CALCULATIONS OF PHONON DISPERSION CURVES

AND

DENSITY OF STATES.

A THESIS SUBMITTED TO THE POST GRADUATE SCHOOL OF AHMADU BELLO UNIVERSITY, ZARIA, IN PARTIAL FULFILMENT FOR THE AWARD OF THE MASTER OF SCIENCE (M.SC) DEGREE IN PHYSICS.

BY

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June, 1999.

DECLARATION

This is to certify that:

(i) The work reported in this thesis was carried out by me, Lawan Sani Taura, at Department of Physics, Alunadu Bello University, Zaria, Nigeria.

(ii) This thesis has not been submitted in any form to any institution, both establishment or organization other then Ahmadu Bello University, Zaria, Nigeria, for the award of degree of master of science.

(iii) All authers whose works are cited and referenced in this project report are duly acknowledged.

Lawan Sani Taura.
01/02/99
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CERTIFICATION

This project report, entitled " Calculation of Phonon Dispersion Curves and Density of States " meets the regulation governing the award of master of science of Ahmadu Bello University, Zaria, and is approved for its contribution to knowledge and literary presentation.

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DEDICATION:

IN THE NAME OF ALLAH, THE BENEFICIENT, THE MERCIFUL, GLORY BE TO ALLAH, THE MOST HIGH.

This work is dedicated to my father late Muhammad Sani Abdullahi. I pray for Allah to forgive him and reward him on the kind of training he gave me from childhood to Adulthood. (Ameen).

Date:

Lawan Sani Taura.

ABSTRACT:

The phonon density of states and dispersion relations of one and two atoms crystal structures are studied for SC and BCC lattices with interatomic interaction up to and including second neighbours. Analytical expression for dispersion relations in the principal symmetry directions are 'derived. The force constants of one and two (CsCl) crystals are determined by an optimization procedure using the dispersion in the [100], [110], [111] directions. The dispersion curves calculated with a two- neigbour, six- parameter give a reasonable fit to the dispersion data in the principal symmetry directions.

The secular equation containing three directional symmetry calculated for the eigenfrequencies of wave vectors also served to establish a histogram of the frequency of the normal modes in which the singularities caused by the critical points are explicitly included.

The FORTRAN code which is used in the computation of the density of states and dispersion curves was obtained from the Boardman Physics Program book, and modified substantially for adaptation for the Personal Computer (PC). The cited standard subroutine libraries which are not available were substituted with our own written programs. The output of the program was also redesigned to produce numbers appropriate for use in a plotting software. To avoid singularities inherent in the original code we converted it to doubled precision and added numbers whicbj§o not noticeably affect the result.

The program can be used for any lattice phonon dispersion and density of states calculation once the relative dynamic matrix has been determined.

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CHAPTER ONE

1.0 Introduction

Atoms in crystalline solids vibrate about their mean equilibrium positions at all temperatures. These vibrations are responsible for a number of important properties of crystalline solids, such as the thermodynamics, Mechanical, heat transport and related physical behaviors of solids. The study of these lattice vibrations whose quanta are called phonons requires a knowledge of the phonon dispersion curves and density of states.

In spite of the fundamental role played by the density of states, it is very difficult to measure directly and is almost invariably computed. Experimental data will normally give information on the phonon dispersion curves, and these will then be used to determine the interatomic force constants, by comparing the experimental curves with those calculated from the force constants. Even when these have been determined, it is by no means simple to calculate the density of states analytically, but modern computing methods have proved an ideal tool for solving the problem numerically.

1.1 Aim and Scope of the research:

The aim of this research is to determine the force constants by solving the secular determinant along the symmetry directions and varying the constants to obtain the best fit to the experimental data. In chapter two we describe the theory of lattice vibration. In chapter three the theory of density of states is given. Chapter four contains the main research carried out. A simulation program is used and the ratio of the two force constants is sets so as to generate a theoretical set of dispersion curves and examine the effect of the two constants on the dispersion curves. We also choose values for the force constant in the secular determinant and evaluate the determinant over a mesh of points in k-space. We built up a histogram of the density of states.

One can extend this procedure to allow the determination of the general interatomic force constants by matching appropriate solutions of the secular equation to these measured dispersion curves.

CHAPTER TWO

2.0 LATTICE VIBRATION:

The easiest way to visualise lattice vibrations is to consider a large number of spheres, each connected to its neighbour by springs. These vibrations occur at any temperature, even at absolute zero. Restoring forces are induced on the spheres when they are displaced from their equilibrium positions. Springs connecting nearest neighbours characterise short-range forces (so that Hooke's law is obeyed), while the spring reaching the second and more distant particle represented by the spheres is imagined to be vibrating about its equilibrium position, a fairly accurate picture of the lattice vibrations emerges.

There are a number of things we can learn about the complete lattice vibrational spectrum of a solid most appropriately by considering the periodic nature of a crystalline material. The continuum approach fails to alert us to the changing conditions encountered when the wavelength is not many times greater than interatomic spacing, whereas a description in terms of atomic force constants is equally valid for low and high frequencies.

A lattice vibrational wave in a crystal is a repetitive and systematic sequence of atomic displacements (longitudinal, transverse, or some combination of the two) which can be characterized by;

(i) A propagation velocity V

(ii) A wavelength λ or wave vector $|k| = (2\pi/\lambda)$ and

(iii) A frequency ν or angular frequency $\omega = (2\pi\nu) = Vk$

So by considering the restoring forces on displaced atoms we can produce an equation of motion for any displacement, and generate a dispersion relationship between frequency and wavelength, but more frequently to the companion relationship between angular frequency and wave vector.

2.1 BOUNDARY CONDITIONS:

2.1.1 Fixed boundary conditions:

Consider a line of length L fixed at both ends. The wave motion on this line can be represented by

$$U = U_o \exp ikx = U_o (\cos kx + i\sin kx) \tag{2.1}$$

KAS.

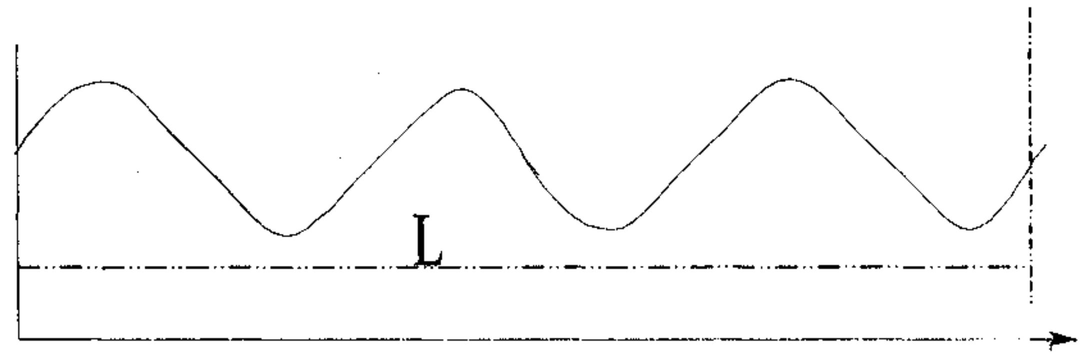

Figure 2.1 A line of length L

Because of the fixed boundaries

$U = 0$ at $x = 0$; so

$$U = U_o \sin kx \tag{2.2}$$

And

$U = 0$ at $x = L$; so $U_o \sin kL = 0$

$kL = n\pi$, $k = n\pi/L$ where $n = 1, 2, 3, \ldots, N$

$$\therefore \; U = U_o \sin n\pi/L \tag{2.3}$$

If the line is a lattice of atoms spaced a distance 'a', the maximum value of k is

$$k_{max} = n\pi/L = N\pi/L$$

$$= N\pi/ Na = \pi/a$$

($\because$ the maximum value of n is N)

The solution $k_{max} = \pi/a$ has

$$U_n = U_o \sin\pi L/a = U_o \sin\pi(Na)/a$$

$$= U_o \sin N\pi = 0 \tag{2.4}$$

That is the solution $k = N\pi/L$ permits no motion of any atom.

Thus there are (N - 1) allowed independent values of k i.e

$k = \pi/L,\ 2\pi/L,\ 3\pi/L, \ldots\ (N-1)\pi/L$.

This is called the case of fixed boundary conditions.

