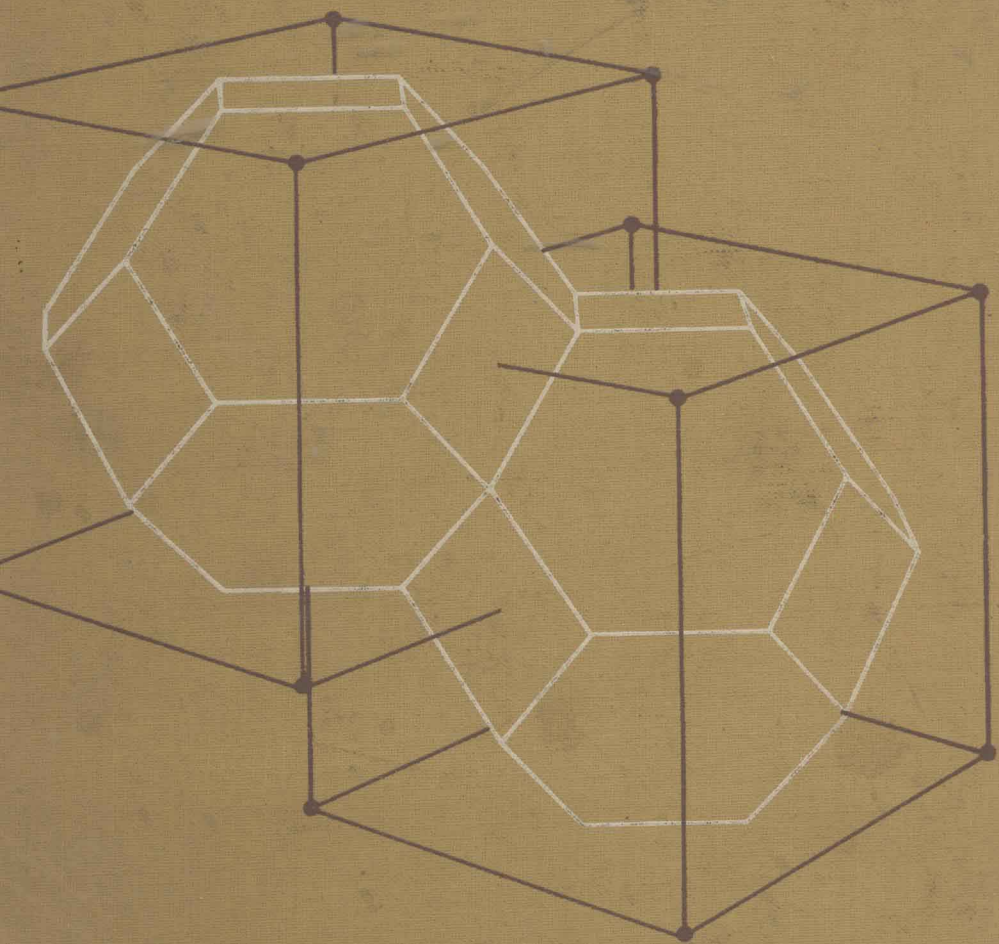


An Introduction to

Lattice Dynamics

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an introduction to Lattice Dynamics

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Dedicated to Our Parents

Preface

Lattice dynamics now forms an important part of any course in solid state physics. Though all textbooks on solid state physics contain a few chapters on it, this topic is not adequately treated. The main reason for this may be that in a regular textbook, space has to be equitably distributed between different aspects of solid state physics. The authors and some other teachers have always felt that in teaching lattice dynamics to postgraduate classes it was necessary to supplement the textbooks by review articles and by proceedings of conferences on neutron scattering.

The Physics Panel of the National Council of Science Education (India) asked us to prepare a monograph on some topic of interest to us and which will also be useful to postgraduate students and teachers. Having earlier felt the necessity of a text on lattice dynamics, which will discuss neutron scattering experiments in some detail, we decided to write a monograph on this topic. Another reason for choosing this topic was that a number of physicists in India have made important contributions to it.

