{17.5}$$

since the term

$$C_{0rr}(y_{n,r} - y_{n,r}) = 0$$

and does not enter any of the calculations.

The total force acting on particle r in cell n will be given by

$$f_{n,r} = \sum_p \sum_s f_{n,r,n+p,s} = \sum_p \sum_s C_{prs}(y_{n+p,s} - y_{n,r}) \tag{17.6}$$

We assume a wave solution to Eq. (17.6) of the form

$$y_{n,r} = A_r e^{2\pi i(\nu t - ax)} \tag{17.7}$$

A_r is to be complex so as to contain the phase difference of particle r with particle 0, *while x is the distance of the origin of the cell from the origin of the lattice.*

$$x = nd$$

We may thus write Eq. (17.7) in the form

$$y_{n,r} = A_r e^{i(\omega t - kn)} \qquad \left\{\begin{matrix}\omega = 2\pi\nu \\ k = 2\pi ad\end{matrix}\right\} \tag{17.8}$$

$y_{n,r}$ therefore has period $1/d$ in a and 2π in k as in Sec. 4. This means that k may be replaced by $k' = k + 2\pi p$ without affecting the solution. Substitution of Eq. (17.8) into Eq. (17.6) gives

$$\begin{aligned} f_{n,r} &= e^{i(\omega t - kn)} \sum_{p,s} C_{prs}(A_s e^{-ikp} - A_r) \\ &= M_r \frac{d^2 y_{n,r}}{dt^2} = -\omega^2 M_r A_r e^{i(\omega t - kn)} \end{aligned} \tag{17.9}$$

from which we obtain the following relation between ω and k:

$$\sum_s D_{r,s}(k) A_s = -\omega^2 M_r A_r \tag{17.10}$$

where the function $D_{r,s}(k$ is defined by

$$\left.\begin{aligned} D_{r,s}(k) &= \sum_p C_{prs} e^{-ikp} \qquad r \neq s \\ D_{r,r}(k) &= -\sum_{ps} C_{prs} + \sum_p C_{prr} e^{-ikp} \end{aligned}\right\} \tag{7.11}$$

The sum over s is to be taken over all atoms in a given cell and the sum over p is to be taken over all the cells.

The acoustical branch gives $A_r = A_s$ at $k = 0$, and hence

$$\begin{aligned} \omega^2 M_r &= \sum_s D_{r,s}(0) = \sum_{s \neq r} D_{r,s}(0) + D_{r,r}(0) \\ &= \sum_{s \neq r} \sum_p C_{prs} - \sum_{ps} C_{prs} + \sum_p C_{prr} \\ &= \sum_{s \neq r} \sum_p C_{prs} - \sum_{p,s \neq r} C_{prs} = 0 \\ \omega &= 0 \end{aligned}$$

For other values of k we write Eq. (17.10) as

$$\sum_s [D_{r,s}(k) + \omega^2 M_r \delta_{rs}] A_s = 0 \tag{17.12}$$

where δ is the Kronecker δ, defined by

$$\delta_{rs} = \begin{cases} 0 & r \neq s \\ 1 & r = s \end{cases}$$

Equation (17.12) gives N linear homogeneous equations for A_s, and the condition that they be consistent is that the determinant of the coefficients vanish; *i.e.*,

$$|D_{r,s}(k) + \omega^2 M_r \delta_{rs}| = 0 \tag{17.13}$$

Equation (17.13) is an equation of degree N in ω^2, and hence there will be N values of ω^2 for a given k, *i.e.*, there will be N branches in the ω vs. k curve or the ν vs. a curve. One of these branches will be the acoustical branch, and the remaining $(N - 1)$ will be optical branches. ω^2 will be a periodic function of k since $D_{rs}(k)$ is a periodic function of k.

If we let $N \to \infty$, the number of optical branches becomes infinite, since we must have the total number of branches equal to the number of degrees of freedom of the system. The lattice will become a continuous string with some sort of periodic structure. We shall discuss the problem of the continuous periodic

string in a later chapter. If the string is continuous and uniform, ω is a linear function of k. Figure 17.2 shows the general appearance of the ω vs. k curves. The dotted curves are ω vs. k for a uniform continuous string.

The transition from the uniform continuous string to the continuous string with periodic structure (a loaded string, for

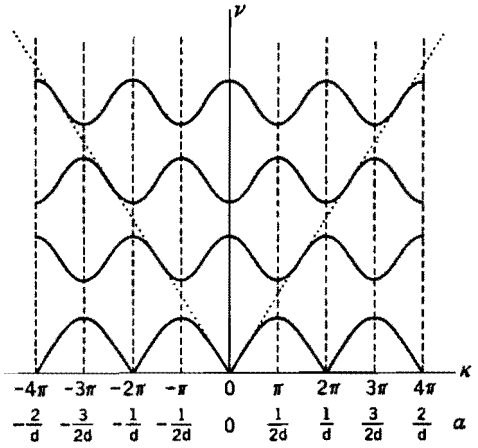


FIG. 17.2.

instance) is one of the problems of periodic perturbation sketched at the end of Sec. 16, and for the discussion of which the example of Sec. 16 will be used as a model. The change from the V-shaped dotted curve in Fig. 17.2 to the wavy curves occurs in a way similar to the change from the single dotted sine curve to the two solid curves in Fig. 16.1.

CHAPTER V

ENERGY VELOCITY, ENERGY FLOW, AND CHARACTERISTIC IMPEDANCE

18. General Discussion; Phase Velocity

So far we have discussed infinite lattices only. If we wish to apply our results to a finite lattice, we must add forces at the ends that will satisfy the boundary conditions. At the left end we must have a source of energy that will supply to the first particle the power that would have come to it if the lattice had extended indefinitely to the left. Then the propagation will depend on the frequency as noted at the end of Sec. 16. On the right end we must have a device that will absorb the energy that would have been absorbed by the omitted portion of the lattice extending indefinitely to the right. To set up the boundary conditions rigorously requires a discussion of the energy density, energy flow, and energy velocity in the lattice. This discussion will be carried on in the next few sections.

The one-dimensional mechanical lattice is an academic rather than a practical problem, and the only important instance of one-dimensional structures is found in electric lines, a discussion of which will be given in detail in the last chapters. It is, however, very useful to know how to set up the boundary conditions for the applications of the theory to two- and three-dimensional lattices. The method developed in this chapter is general and will be extended later to these problems, but it is easier to understand in the one-dimensional case.

The problems discussed are closely connected with the property of the structures of exhibiting *dispersion*. The wave velocity defined in the preceding chapters is known as *phase velocity*, since it is obtained from a comparison of the relative phase of the oscillations of two neighboring atoms. This phase velocity is the one to be used in formulas like

$$\lambda = V\tau, \qquad V = \frac{\nu}{a}, \qquad \nu = \frac{1}{\tau}, \qquad a = \frac{1}{\lambda} \tag{18.1}$$