2.1.2 Periodic Boundary Condition

For a line whose ends are not fixed but are joined so that the line forms a circle we have cyclic or periodic boundary conditions. In this case the only requirement is that,

$$U(x) = U(x+L) \tag{2.5}$$

Since we have $Ux) = U_o \exp(ikx)$;

$$\therefore U(x+L) = U_o \exp ik(x+L)$$

$$= U_o \exp(ikx) \times \exp(ikL)$$

$$\therefore U(x+L) = U(x)\exp(ikL), \text{ since } U(x+L) = U(x)$$

$$\therefore \exp(ikL) = 1 = \exp(i2\pi n),\ kL = 2\pi n$$

$$k = 2\pi n/L \tag{2.6}$$

So $U = U_o \exp i(2\pi nx/L)$, a travelling wave. The allowed values of n are $\pm1, \pm2, \pm3 \ldots$ In order that the total number of modes shall be equal to N, n must have N different values i.e.

$$n = 0, \pm1, \pm2, \pm3, \ldots, \pm N/2.$$

2.2 Vibration of Monatomic Linear Chain

Consider a linear chain of atoms of mass m bound to each neighbour by a spring obeying Hooke's law (see figure 2.2) we assume there are N atoms and periodic boundary conditions so that atom N is attached to atom 1 as if it were atom N + 1 (i.e the chain is bent into a ring), and we can then define interatomic force constant γ_1 such that if U_1 denotes the displacement of the 1^{th} atom, then the force on the atom at the origin due to the displacement U_1 is

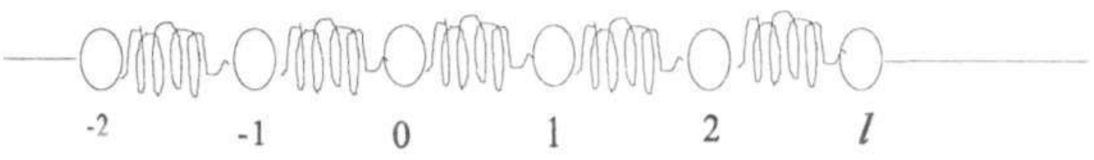

Figure 2.2 Linear chain of identical atoms, with interatomic forces between nearest neighbours only.

$$F_o = +\gamma_1 \ (u_1 - u_o) \tag{2.7}$$

Summing over all atoms (+ve and -ve) the equation of motion of the atom at the origin is

$$m\frac{\partial^2 uo}{\partial t^2} = \sum_{l\neq 0} \gamma \left(u_l - uo\right) \tag{2.8}$$

if we look for a solution for u_o in the form of a wave of frequency ω and wave number $k = 2\pi/\lambda$ travelling in the x -

direction, this will have the general form.

$$u(x) = Ae^{i(\omega t - kx)} \tag{2.9}$$

However, we need only to consider displacements at actual atomic sites, so if the lattice spacing is a,

$u_l = A \exp i(\omega t - kLa)$ giving

$$-m\omega^2 A e^{i\omega t} = \sum_{l \neq 0} \gamma_l A \left\{ e^{i(\omega t - kla)} - e^{i\omega t} \right. \tag{2.10}$$

Since by symmetry $\gamma_l = \gamma_{-l}$, then equation (2.10) can be written after cancellation as:

$$m\omega^2 = \sum_{l>0} 2\gamma_l \{1 - \cos ka\} \tag{2.11}$$

By considering the simple example of nearest neighbour interactions only, we have ($\gamma_1 = \gamma$, $\gamma_2 = \gamma_3 = \ldots = 0$)

Then equation (2.11) becomes

$$\omega^2(k) = \frac{2\gamma}{m}\{1 - \cos ka$$

But $\cos ka = 1 - 2\sin^2 \frac{1}{2}ka$, so that

$$\omega^2(k) = \frac{4\gamma}{m}\sin^2(ka/2)$$
$$\omega(k) = \pm 2\sqrt{\gamma/m}\,\sin(ka/2) \tag{2.12}$$

Thus the ω-k relationship, which is called the dispersion relation, is periodic in k, as shown in Figure (2.3). However, let us consider the physical significance of this periodicity:

(1) by looking at the relative motion of two successive atoms:

$$\frac{u_1}{u_o} = \frac{A\exp i(\omega t - ka)}{A\exp i\omega t} = \exp\text{-}ika \qquad (2.13)$$

Thus a range of values of k = $2\pi/a$ cover all possible values of u_1/u_o. Since k must be allowed both positive and negative values to represent waves propagating in either direction, the range of independent values of k is

$$\frac{-\pi}{a} < k \leq \frac{\pi}{a} \qquad (2.14)$$

and this is called the first Brillouin zone

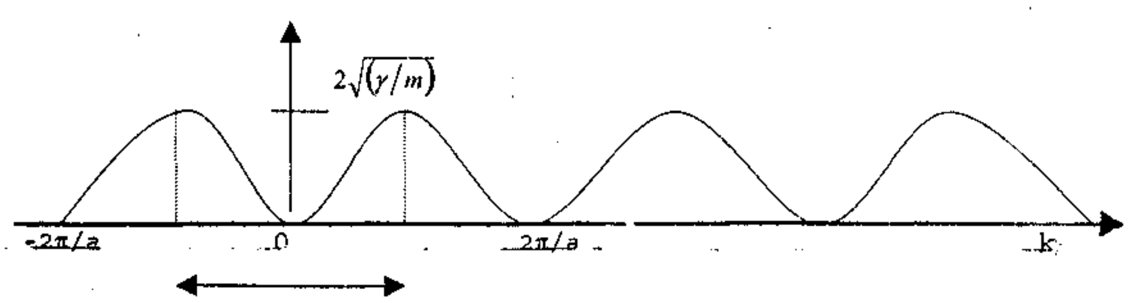

Fig.2.3 Plot of ω versus k (phonon dispersion curve) for a linear chains of atoms with interatomic spacing **a** *between nearest neighbours only.*

(2) At maximum frequency $\sin\left(\frac{1}{2}ka\right)$ will be equal to 1, since the maximum value of sine is 1.

$$\therefore\ \omega_{\max}(k) = 2\sqrt{\gamma/m} \qquad (2.15)$$

This maximum frequency $2\sqrt{\gamma / m}$ is a natural cut-off frequency for the lattice; for frequencies above this value k must be imaginary to satisfy equation (2.12) so that we have an exponentially decaying motion that does not propagate into the lattice.

(3) At low frequencies $k \to 0$, the long-wavelength limit $\sin x \to x$ and we have

$$\omega(k) = \sqrt{4\gamma / m}\sin ka/2$$

$$= 2\sqrt{(\gamma / m)}ka/2$$

$$= a\sqrt{(\gamma / m)}k$$

$$\omega(k) = v_o k \qquad (2.16)$$

where $v_o = a\sqrt{(\gamma / m)}$

$$V_p = \text{phase velocity} = \omega/k = v_o \qquad (2.17)$$

From the relation $\omega = v_o k$, we can have the group velocity as

$$d\omega/dk = v_o \qquad (2.18)$$

We see from eqs (2.17) and (2.18) that the group velocity and phase velocities are equal. This is to be expected because waves of long wavelength would not be sensitive to the discreteness of the structure that is, large number of atoms would participate in all displacements.

(4) At higher frequencies, the group velocity and phase velocities are no longer equal: since $\omega(k) = 2\sqrt{(\gamma/m)}\,\mathrm{sin}ka/2$ therefore, the group velocity

$$V_g = d\omega/dk = a\surd(\gamma/m)\ \mathrm{cos}ka/2 = v_o\mathrm{cos}ka/2$$

$$V_g = v_o\ \cos(ka)/a \qquad (2.19)$$

if $k \to 0$, $V_g = v_o$

if $k \to \pi/a$, $V_g = 0$

and the phase velocity is

$$V_p = \omega/k = \frac{2\sqrt{\gamma}/m\ sinka/2}{k}$$

$$V_p = \frac{2a\sqrt{\gamma}/m\ sinka/2}{ka} = \frac{V_o sinka/2}{ka/2} \qquad (2.20)$$

$$\therefore V_p = \frac{V_o sinka/2}{ka/2}$$

if $k \to 0$, $V_p \to 0$

$k \to \pi/4$, $V_p \to 2v_o/\pi$

At $k = \pi/a$, no signal or energy is propagated; the wave is a standing wave, because $k = \pi/a$ gives $\lambda = 2a$ (the maximum frequency); alternate atoms oscillate in anti - phase, so that mid - points of each spring is at rest. The masses therefore behave as if held by two springs each of spring constant 2γ, giving the frequency $\omega(k) = \sqrt{(4\gamma/m)}$.

The simple form of dispersion curve shown in figure (2.3) is as a result of assuming nearest - neighbour forces only. Extension to further neighbours is quite simple in one dimension. For instance, if $\gamma_1 \neq 0$ and $\gamma_2 \neq 0$ equation (2.11) gives

$$\omega^2(k) = \frac{2}{m}(\gamma_1 + \gamma_2 - \gamma_1 \cos ka - \gamma_2 \cos 2ka) \qquad (2.21)$$

2.3 Vibration of Diatomic Linear Chain:

Consider a linear chain with two types of atoms with masses m_1 and m_2 alternating regularly. Variations may occur in the force constants, and the atomic spacing. However, the essential features can be illustrated if we assume even atomic spacing, a single nearest - neighbour force constant γ, but different atomic masses, as shown in figure 2.4.