In this monograph we have discussed topics which tie up closely with lattice dynamics and its study by neutron scattering experiments. Ionic crystals have not been discussed in great length. We would have liked to include a chapter on Mössbauer effect, but a separate monograph is being planned on this topic under the NCSE program.

Some problems have been added at the end of most chapters. These problems are intended to amplify the points which we thought would be difficult to include in the main text. References of a general nature are indicated by an asterisk.

The authors are indebted to Prof. F. C. Auluck, Prof. R. N. Dogra, Prof. M. S. Sodha, and Prof. S. C. Jain for their interest and support of this work. The authors are grateful to Dr. R. D. Deshpande for his interest in the publication of this monograph. Thanks are also due to Mr. V. N. Wanchoo and Dr. N. K. Bansal for their help in the early stages of the preparation of the manuscript. The authors would also like to thank Dr. J. Mahanty, Dr. S. K. Joshi, Dr. B. Sharan, and Dr. B. B. Tripathi for their comments and suggestions. Finally, the efficient typing of Mr. V. N. Sharma, Mr. T. N. Gupta, and Mr. O. P. Virmani is gratefully acknowledged.

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Introduction

The study of lattice dynamics now forms an important part of any course in solid state physics. The vibrations of atoms in a crystal not only determine its thermal properties but also govern phenomena like diffuse scattering of X-rays, neutron scattering, spin-lattice relaxation, etc. In order to understand any of these phenomena it is necessary to develop the theory of vibration of atoms, that is, the theory of lattice dynamics.

In 1819 Dulong and Petit discovered empirically that the specific heat per gram atom of a crystal of any element was $3R$, R being the gas constant. This law was found to hold for most elements at room temperature and above. It was, however, soon discovered that at low temperatures the specific heat of crystals was considerably lower. In 1907 Einstein for the first time developed the quantum theory of specific heat of crystals. He assumed that the atoms in a crystal behaved like quantum oscillators, vibrating with a fixed frequency. All oscillators were supposed to vibrate independently without any interaction with each other. Based on this hypothesis, Einstein developed his theory of specific heat. This theory did explain the decrease in specific heat with decreasing temperature, but it turned out that the decrease predicted by theory was far more rapid than what was observed. This discrepancy between theory and experiment was removed in 1912 by Debye and almost simultaneously by Max Born and von Kármán. They argued that because of the strong binding between different atoms in a crystal it was incorrect to assume all atoms to be independent oscillators. When one atom starts to oscillate it sends a wave through the entire crystal, causing many other atoms to oscillate. On the basis of this hypothesis Debye developed the theory of specific heat that was remarkably successful in explaining the temperature variation of specific heat of most metals. However, a few exceptions, such as graphite, bismuth, selenium, and tellurium, were discovered and we now understand why the Debye theory fails in these cases.

It was realized fairly early that since specific heat was an integral measurement, the agreement between theory and experiment could not be regarded as a sensitive test for Debye's theory of lattice dynamics. This theory was also used successfully to explain the effect of temperature on the intensity of Laue spots in X-ray diffraction studies. Even so, since this effect also depended on the overall frequency spectrum of the crystal, one could not deduce the details of the spectrum from such a study. Some attempts have been made to devise methods for obtaining the fre-

quency distribution function directly from the specific heat data, but they have not been very successful.

With the availability of high intensity thermal neutron beams from reactors, the very nature of the problem was changed. It became possible to study processes involving single lattice waves, and the frequency distribution function and the dispersion relation could be experimentally determined. This stimulated much work both in theory and experiment. It turned out that the theory of lattice dynamics was not as simple as was thought at one time. A number of models have been proposed for describing the atomic vibrations, and a good amount of work in this field has been done by physicists in India.