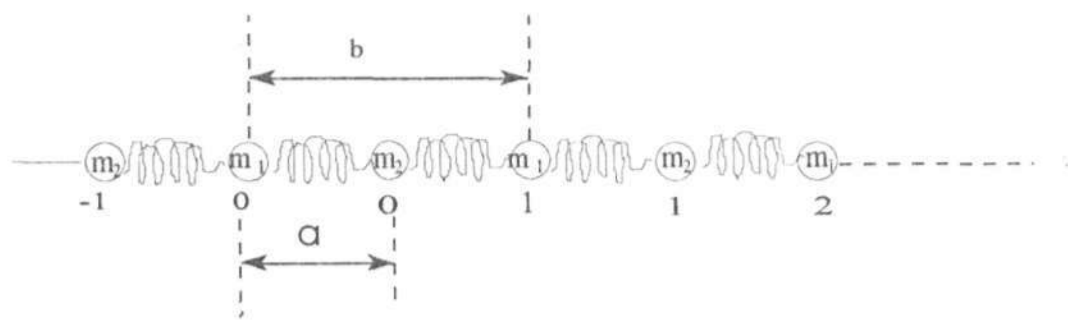

Fig. 2.4. linear chain of atoms of two spacies, having different masses but identical spacing and force constants.

The lattice spacing b is now the distance between like atoms (i.e. b = 2a), since the unit cell now contains two atoms. Thus we have two equations of motion, for two types of atoms:

$$\begin{aligned} m_1 \frac{\partial^2 u_o(1)}{\partial t^2} &= \gamma\left(u_o(2) - u_o(1)\right) + \gamma\left(u_{n-1}(2) - u_o(1)\right) \\ &= \gamma\left(u_o(2) + u_{n-1}(2) - 2u_o(1)\right) \end{aligned} \tag{2.22}$$

$$\begin{aligned} m_2 \frac{\partial^2 u_o(2)}{\partial t^2} &= \gamma[u_1(1) - u_o(2)] + \gamma[u_o(1) - u_o(2)] \\ &= \gamma[u_1(1) + u_o(1) - 2u_o(2)] \end{aligned} \tag{2.23}$$

We now use, in equations (2.22) and (2.23), the plane wave solution:

$$u_l(1) = Ae^{i(\omega t - klb)}$$

$$u_l(2) = Be^{i[\omega t - k(l + \frac{1}{2})b]} \qquad (2.24)$$

Therefore

$$\frac{\partial U_l(1)}{\partial t} = iA\omega\, e^{i}(\omega t - klb)$$

$$\frac{\partial^2 U_l(1)}{\partial^2 t} = -A\omega^2 e^{i}(\omega t - klb) \qquad (2.25)$$

Similarly

$$\frac{\partial^{2_l}(2)}{\partial^2 t} = -B\omega^2 e^{i[\omega t - k(l + 1/2)b]}$$

Substituting eq. (2.25) into eqs. (2.22) and (2.23) we have

$$-m_l A\omega^2 e^{i\omega t} = \gamma\left\{B\, e^{i(\omega t - 1/2kb)} + Be^{i(\omega t + 1/2kb)} - 2A\, e^{i\omega t}\right\}$$

$$-m_l\omega^2 = \gamma\left\{B\, e^{-i/2kb} + B\, e^{i/2kb} - 2A\right\} \qquad (2.26)$$

$$-m_l A\omega^2 = -2\gamma\left\{A - B\cos 1/2kb\right\}$$

and

$$-m_2 B\omega^2 e^{i(\omega t - 1/2kb)} = \gamma\left\{A e^{i(\omega t - kb)} + A e^{i\omega t} - 2B e^{i(\omega t - 1/2kb)}\right\}$$

$$-m_2 B\omega^2 e^{i(\omega t - 1/2kb)} = \gamma e^{i\omega t - 1/2kb}\left\{A e^{-i/2kb} + A e^{i/2kb} - 2B\right\} \qquad (2.27)$$

$$-m_2 B\omega^2 = -2\gamma\{B - A\cos 1/2kb\}$$

eqs. (2.26) and (2.27) give

$$-m_1 A\omega^2 = -2\gamma\ \{A - B\cos\tfrac{1}{2}kb\}$$

$$-m_2 B\omega^2 = -2\gamma\ \{B - A\cos\tfrac{1}{2}kb\} \qquad (2.28)$$

The condition for equation (2.28) to have non- - trivial solution for A and B is that the determinant of coefficients of A and B must vanish i.e.

$$\begin{vmatrix} 2\gamma - m_1\omega^2 & -2\gamma\cos\frac{1}{2}kb \\ -2\gamma\cos\frac{1}{2}kb & 2\gamma - m_2\omega^2 \end{vmatrix} = 0 \qquad (2.29)$$

giving

$$4\gamma^2 - 2\gamma m_2\omega^2 - 2\gamma m_1\omega^2 + m_1m_2\omega^4 - 4\gamma^2\cos^2(½kb) = 0$$

$$4\gamma^2(1 - \cos^2(½kb)) - 2\gamma\omega^2(m_1 + m_2) + m_1m_2\omega^4 = 0$$

$$\therefore \quad 4\gamma^2\sin^2(½kb) - 2\gamma\omega^2(m_1 + m_2) + m_1m_2\omega^4 = 0$$

Dividing through by m_1m_2 we have

$$\omega^4 - 2\gamma(1/m_1 + 1/m_2)\omega^2 + 4\gamma^2/m_1m_2\sin^2(½kb) = 0$$

The above equation is a quadratic equation in ω^2 and this may be written as

$$\omega^2 = \gamma\left(\frac{1}{m_1} + \frac{1}{m_2}\right) \pm \omega\left[\left(\frac{1}{m_1} + \frac{1}{m_2}\right)^2 - \frac{4\sin^2\left(\frac{1}{2}kb\right)}{m_1m_2}\right] \qquad (2.30)$$

$$\omega^2 = \frac{1}{2}\omega_o^2\left[1 \pm \sqrt{1 - C\sin^2\left(\frac{1}{2}kb\right)}\right] \qquad (2.31)$$

where $\omega_o^2 = 2\gamma(1/m_1 + 1/m_2)$ and C is commonly called a coupling coefficient, defined as

$$c = \frac{4m_1m_2}{(m_1 + m_2)^2} = \frac{4\rho}{(1+\rho)^2} \qquad (2.32)$$

where $\rho = m_1/m_2$

Equation (2.30) expresses the dispersion relation between ω and k. The dispersion curve is shown in Figure (2.5).

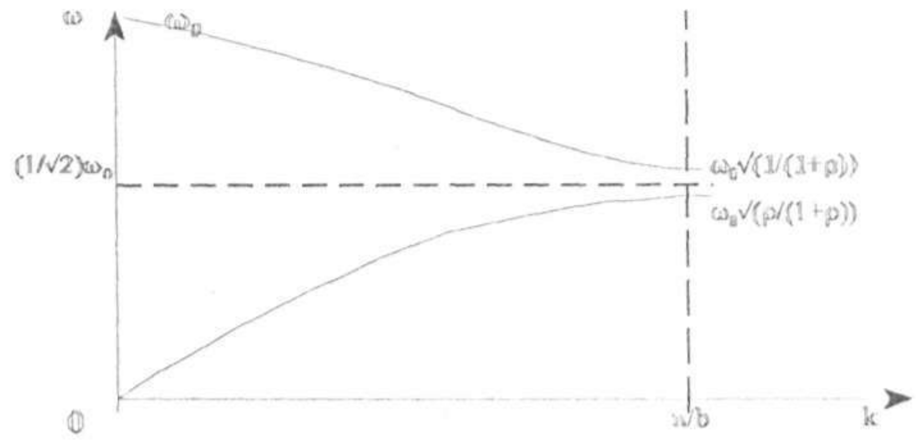

Fig. 2.5: Phonon dispersion curve for a diatomic linear chain, with atoms of different masses m_1 and m_2 (where $\rho = m_1/m_2$, m_1 being the smaller mass)

While discussing the monatomic lattice, there was solution for ω > 0 and for ω < 0. But the diatomic case evidently has two solutions as shown in Eq (2.30). We consider first the sum (+) case:

For k → 0, we can neglect the sine term in eq (2.30), so we have

$$\omega_+^2 = \gamma\left(\frac{1}{m_1} + \frac{1}{m_2}\right) + \gamma\left[\left(\frac{1}{m_1} + \frac{1}{m_2}\right)^2\right]^{\frac{1}{2}}$$

$$= 2\gamma\left(\frac{1}{m_1} + \frac{1}{m_2}\right)$$

But

$$\omega_o^2 = 2\gamma\left(\frac{1}{m_1} + \frac{1}{m_2}\right)$$

Hence

$$\omega_+^2 = \omega_o^2 \qquad (2.33)$$

This shows that at $k \to 0$, $\omega_+^2 = \omega_o^2$, which is the optical branch.

For $k \to \pi/b$. The sine term in Eq (2.30) becomes $-4/m_1m_2$, which changes the term under the radical to $(1/m_1 - 1/m_2)^2$, i.e.

$$\omega_+^2 = \gamma\left(\frac{1}{m_1} + \frac{1}{m_2}\right) + \gamma\left[\left(\frac{1}{m_1} + \frac{1}{m_2}\right)^2 - \frac{4}{m_1 m_2}\right]^{\frac{1}{2}}$$

Or

$$\omega_+^2 = 2\frac{\gamma}{m_1}$$

But

$$\omega_o^2 = 2\gamma\left(\frac{1}{m_1} + \frac{1}{m_2}\right)$$

which implies that

$$2\gamma = \omega_o^2 \frac{m_1 m_2}{m_1 + m_2}$$

Therefore

$$\omega_+^2 = \omega_o^2\left(\frac{1}{1+\rho}\right) \_ \omega_+ = \omega_o\sqrt{\frac{1}{1+\rho}} \quad ; \quad optical \tag{2.34}$$

Now by considering the difference sum (-) case:

For k → 0, the sine term in eq (2.30) becomes $4k^2b^2/m_1m_2$

$$\omega_-^2 = \gamma\left(\frac{1}{m_1}+\frac{1}{m_2}\right) - \gamma\left[\left(\frac{1}{m_1}+\frac{1}{m_2}\right)^2 - \frac{4k^2b^2}{m_1m_2}\right]^{\frac{1}{2}}$$

$$= \gamma\left(\frac{1}{m_1}+m_2\right)\left[1-\left(1-\frac{4m_1m_2k^2b^2}{m_1+m_2}\right)^{\frac{1}{2}}\right]$$

$$= \frac{1}{2}\omega_o^2\left[1-\left(1-\frac{4\rho k^2b^2}{(1-\rho)^2}\right)^{\frac{1}{2}}\right]$$

Using binomial expansion, we get

$$\omega_-^2 = \omega_o^2 k^2 b^2 \tag{2.35}$$

For k → π/b, the solution is

$$\omega_-^2 = \gamma\left(\frac{1}{m_1}+\frac{1}{m_2}\right) - \gamma\left[\left(\frac{1}{m_1}+\frac{1}{m_2}\right)^2 - \frac{4}{m_1 m_2}\right]^{\frac{1}{2}}$$

Or

$$\omega_-^2 = \frac{2\gamma}{m_2}$$

But

$$2\gamma = \omega_o^2 \frac{m_1 m_2}{m_1 + m_2}$$

Hence,

$$\omega_-^2 = \omega_o^2\left(\frac{m_1}{m_1+m_2}\right) \_ \ \omega_- = \omega_o \sqrt{\frac{\rho}{1+\rho}} \quad \textit{Acoustical} \qquad (2.36$$

The upper ω_+ and lower ω_- branches of the curve are referred to as the optical and acoustical branches respectively, and the curves are symmetrical at $\omega_o^2/2$. The two branches join and become degenerate at $k = \pi/b$. Thus for the limiting case $m_1 = m_2$ the upper curve has been artificially `folded back' from that part of the Brillouin zone where $\pi/b < k \le \pi/a$ as shown in Figure (2.6)

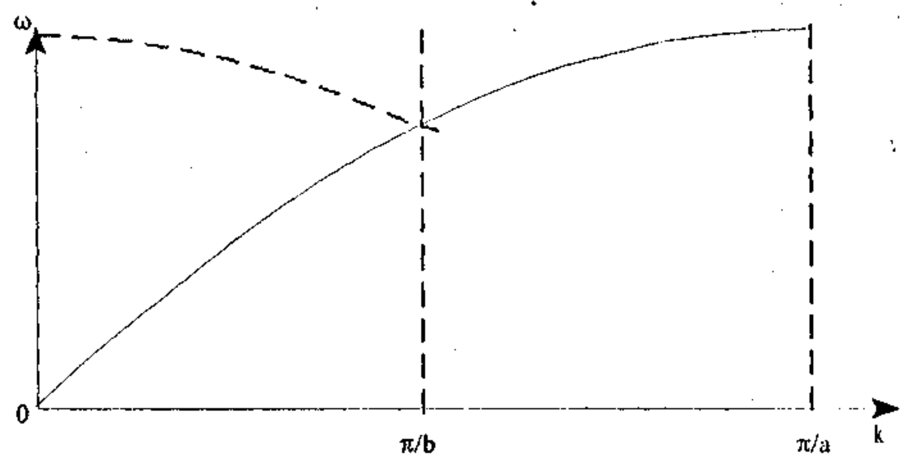

Figure 2.6: *The true phonon dispersion curve for a monatomic linear chain (solid line) and when treated as the limiting case $m_1 = m_2$ for a diatomic linear chain (broken line)*

The optical branch represents a completely different form of wave motion. the physical difference of the two branches can be calculated as $k \to 0$.

For the optical branch, $\cos(kb/2) \to 1$

Therefore eq(2.28) gives

$$-m_1 A\omega^2 = -2\gamma A - 2\gamma B$$

or

$$\frac{\omega^2}{2\gamma} = \frac{(A-B)}{Am_1} \qquad (2.37)$$

and

$$-m_2 B\omega^2 = -2\gamma(B-A)$$

Or

$$\frac{\omega^2}{2\gamma} = -(A-B)/m_2 B \tag{2.38}$$

comparing eqs(2.37) and (2.38)

$$\frac{A}{B} = -\frac{m_2}{m_1} \tag{2.39}$$

This shows that the neighbouring atoms are moving in opposite directions in such a way that the common centre of mass for a neighbour pair does not move. If $m_1 = m_2$, we find $A/B = -1$ for the optical branch.

The corresponding calculations for the acoustical branch is: as $k \to 0$, $\cos(kb/2) = 1 - 2\sin^2(kb/2) = 1 - (k^2b^2)/2$.

Therefore, eq(2.28) can be written as

$$-m_1 A\omega^2 = -2\gamma[A - B(1 - \frac{k^2b^2}{2})]$$

$$-m_1 A\omega^2 = 2\gamma B[1 - \frac{k^2b^2}{2}] - 2\gamma A \tag{2.40a}$$

$$-m_2 B\omega^2 = -2\gamma[B - A(1 - \frac{k^2b^2}{2})]$$

$$-m_2 B = 2\gamma A[1 - \frac{k^2b^2}{2}] - 2\gamma B \tag{240b}$$

But

$$\omega^2 = (\frac{2\gamma}{m_1 + m_2}) k^2 b^2$$

Substituting into Equations (2.40a) and (2.40b) we get

$$-m_1 A(\frac{2\gamma}{m_1 + m_2}) k^2 b^2 = 2\gamma B(1 - \frac{k^2 b^2}{2}) - 2\gamma A$$

$$-m_2 B(\frac{2\gamma}{m_1 + m_2}) k^2 b^2 = 2\gamma A(1 - \frac{k^2 b^2}{2}) - 2\gamma B \qquad (2.41)$$

Adding Equations (2.41) we have

$$-\frac{1}{m_1 - m_2}(m_1 A + m_2 B) = -\frac{1}{2}(A + B)$$

which leads to A/B = +1

In this case the neighbouring atoms go in the same direction as shown in the figure (2.7) below

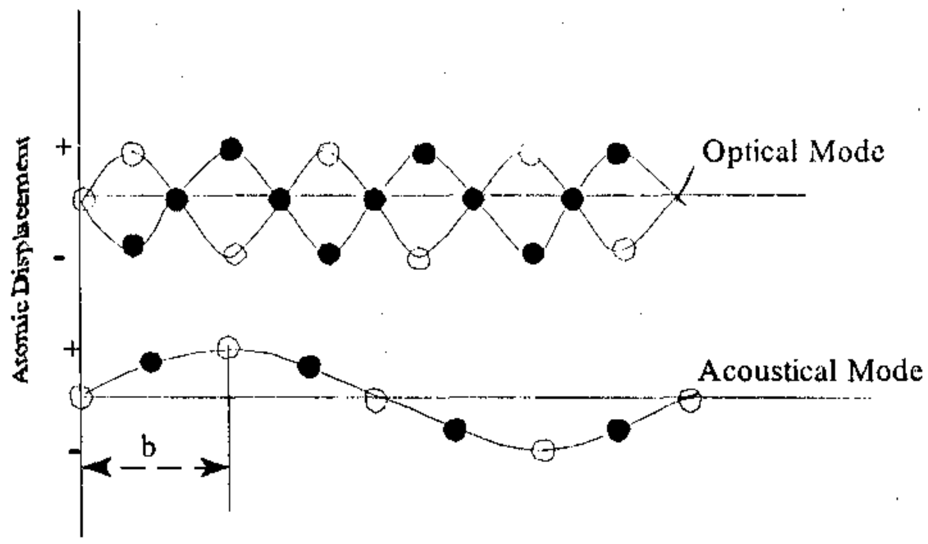

Fig: (2.7) *The difference between the acoustical and optical modes.*

The acoustic branch can be stimulated by some kind of force that makes all the atoms to go in the same direction, such as a compressional wave or sound wave. This is why it is called the Acoustic branch. A monatomic lattice can respond only to this kind of excitation.