The atomic vibrations in a crystal can be quantized, and this gives rise to quasi-particles called *phonons*. Neutron scattering from a crystal is usually analyzed in terms of the number of phonons exchanged with the crystal. Zero phonon process corresponds to elastic scattering, since no energy change of the crystal is involved. This is the usual Bragg scattering, and a study of this scattering process gives us information about the structure of the crystal. Inelastic scattering, that is, the scattering process in which one or more phonons are either created or absorbed in the crystal, gives us information about lattice dynamics. This is discussed in detail in Chapter 9.

In Chapter 2 we have developed the theory of lattice dynamics, under the harmonic approximation, that is, in writing the potential energy of a vibrating atom we retain terms only up to the second power in the displacement of the atom. This implies that there is no phonon-phonon interaction and hence these quasi-particles have an infinite lifetime. This also means that the energy of a phonon is exactly defined. The neglect of higher-order terms will prevent us from discussing *anharmonic* effects, that is, the phonon-phonon interaction which leads to finite lifetime for a phonon. The finite lifetime of a phonon implies a spread in its energy and when a neutron with a well-defined energy is scattered by the absorption or emission of a phonon, it will also show a spread in energy corresponding to the spread in energy of the phonon.

In Chapter 3, the lattice modes are quantized and the concept of phonon is justified. Interesting information about the propagation of low-frequency waves through a crystal can also be obtained from the macroscopic theory of elasticity. This is considered in Chapter 4. In Chapter 5 we have considered lattice vibrations of three-dimensional cubic crystals.

In Chapter 6 the phenomenological theory of lattice dynamics is developed and the Debye approximation is justified. We have also evaluated the correction to the Debye approximation that arises from surface modes. This correction becomes important when thermal properties of microcrystallites are considered. In Chapter 7 we discuss the theory of specific heat of solids. The last two chapters deal with neutron scattering and we have tried to explain how neutron scattering experiments are used to determine the frequency distribution function and dispersion relation for lattice modes.

Wave Propagation in One-dimensional Lattices

Before discussing the propagation of elastic waves through a three-dimensional crystal, it is instructive and also simpler to study the vibrations of particles lying along a single straight line. As we shall see, many of the vibrational properties of three-dimensional crystals are, in a qualitative way, also possessed by the one-dimensional chain. An added advantage in discussing the chain first is that we avoid mathematical complexities and can obtain better physical understanding of the results.

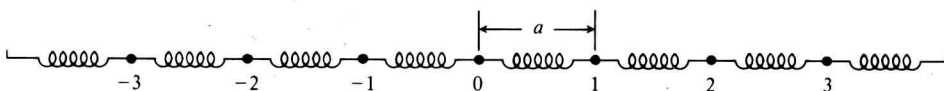


Fig. 2.1. A chain consisting of equally spaced identical particles held together by elastic forces.

Let us consider a lattice consisting of an infinite number of equally spaced identical particles of mass M , lying along a straight line (Fig. 2.1). We assume that the particles are held together by elastic forces obeying Hooke's law. Since the chain is infinite, we may choose any particle as the origin. The particles on the right are successively numbered $1, 2, 3, \dots$, and those on the left of the origin are numbered $-1, -2, -3, \dots$. The equilibrium spacing between the particles will be denoted by a . These particles can vibrate either longitudinally (along the chain) or transversely (at right angles to the chain). We will consider these two types of vibrations separately.

LONGITUDINAL VIBRATIONS

Let us first consider the case in which the particles execute longitudinal vibrations. The displacement of the n th particle from its equilibrium position will be denoted by u_n , so that at any instant of time the coordinate of the n th particle, x_n , will be given by

$$x_n = na + u_n. \quad (2.1)$$

The distance between the n th and the $(n + m)$ th particle will be denoted by

$$\begin{aligned} r_{n, n+m} &= x_{n+m} - x_n \\ &= ma + u_{n+m} - u_n. \end{aligned} \quad (2.2)$$

Since we have assumed that the forces between particles obey Hooke's law, the energy of interaction between any two particles will be a function only of the distance between them:

$$U(r) = U(|x_{n+m} - x_n|). \quad (2.3)$$

This type of interaction is known as the *central force interaction*. A mechanical analogy is a spring where the restoring force is proportional to the change in length of the spring and is independent of any change in direction of the spring (without change in length).

The total potential energy of the lattice, V , will be given by

$$V = \sum_n \sum_{m>0} U(x_{n+m} - x_n), \quad (2.4)$$

where m must be restricted to positive values so that the interaction between a given pair of particles will be counted only once.[†] The displacement of the particles from their respective equilibrium positions is assumed to be very small compared to the interparticle distance. Since $m > 0$, $x_{n+m} - x_n$ will always be positive, and hence we have dropped the absolute sign from the parenthesis in Eq. (2.4). Further, since $u_n \ll a$, we may expand $U(x_{n+m} - x_n)$ in a Taylor series about the point $x = ma$:

$$\begin{aligned} U(x_{n+m} - x_n) &= U(ma + u_{n+m} - u_n) \\ &= U(ma) + (u_{n+m} - u_n)U'(ma) \\ &\quad + \frac{1}{2}(u_{n+m} - u_n)^2 U''(ma) + \dots, \end{aligned} \quad (2.5)$$

where $U'(ma)$ and $U''(ma)$ are $dU(r)/dr$ and $d^2U(r)/dr^2$, evaluated at $r = ma$. Since $u_n \ll a$ we will neglect all terms higher than the second power in Eq. (2.5). This is known as the *harmonic approximation*. There are effects like thermal expansion, which depend entirely on the higher-order terms—the so-called *anharmonic terms*. We will confine ourselves to the harmonic approximation. The expression for the potential energy is therefore,

$$V = V_0 + \sum_n \sum_{m>0} (u_{n+m} - u_n)U'(ma) + \frac{1}{2} \sum_n \sum_{m>0} (u_{n+m} - u_n)^2 U''(ma), \quad (2.6)$$

where

$$V_0 = \sum_n \sum_{m>0} U(ma), \quad (2.7)$$

is the potential energy of the lattice corresponding to the equilibrium configuration. The coefficient $U'(ma)$ of the linear terms in u_n is zero, since the potential energy is a minimum when particles are in their equilibrium positions. This also implies that in the equilibrium position there is no net force on any particle.

[†] If we want to sum over all m , both positive and negative, the expression for V will be

$$V = \frac{1}{2} \sum_n \sum_m U(|x_{n+m} - x_n|).$$

From now on we will assume nearest-neighbor interaction: the energy of interaction is taken to be zero between two particles which, in the equilibrium configuration, are separated by a distance $2a$ or more. This assumption in no way alters the essential character of vibrations of the chain (Problem 2.1). Hence we may write

$$V = V_0 + \frac{1}{2}U''(a) \sum_n (u_{n+1} - u_n)^2. \quad (2.8)$$

If F_p denotes the force acting on the p th particle, then it will be given by:

$$F_p = -\frac{\partial V}{\partial u_p} = -\frac{1}{2}U''(a) \frac{\partial}{\partial u_p} [(u_p - u_{p-1})^2 + (u_{p+1} - u_p)^2], \quad (2.9)$$

since none of the other terms of the sum in Eq. (2.8) will contain u_p . Thus

$$F_p = U''(a) [u_{p+1} - 2u_p + u_{p-1}]. \quad (2.10)$$

Equation (2.10) can readily be written down from simple physical arguments. We assume the interaction between nearest neighbors to be given by Hooke's law with force constant f . The expression for F_p in such a case must be

$$\begin{aligned} F_p &= -f(u_p - u_{p-1}) - f(u_p - u_{p+1}) \\ &= f(u_{p+1} - 2u_p + u_{p-1}), \end{aligned} \quad (2.11)$$

where $f(u_p - u_{p-1})$ is the restoring force acting on the p th particle because of its relative displacement from the $(p-1)$ th particle. If we compare Eq. (2.10) with Eq. (2.11) we find that U'' plays the role of the force constant, provided it is assumed that the force between the particles obeys Hooke's law. However, a detailed derivation of Eq. (2.10) is necessary to bring out the significance of harmonic approximation.