The optical branch, on the other hand, can be excited by an excitation that has an opposite effect on the two atoms. However, the existence of optical type vibrations does not necessarily depend on a mass difference or even on oppositely charged ions. It depends only on they're being two atoms per primitive cell so that they can vibrate in and out from the centre of mass. There are some interesting facts about diatomic lattice to be noted.

(i) If the masses are all equal, the frequency range is the same in the monatomic and diatomic lattices, and there is no forbidden gap.

(ii) At $k = \pi/2a$, only one of the sub-lattice is vibrating. In the optical branch, it is the light atom while in the acoustical branch it is the heavy atom. Both branches represent standing waves, which have a phase difference of $\pi/2$. The frequency difference between the two modes arises entirely from the masses of the two atoms.

(iii) If the heavy mass $m_2 \to \infty$, the acoustical branch disappears. The optical branch flattens in such a way that all k values have the same frequency $(2\gamma/m_1)^{1/2}$ as can be seen from eq(2.36). Physically, this means that each atom is completely independent of its neighbours and each oscillates at its own natural uncoupled frequency.

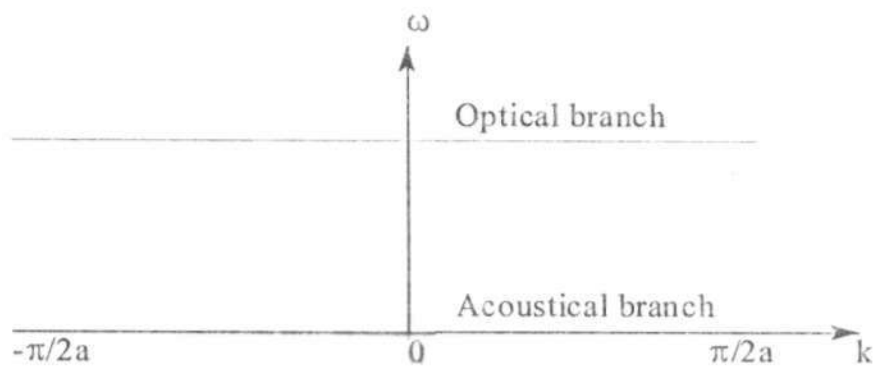

Fig: 2.8 Acoustical branch as $M_2 \rightarrow \infty$ (disappears).

In this case, the midpoint between each atom is tied down, isolating the atoms from one another.

(iv) If the light mass $m_1 \rightarrow 0$, the optical branch disappears upward, the acoustical branch is unchanged, and we return to the monatomic lattice constant `2a'.

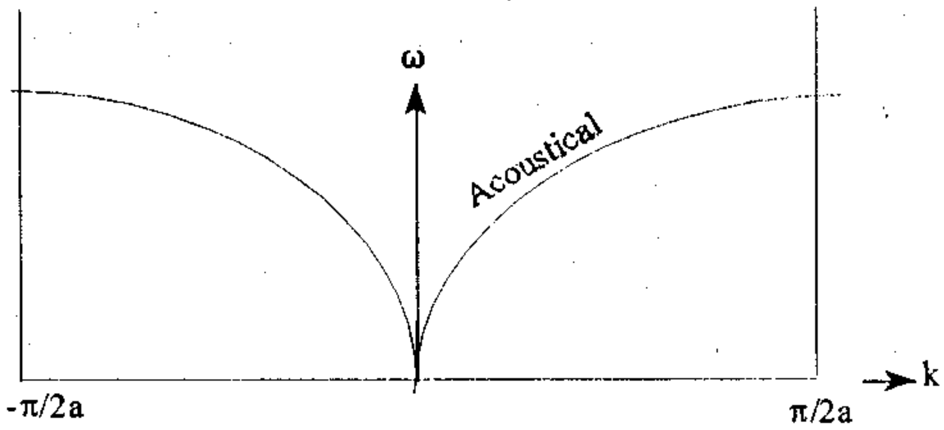

Fig:2.9 Optical branch as M1 → 0(disappears).

(v) The optical modes are essentially the natural frequency of light atoms, perturbed by the heavy sub-lattice. At k =π/2a, the heavy sub-lattice is stationary, and the light atoms vibrate at their natural frequency (2 /m). As k decreases, the perturbation increases, until at k = 0 the two sub-lattices are actually vibrating rightly against each other as shown in the Figure (2.9)

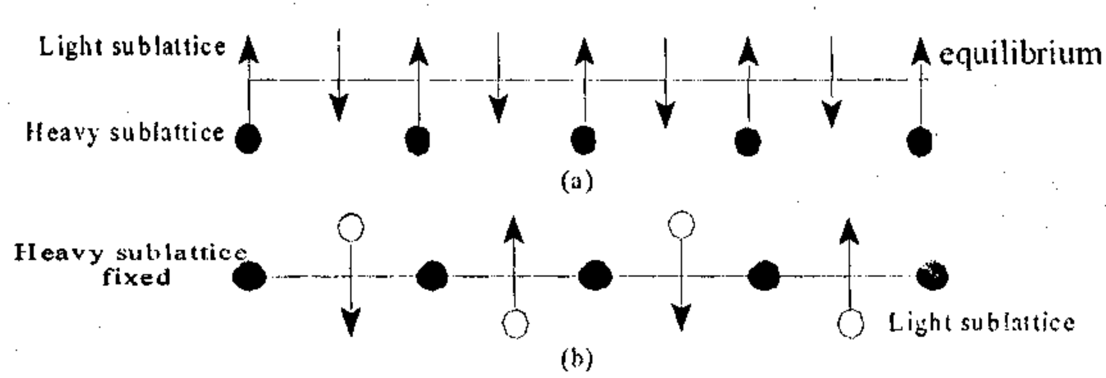

Fig. 2.10: *Optical modes (a) at $k = 0$ and (b) $k = \pi/2a$ showing vibrating of these light and heavy sub-lattices*

The increase in frequency as k decreases is due to an effectively larger spring constant $\{\gamma \rightarrow \gamma(1 + m_1/m_2)\}$ for the larger atoms, which results from the counter-vibrating heavy sub-lattice.

CHAPTER THREE

3.0 Density of States

Any vibrational pattern is possible for an elastic continuum. There is a limit to the number of distinguishable modes of vibration for a lattice of finite size made up of discrete atoms.

The linear monatomic chain of $(N + 1)$ atoms , which will have a length of Na, the distribution of modes with respect to frequency or wave-vector either longitudinal or transverse vibrations can exist for which there are 1, 2, 3, ... or N half-wavelengths in the distance Na. These permitted vibrational modes are situations for which the wave-vector is

$$k = \pi/Na,\ 2\pi/Na,\ 3\pi/Na,\ \ldots \text{ or } \pi/a \qquad (3.0)$$

and the spacing is linear.

The spacing will be very small if N is a large number, and it will then be appropriate to describe the number of states (number of distinguishable vibrational modes) lying between k and $k + dk$ as $(Na/\pi)dk$. Then the number of states per unit length of our one-dimensional crystal, in an interval dk, is simply

$$\begin{aligned} G(k).dk &= (1/\pi).dk, && k \leq \pi/a \\ &= 0 && k \geq \pi/a \end{aligned} \qquad (3.1)$$

we refer to $G(k)$ as the density of states (per unit length, per unit interval k) with respect to k. For one-dimensional example chosen, we see that $G(k)$ does not depend on k within the permitted spectral range.

Our evaluation of a density of states was weakened by our assumption that the end atoms in the chain were motionless (since such an assumption permits solutions only for standing waves rather than running waves). Alternatively, we might suppose an infinite linear chain of atoms with atomic spacing a, subject to the restriction that any permitted mode repeats its set of displacements after the distance $L = Na$. Modes which can propagate subject to this restriction must have wave vectors

$$k = \pm 2\pi/L,\ \pm 4\pi/L,\ \pm 6\pi/L,\ \ldots \text{ or } \pm \pi/a \qquad (3.2)$$

A comparison of eqs(3.0) and (3.2) makes it obvious that the density of states $G(k)$ in terms of unit change in k is $1/\pi$ for a one-dimensional crystal. Indeed we can assert that the density of states for an infinite chain is independent of the boundary conditions applied. Now an infinite linear chain of atoms is not the kind of crystal we study experimentally. However, by demonstrating the unimportance of boundary conditions for a linear chain we can go on to assert that the density of states with respect to wave-vector, frequency, or energy in a real three-dimensional crystal will not depend on the shape or nature of the surface, provided only that the crystal is large compared with atomic dimensions.