Thus the equation of motion of the p th particle is

$$M \frac{d^2 u_p}{dt^2} = U''(a) [u_{p+1} - 2u_p + u_{p-1}]. \quad (2.12)$$

We attempt to solve this equation by assuming a solution of a running wave type†

$$u_p = A \exp[-i(\omega t - q\xi_p)], \quad i = \sqrt{-1}, \quad (2.13)$$

† Classically it does not matter whether we take $-i$ or $+i$ in the exponent of Eq. (2.13). However, in quantum mechanics the momentum operator p_x is represented by $-i\hbar(\partial/\partial x)$ and the momentum of the wave will be given by

$$p u_p = -i\hbar \frac{\partial}{\partial x} u_p$$

(for our case ξ_p is x), or

$$\begin{aligned} p u_p &= -i\hbar A(iq) \exp[-i(\omega t - qx)] \\ &= \hbar q u_p, \end{aligned}$$

or

$$p = \hbar q.$$

We thus get positive momentum for the wave traveling in the positive x -direction. Had we taken $+i$, instead of $-i$ in Eq. (2.13), we would have obtained negative momentum for the wave traveling along the positive x -direction.

where A is amplitude of the wave, $\xi_p (= pa)$ represents the equilibrium position of the p th particle, and $\omega (= 2\pi\nu)$ and q denote the angular frequency and wave vector of the wave respectively. By substituting in Eq. (2.12) we get

$$\begin{aligned} -M\omega^2 &= U''(a) [e^{-iqa} - 2 + e^{iqa}], \\ &= -4U''(a) \sin^2 \frac{qa}{2}, \end{aligned}$$

or

$$\omega = \omega_{0L} \left| \sin \frac{qa}{2} \right|, \quad (2.14)$$

where

$$\omega_{0L} = \left[\frac{4U''(a)}{M} \right]^{\frac{1}{2}}, \quad (2.15)$$

and the subscript L denotes the fact that the vibrations are longitudinal. Equation (2.14), which gives us a relation between the angular frequency ω and the propagation vector q , is known as the *dispersion relation*.

We impose the condition that ω , the angular frequency, always be positive. This explains why we take the modulus of the sine function in Eq. (2.14). Because of this, ω is a periodic function of q with period $2\pi/a$ (rather than $4\pi/a$). This point is discussed in detail later.

TRANSVERSE VIBRATIONS

We will now consider transverse vibrations of an infinite chain. We first show that central forces alone cannot give rise to harmonic transverse vibrations. Let v_n be the displacement of the n th particle in a direction normal to the chain. The displacements of all the particles are assumed to be in the same plane. Thus the relative distance between the displaced particles at sites $n + m$ and n will be given by

$$d = |x_{n+m}\hat{i} + v_{n+m}\hat{j} - x_n\hat{i} - v_n\hat{j}|, \quad (2.16)$$

where \hat{i} is a unit vector along the chain and \hat{j} is a unit vector normal to the chain — in the direction of the displacement. We will assume that there is no displacement of the particles along the chain, so that $x_{n+m} - x_n = ma$. Therefore

$$\begin{aligned} d &= [\{ma\hat{i} + (v_{n+m} - v_n)\hat{j}\}^2]^{\frac{1}{2}} \\ &= \left[m^2a^2 \left\{ 1 + \frac{(v_{n+m} - v_n)^2}{m^2a^2} \right\} \right]^{\frac{1}{2}}, \end{aligned}$$

(because $\hat{i} \cdot \hat{j} = 0$). Thus to lowest power in $(v_{n+m} - v_n)^2$, we have

$$d \simeq ma + \frac{(v_{n+m} - v_n)^2}{2ma}. \quad (2.17)$$

This expansion is justified because the displacements are very small compared to the interparticle distance. If we assume that only the interactions among nearest neighbors are important, the expression for the potential energy becomes

$$V_T = \sum_n U \left[a + \frac{(v_{n+1} - v_n)^2}{2a} \right],$$

where the subscript T denotes transverse vibrations. Expanding U in a Taylor series, we obtain

$$V_T = \sum_n \left[U(a) + \frac{(v_{n+1} - v_n)^2}{2a} U'(a) + \frac{1}{2} \frac{(v_{n+1} - v_n)^4}{4a^2} U''(a) + \dots \right]. \quad (2.18)$$

Since $U'(a) = 0$, we have

$$V_T = V_0 + \frac{1}{2} U''(a) \sum_n \frac{(v_{n+1} - v_n)^4}{4a^2}. \quad (2.19)$$

We observe that for the transverse case the potential energy depends on the fourth power of the relative displacement. Therefore, if we consider only central forces, the equation of motion of a chain that vibrates transversely will be entirely different from that of a chain that vibrates longitudinally. Hence *the usual type of transverse modes cannot be explained on the basis of central forces and harmonic approximation alone.*

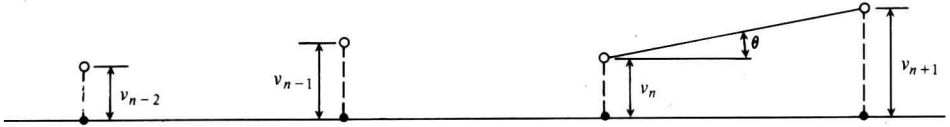


Fig. 2.2. Transverse vibrations of a one-dimensional chain consisting of equally spaced identical particles. The open and the solid circles represent, respectively, the displaced and the equilibrium positions of the particles.

However, since transverse vibrations of chains are observed, some other form of restoring force must also exist. The other force is the so-called *angular force*, which depends on the angle which the line joining the moving particles makes with the equilibrium position of the line.† Figure 2.2 shows the transverse displacement of the particles. It is clear that when the particles $n + 1$ and n are in the positions shown, the angle θ through which they have turned will be given by

$$\theta \approx \frac{v_{n+1} - v_n}{a}. \quad (2.20)$$

Let us assume that the angular force is proportional to θ , with f_T as the proportionality constant. This force is always directed towards the equilibrium site

† The vibrations of a layer lattice taking account of angular forces have been studied by Kothari *et al.* (1971).

8 Wave propagation in one-dimensional lattices

and hence acts normally to the direction of the chain. Thus, assuming interaction between nearest neighbors only, the force on the p th particle will be given by

$$F_p = -f_T \frac{v_p - v_{p+1}}{a} - f_T \frac{v_p - v_{p-1}}{a}. \quad (2.21)$$

Consequently, the equation of motion will be

$$M \frac{d^2 v_p}{dt^2} = \frac{f_T}{a} [v_{p+1} - 2v_p + v_{p-1}]. \quad (2.22)$$

As in the case of longitudinal vibrations, we solve the above equation by assuming a running wave solution of the type given by Eq. (2.13). This leads to the following dispersion relation