3.1 Density of Modes for Monatomic Linear Chain

From the monatomic linear chain treatment, it shows that all values of k are possible. So in this case the chain must be bounded and the appropriate boundary conditions can be applied. The particular choice of boundary condition affects only the time details of the density of states, which is for the solution to be periodic over a very large number of lattice spacings, N. Thus $u_l = u_{l+N}$, eq(2.5) then

$Exp-(ikla) = \exp\{-ik(l+N)a\}$ or $e^{-ikNa} = 1$

Hence, $kNa = 2n\pi$, where n is any integer, or

$$k = 0, \frac{2\pi}{aN}, \frac{2\pi}{a}\frac{2}{N}, \dots \pm \frac{2\pi}{a}\frac{\frac{1}{2}N}{N} \qquad (3.3)$$

i.e., there are approximately N possible values of k, evenly distributed throughout k-space with an interval $2\pi/Na$.

Thus the density of states in k-space, $\omega(k)$ - that is, the number of possible modes of vibration per unit interval in k-space is a constant given by

$2\pi\omega(k)/Na = 1 \rightarrow \omega(k) = Na/2\pi$

On the other hand, if the density of states is a function of frequency, $D(\omega)$. Now the number of states in a small frequency interval $d\omega$ will be

$$D(\omega)d\omega = \omega(k)dk = \omega(k)\frac{dk}{d\omega}d\omega \qquad (3.4)$$

Therefore

$$D(\omega) = \frac{\omega(k)}{d\omega/dk} \qquad (3.5)$$

For the one-dimensional linear chain with nearest-neighbour interactions, it is easy to show that eq(2.22) becomes

$$D(\omega) = \frac{Na/2\pi}{d\omega/dk}$$

but

$$\omega^2 = \frac{4\gamma}{m}\sin^2 ka/2$$

$$\omega = 2\sqrt{\frac{\gamma}{m}}\sin ka/2$$

$$d\omega/dk = a\sqrt{\gamma/m}\cos ka/2$$

Therefore

$$D(\omega) = \frac{Na/2\pi}{a\sqrt{\gamma/m}\ coska/2}$$

and

$$D(\omega) = \frac{N}{2\pi\left(1-\sin^2 ka/2\right)\sqrt{\gamma/m}}$$

From eq(2.11)

$$\sin^2 ka/2 = \frac{m\omega^2}{4\gamma}$$

$$D(\omega) = \frac{2N}{\pi(\omega_{\max}^2 - \omega^2)^{1/2}} \qquad (3.6)$$

where

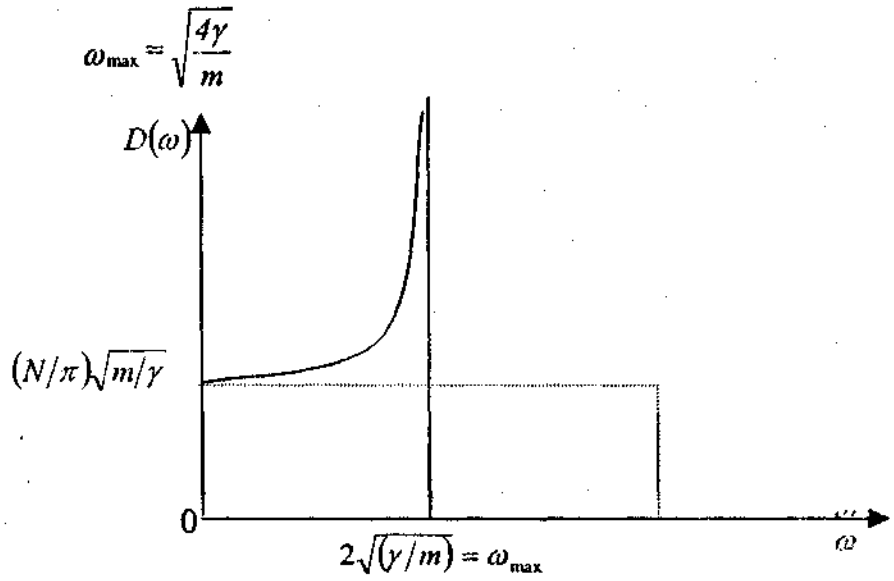

Fig. 3.1 density of states for a chain of atoms.

The factor 2 arises because ω is always positive, so the negative and positive regions of k-space both contribute to the range dω.

We notice that it tends to infinity as the cut-off frequency $2\sqrt{\gamma/m}$ is approached from below, because the group velocity dω/dk tends to zero here. If the dispersion of sound at short wavelength is ignored we will obtain the constant density of states shown by the broken line in Figure(3.1), for which the total number of states does not reach the value N until frequency $\omega = \pi(k/m)^{1/2}$

3.2 Density of States in Three Dimensions

Since the result of the one-dimensional example (as discussed above) cannot be compared with experiment, therefore, we apply periodic boundary conditions over N^3 primitive cells within a cube of side L, so that k is determined by the condition

$$\exp[i(k_x x + k_y y + k_z z)]$$

$$\equiv \exp\{i[k_x(x+L) + k_y(y+L) + k_z(z+L)]\} \qquad (3.7)$$

where

$$k_x,\ k_y,\ k_z = 0,\ \pm 2\pi/L,\ \pm 4\pi/L,\ \ldots,\ N\pi/L \qquad (3.8)$$

Therefore, there is one allowed value of k per volume $(2\pi/L)^3$ in k-space, or

$$\left(\frac{L}{2\pi}\right)^3 = \frac{V}{8\pi^3} \qquad (3.9)$$

allowed values of k per unit volume of k-space, for each polarization and for each branch. The volume of the specimen is $V = L^3$.

In the continuum or Debye approximation the velocity of sound is constant: $\omega = vk$. The total number of modes with wave-vector less than k is given by $(L/2\pi)^3$ times the volume of a sphere of radius k, so that

$$N = \left(\frac{L}{2\pi}\right)^3 \frac{4\pi}{3} k^3 = \left(\frac{L}{2\pi}\right)^3 \frac{4\pi\omega^3}{3v^3} \qquad (3.10)$$

since $k = \omega/v$

$$N = \frac{V\omega^3}{6\pi^2 v^3} \qquad (3.11)$$

$$d^3k = dk_n ds_\omega \tag{3.16}$$

The gradient of ω, which is ∇k_ω is also normal to the surface ω constant, and the quantity

$$|\Delta_k \omega| dk_n = d\omega \tag{3.17}$$

Thus the element of the volume is

$$d^3k = \frac{d\omega\, ds_\omega}{|\Delta_k \omega|} \tag{3.18}$$

Substituting eq(3.18) into eq(3.15) we have

$$D(\omega)d\omega = \left(\frac{L}{2\pi}\right)^3 \int \frac{ds_\omega}{\nabla_k \omega} d\omega \tag{3.19}$$

One significant importance of eq(3.19) is that

$$D(\omega)d\omega = \left(\frac{L}{2\pi}\right)^3 \int \frac{ds_\omega}{\nabla_k \omega} d\omega \tag{3.20}$$

where $v_g = |\nabla k\omega|$ is the group velocity.

For the monatomic linear chain eq(2.12) the sound velocity is easily calculated as

$$\omega^2 = (4\gamma/m)\sin^2 ka/2$$

$$\frac{d\omega}{dk} = a\sqrt{\gamma/m}\cos ka/2$$

$$= a\sqrt{(\gamma/m)}\left\{1 - \sin^2\left(\frac{ka}{2}\right)\right\}^{1/2}$$

$$= a\sqrt{\frac{\gamma}{m}}\left\{1 - \frac{m\omega^2}{4\gamma}\right\}^{1/2}$$

for each polarization type. The density of modes for each polarization type is

$$D(\omega)=\frac{dN}{d\omega}=\frac{V\omega^2}{2\pi^2 v^3} \tag{3.12}$$

If there are N primitive cells in the specimen, the total number of acoustic phonon modes is N, and a cut-off frequency ω_D is determined from the eq(3.11) as

$$N=\frac{V\omega^3}{6\pi^2 v^3} - \omega_D^3=\frac{6\pi^2 v^3 N}{V} \tag{3.13}$$

To this frequency there corresponds a cut-off wave-vector in k-space:

$$k_D=\omega_D/v=\left(6\pi^2 N/V\right)^{1/3} \tag{3.14}$$

The general expression for D(ω), the number of modes per unit frequency range given the phonon's dispersion relation ω(k) can be found.

From eq(3.9) the number of allowed values of k for which the phonon frequency is between ω and ω + dω is

$$D(\omega)d\omega=\left(\frac{L}{2\pi}\right)^2 \int_s d^3 k \tag{3.15}$$

Here we restrict ourselves to a particular value of s and consider the constant frequency surfaces for ω and ω +dω. If ds_ω is an element of area of the constant frequency surface ω, and the distance between that surface and that corresponding to ω + dω is dk_n (n for normal), then

$$\frac{d\omega}{dk} = \frac{a}{2}\left\{\frac{4\gamma}{m} - \omega^2\right\}^{1/2} \tag{3.21}$$

For long wavelength

$$\frac{d\omega}{dk} = \frac{a}{2}\left(\frac{4\gamma}{m}\right)^{1/2} = a\left(\frac{\gamma}{m}\right)^{1/2} \tag{3.22}$$

which is the sound velocity in a string whose mass per unit length is m/a and tension is γa.