$$\omega = \omega_{0T} \left| \sin \frac{qa}{2} \right|, \quad (2.23)$$

where

$$\omega_{0T} = \left[\frac{4f_T}{aM} \right]^{\frac{1}{2}}. \quad (2.24)$$

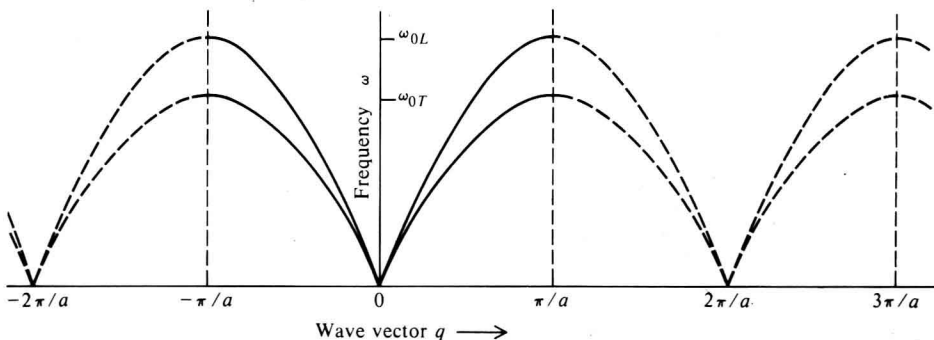


Fig. 2.3. The dependence of frequency on the wave vector for a one-dimensional chain.

We notice that the dispersion relation for the transverse mode is similar to the one derived for the longitudinal mode, except for the maximum frequency ω_{0T} , which is usually less than ω_{0L} . The ω -vs- q curve is plotted in Fig. 2.3 and the transverse branch is shown to lie below the longitudinal branch (because ω_{0T} is assumed to be less than ω_{0L}). In general, for a linear chain of identical particles there will be one longitudinal branch and two transverse branches corresponding to the two independent mutually perpendicular directions of vibration of the particles.

From Eqs. (2.14) and (2.23), we find that corresponding to each branch there exists a certain maximum frequency (ω_{0L} for longitudinal vibrations and ω_{0T} for transverse vibrations) beyond which no waves can be propagated through the

chain (Fig. 2.3). The chain may thus be considered as a low-pass filter which would transmit only in the frequency range between zero and ω_{\max} . (We will later discuss a system which transmits frequencies in the ranges $0 < \omega < \omega_3$ and $\omega_2 < \omega < \omega_1$ [$\omega_1 > \omega_2 > \omega_3$], but not in the range $\omega_3 < \omega < \omega_2$.)

Let us consider what happens if a longitudinal wave with ω exceeding ω_{0L} is imposed on the chain. Since

$$\omega^2 = \omega_{0L}^2 \sin^2 \frac{qa}{2},$$

it is obvious that q must be complex. Let

$$q = \alpha + i\beta \quad (2.25)$$

(where α and β are real), so that†

$$\sin \frac{qa}{2} = \sin \frac{\alpha a}{2} \cosh \frac{\beta a}{2} + i \cos \frac{\alpha a}{2} \sinh \frac{\beta a}{2}. \quad (2.26)$$

Since ω^2 is real, we must have

$$\cos \frac{\alpha a}{2} \sinh \frac{\beta a}{2} = 0.$$

If $\sinh(\beta a/2) = 0$, then $\beta a = 0$; which implies that q must be real and therefore $\omega < \omega_{0L}$. Hence for ω to be greater than ω_{0L} , $\cos(\alpha a/2)$ must be zero, or $\alpha a/2 = \pi/2$. Thus

$$\alpha = \text{real part of } q = \frac{\pi}{a}.$$

This leads to

$$\omega^2 = \omega_{0L}^2 \cosh^2 \frac{\beta a}{2}. \quad (2.27)$$

The variation of the real and imaginary parts of q with ω is shown in Fig. 2.4. Substituting the value of q from Eq. (2.25) with $\alpha = \pi/a$ in Eq. (2.13), we obtain

$$u_p = A(-1)^p \exp[-i\omega t - p a \beta].$$

From this we see that all frequencies above ω_{0L} will be attenuated, the attenuation being stronger for larger ω . We will be interested only in the frequency range $0 < \omega < \omega_{\max}$, that is in waves that are propagated through the lattice.