3.3 Van Hove Critical Points

For the analytical expression for the density of states in one dimension, eq(3.6) has a singularity at $\omega = \omega_{max}$. The reason for this is easy, in Figure (3.1) the density of points in k-space is uniform, so that at any point on the curve where the slope approaches zero there will be a very large density of points in ω-space. This occurs at the Brillouin zone boundary, where $\omega = \omega_{max}$. However, any point on a dispersion curve where the slope is zero will create a singularity in the density of states and these are known as van Hove singularities.

In three dimensions a similar feature occurs where ever $\nabla_k(\omega) = 0$.

4.0 Normal Modes

We can now write the equation of motion, still for simplicity confining our attention to the force in one dimension as

$$F_0 = +\gamma\left(u_1 - u_o\right)$$

which may be written as

$$F_0 = \sum_{l\neq 0}\gamma_l\left(u_l - u_0\right) = \sum_{l\neq 0}\gamma_l u_l - \sum_{l\neq 0}\gamma_l u_0 \qquad (4.1)$$

If we define a special quantity γ_0 as

$$\gamma_0 = -\sum_{l\neq 0}\gamma_l$$

then eq(4.1) reduces to

$$F_0 = \sum_{l\neq 0}\gamma_l u_l + \gamma_0 u_0$$

$$F_0 = \sum_{l=-\infty}^{+\infty}\gamma_l u_l \qquad (4.2)$$

The physical significance of γ_0 is simply that it represents the restoring force on the atom at the origin due to a displacement of itself.

4.1 Normal Mode Frequencies in Three Dimensions

In three dimensions, eq(4.2) can be generalized to

$$\vec{F}_0 = \sum_l \vec{\Phi}_l \bullet \vec{u}_l \qquad (4.3)$$

(the minus sign is introduced simply for convenience, because Φ then represents the second derivatives of the equilibrium crystal potential energy).

If we use α and β as coefficients to represent the cartesian components of the vectors, the force equation(4.3) can be written

$$F_{0,\alpha} = -\sum_l \sum_{\beta=1}\Phi_{l,\alpha\beta}u_{l,\beta}, \alpha = 1,2,3 \qquad (4.4)$$

There are now three equations of motion for each atom, corresponding to the three degree of freedom.

$$m\frac{\partial^2}{\partial t^2}u_{0,\alpha} = -\sum_{l}\sum_{\beta=1}^{3}\Phi_{l,\alpha\beta}u_{l,\beta} \tag{4.5}$$

and the three-dimensional form of a plane wave is

$$u_{l,\alpha}\left(\vec{k}\right) = A_\alpha \exp\left[i\left(\omega t - \vec{k}\bullet\vec{r}_l\right)\right] \tag{4.6}$$

therefore eqn(4.5) becomes

$$-m\omega^2 A_\alpha \exp(i\omega t) = -\sum_{l}\sum_{\beta=1}^{3}\Phi_{l,\alpha\beta}A_\beta \exp\left[i(\omega t - k.r)\right] \tag{4.7}$$

To facilitate the generalization to a unit cell containing more than one atom, it is convinient at this point to make two new definitions.

$$B_\alpha = m^{1/2}A_\alpha, D_{\alpha\beta} = \frac{1}{m}\sum_{l}\Phi_{l,\alpha\beta}\exp\left(-i\vec{k}\bullet\vec{r}_l\right) \tag{4.8}$$

Substituting eq(4.8) into eq(4.7) gives

$$m^{\frac{1}{2}}A_\alpha\omega^2 = \frac{1}{m}\sum_{l}\sum_{\beta=1}^{3}\Phi_{l,\alpha\beta}A_\beta\exp\left[-ik.r_l\right]\times m^{\frac{1}{2}}$$

$$\omega^2 B_\alpha = \sum_{\beta=1}^{3}D_{\alpha\beta}B_\beta, \alpha = 1,2,3 \tag{4.9}$$

or in matrix form

$$\omega^2\vec{B} = D\cdot\vec{B} \tag{4.10}$$

This is a typical eigenvalue problem and the solutions for ω^2 are the roots of the determinantal equation

$$\mathrm{Det}\,(D - \omega^2 I) = 0 \tag{4.11}$$

The matrix **D** is commonly called the dynamical matrix, and the determinant is called the secular determinant.

4.2 Calculation of dynamical matrix for a BCC lattice with one atom Unit Cell

In this part, we have to specify the type of lattice and force constants. In the case of a body-centered cubic (BCC) lattice which can be described by

$$\vec{r}_l = \vec{a}\vec{l}\ ,\ l=(l_1, l_2, l_3), \qquad (4.12)$$

where l_1, l_2, and l_3 are either all odd or all even integers.

For simplicity, the interatomic force constants are purely radial, and that only nearest- and second nearest neighbour interactions are significant, with force constants γ and $R\gamma$, so that R represents the ratio of second nearest to nearest force constsants. We need to calculate the matrices Φ_l for each nearest and second nearest neighbour (l=1,-14) and for l=0.

If the atom O lies at the center of a cube of side 2a, then the eight nearest neighbours lie on the corners of the cube, along the [111], type directions as shown in Figure (4.1). Consider atom 1, lying on the [111]-direction. Referring back to ecquation (4.4), we see that $-\Phi_{l,\alpha\beta}$ is the force on atom O in the α-direction resulting from unit displacement of atom 1 in the β-direction.

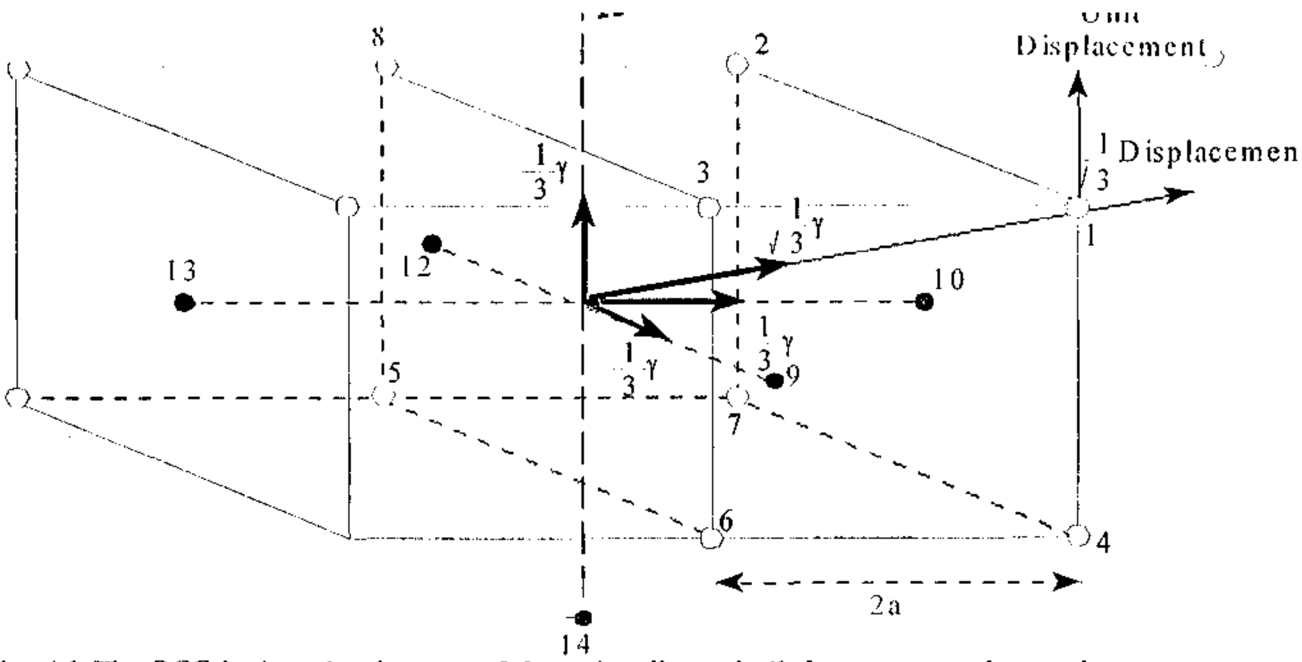

Fig: 4.1 The BCC lattice, showing two of the unit cells, and all the nearest and second-nearest neighbours of the atom at the center of the right hand cell.