Returning to Eqs. (2.14) and (2.23), we find that if $qa \ll 1$

$$\omega \simeq \omega_0 \frac{qa}{2}. \quad (2.28)$$

That is, the frequency is proportional to the wave vector q . (We have dropped the subscript T or L , as the present consideration is equally valid for both transverse

† $\sin i\theta = i \sinh \theta$, $\cos i\theta = \cosh \theta$.

and longitudinal vibrations.) Since for a continuous string the frequency is always proportional to the wave vector, we note that an array of point particles and a continuous string give the same results only if $qa \ll 1$ — that is, when the wavelength is large compared to the interparticle distance. The same holds for sound waves in a solid. The maximum frequency ω_0 is usually of the order of 10^{13} sec^{-1} , whereas

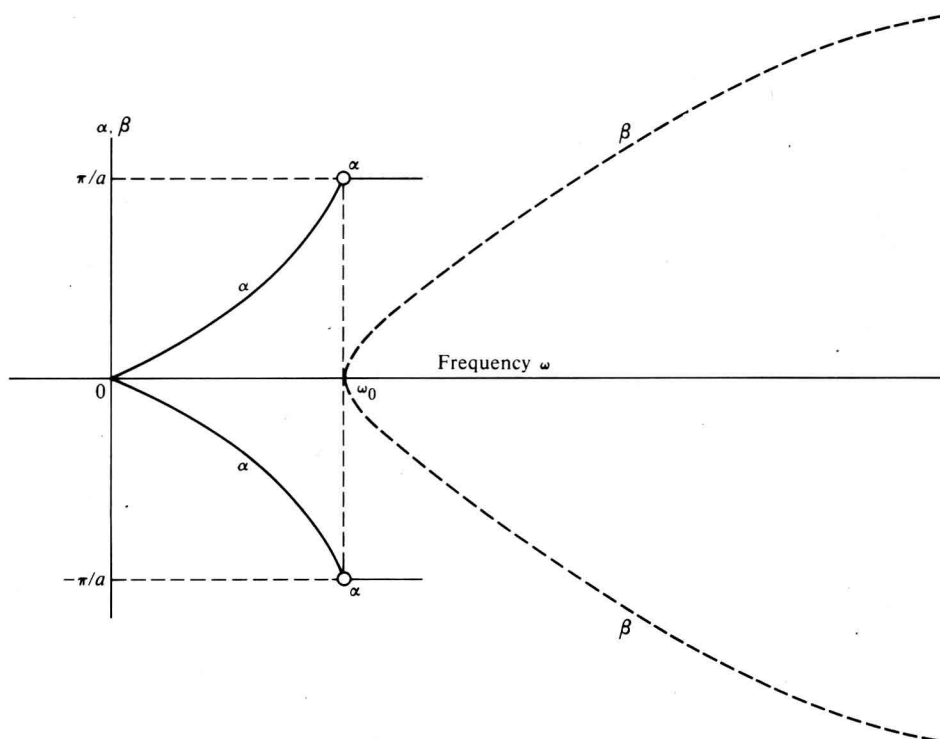


Fig. 2.4. The variation of the real and imaginary parts of the wave vector with frequency.

the highest frequency that can be artificially generated (by a thin slice of quartz crystal) is nearly 10^9 sec^{-1} . Thus if one is concerned with sound waves propagating through a solid one need consider only a very small range of frequencies near zero and hence the assumption $qa \ll 1$ will be a very good approximation.

From Eqs. (2.14) and (2.23) we notice that if q is replaced by

$$q_m = q + \frac{2\pi m}{a}, \quad (2.29)$$

with $m = \pm 1, \pm 2, \dots$, the equation remains the same. Thus the state of vibration of an array of mass points corresponding to a wave vector q will be identical to the state corresponding to any of the other wave vectors $q + 2\pi m/a$. Thus, if we want to have one-to-one correspondence between the states of vibration of a