Let us consider the unit displacement of atom 1 in the x-, y- or z- direction. In each case this results in a radial component of displacement

$$R = \sqrt{x^2 + y^2 + z^2}$$

For unit displacement

$$R = \sqrt{1+1+1} = \sqrt{3}$$

and since only radial forces are being considered, the resultant force on atom O is $(1/\sqrt{3})\gamma$. If the force is resolved into three certasian components, these can be written as $F_{ox} = F_{oy} = F_{oz} = \gamma/3$. Thus each cartesian component of force due to unit displacement along any cartesian axis is $\gamma/3$, and this means that $-\Phi_{1,\alpha\beta} = \gamma/3$ for all α and β. Thus, the matrix is given as

$$-\Phi_1 = \frac{1}{3}\gamma\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} \qquad (4.13)$$

Exactly the same will be true for atom 5, in the $[\bar{1}\,\bar{1}\,\bar{1}]$- direction, ie. $-\Phi_5 = -\Phi_1$.

For atom 2 lying on the $[\bar{1}\,1\,1]$-direction is also the same with atom 6 in the $[1\,\bar{1}\,1]$-direction, and the matrix is given as

$$-\Phi_2 = -\Phi_6 = \tfrac{1}{3}\gamma\begin{pmatrix} 1 & -1 & -1 \\ -1 & 1 & 1 \\ -1 & 1 & 1 \end{pmatrix} \tag{4.14}$$

For atom 3 lying on the $\left[1\,\bar{1}\,1\right]$-direction is also the same with atom 7 in the $\left[\bar{1}\,1\,\bar{1}\right]$-direction, and the matrix is given as

$$-\Phi_3 = \Phi_7 = \tfrac{1}{3}\gamma\begin{pmatrix} 1 & -1 & 1 \\ -1 & 1 & -1 \\ 1 & -1 & 1 \end{pmatrix} \tag{4.15}$$

For atom 4, lying on the $\left[1\,1\,\bar{1}\right]$-direction is also the same with atom 8 in the $\left[\bar{1}\,\bar{1}\,1\right]$-direction, and the matrix is given as

$$-\Phi_4 = -\Phi_8 = \frac{1}{3}\gamma\begin{pmatrix} 1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \end{pmatrix} \tag{4.16}$$

The second-nearest neighbours lie on the six faces of a cube of side 4a. thus for atom 9, lying along the $[100]$-direction, a unit displacement in the x-direction gives a force $R\gamma$ in that direction on the atom at O, therefore

$$-\Phi_{9,xx} = -\Phi_{12,xx} = R\gamma \tag{4.17}$$

since they are directly opposite neighbours and orthogonal displacements have no effect.

For atom 10, lying along the $[100]$-direction, a unit displacement in the y-direction gives a force $R\gamma$ in that direction on the atom at O,

$$-\Phi_{10,yy} = -\Phi_{13,yy} = R\gamma \tag{4.18}$$

and orthogonal displacements have no effect.

For atom 11, lying along the $[100]$-direction, a unit displacement in the y-direction gives a force $R\gamma$ in that direction on the atom at O,

$$-\Phi_{11,zz} = -\Phi_{14,zz} = R\gamma \tag{4.19}$$

and orthogonal displacements have no effect.

Finallay to calculate $\Phi_{0,}$ is simply the force on atom O due to unit displacement of itself. Thus a unit displacement of O along Ox is equivalent to a displacement of all the neighbours along –Ox. Adding the components of force due to all the other atoms, we find

$$-\Phi_{0,xx} = -\tfrac{8}{3}\gamma - 2R\gamma, -\Phi_{0,xy} = 0, -\Phi_{0,xz} = 0, \tag{4.20}$$

Also, a unit displacement of O along Oy is equivalent to a displacement of all the neighbours along –Oy. Adding the components of force due to all the other atoms, we find

$$-\Phi_{0,yy} = -\tfrac{8}{3}\gamma - 2R\gamma, -\Phi_{0,yx} = 0, -\Phi_{0,yz} = 0, \tag{4.21}$$

The unit displacement of O along Oz is equivalent to a displacement of all the neighbours along –Oz. Adding the components of force due to all the other atoms, we find

$$-\Phi_{0,zz} = -\tfrac{8}{3}\gamma - 2R\gamma, -\Phi_{0,zy} = 0, -\Phi_{0,zx} = 0, \tag{4.22}$$

Thus the matrix becomes

$$-\Phi_0 = -2\gamma\left(\tfrac{4}{3} + R\right)\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{4.23}$$

We can now calculate D from equation (4.8), ie

$$D_{\alpha\beta} = \sum_l \frac{1}{m}\Phi_{l,\alpha\beta}\exp(-ik\cdot r_l) \tag{4.24}$$

Using figure (4.1): the contributions to mD_{xx} are:

from atoms 1 and 5:

$$-\tfrac{1}{3}\gamma\left[\exp\{-i(k_x a + k_y a + k_z a)\} + \exp\{i(k_x a + k_y a + k_z a)\}\right],$$

from atoms 2 and 6:

$$-\tfrac{1}{3}\gamma\left[\exp\{-i(-k_x a + k_y a + k_z a)\} + \exp\{i(-k_x a + k_y a + k_z a)\}\right],$$

from atoms 3 and 7:

$$-\tfrac{1}{3}\gamma\left[\exp\{-i(k_x a - k_y a + k_z a)\} + \exp\{i(k_x a - k_y a + k_z a)\}\right],$$

from atoms 4 and 8:

$$-\tfrac{1}{3}\gamma\left[\exp\{-i(k_x a+k_y a-k_z a)\}+\exp\{i(k_x a+k_y a-k_z a)\}\right],$$

from atoms 9 and 12:

$$-R\gamma\left[\exp\{-i(k_x 2a)\}+\exp\{i(k_x 2a)\}\right]=2R\gamma\cos 2k_x a$$

and

from atom O

$$+2\gamma\left(\tfrac{4}{3}+R\right)$$

Therefore

$$D_{xx}=-\frac{2}{3}\gamma\left[\cos(k_x a+k_y a+k_z a)+\cos(-k_x a+k_y a+k_z a)\right.$$

$$\left.-\frac{2}{3}\gamma\right[\cos(k_x a-k_y a+k_z a)+\cos(k_x a+k_y a-k_z a)\Big]$$

$$=-\frac{2}{3}\gamma\left[2\cos(k_y a+k_z a)\cos k_x a+2\cos k_x a\cos(k_y a-k_z a)\right]$$

$$=-\frac{4}{3}\gamma\left[\cos k_x a\{\cos(k_y a+k_z a)+\cos(k_y a-k_z a)\}\right]$$

$$=-\frac{4}{3}\gamma\cos k_x a\left[2\cos k_y a\cos k_z a\right]$$

Hence

$$D_{xx}=\frac{2\gamma}{m}\left(-\tfrac{4}{3}Cosk_x aCosk_y aCosk_z a-RCos2k_x a+\tfrac{4}{3}+R\right)\qquad(4.25)$$

The contributions to mD_{xy} are:

from atoms 1 and 5:

$$\tfrac{1}{3}\gamma\left[\exp\{-i(k_x a+k_y a+k_z a)\}+\exp\{i(k_x a+k_y a+k_z a)\}\right],$$

from atoms 2 and 6:

$$-\tfrac{1}{3}\gamma\left[\exp\{-i(-k_x a+k_y a+k_z a)\}+\exp\{i(-k_x a+k_y a+k_z a)\}\right],$$

from atoms 3 and 7:

$$-\tfrac{1}{3}\gamma\left[\exp\{-i(k_x a-k_y a+k_z a)\}+\exp\{i(k_x a-k_y a+k_z a)\}\right],$$

from atoms 4 and 8:

$$-\tfrac{1}{3}\gamma\left[\exp\{-i(k_x a+k_y a-k_z a)\}+\exp\{i(k_x a+k_y a-k_z a)\}\right]$$

Therefore

$$D_{xy}=\frac{2}{3}\gamma\left[\cos(k_x a+k_y a+k_z a)-\cos(-k_x a+k_y a+k_z a)\right]$$

$$-\frac{2}{3}\gamma\left[\cos(k_x a-k_y a+k_z a)-\cos(k_x a+k_y a-k_z a)\right]$$

$$=\frac{2}{3}\gamma\left[-2\sin(k_y a+k_z a)\sin k_x a-2\sin k_x a\sin(k_y a-k_z a)\right]$$

$$=-\frac{4}{3}\gamma\sin k_x a\left[\sin(k_y a+k_z a)+\sin(k_y a-k_z a)\right]$$

$$=-\frac{4}{3}\gamma\sin k_x a\left[2\sin k_y a\cos k_z a\right]$$

$$=-\frac{8}{3}\gamma\sin k_x a\sin k_y a\cos k_z a$$

Hence

$$D_{xy}=D_{yx}=+\tfrac{8}{3}\gamma Sin k_x a Sin k_y a Cos k_z a \qquad (4.26)$$

The contributions to mD_{xz} are:

from atoms 1 and 5:

$$-\tfrac{1}{3}\gamma\left[\exp\{-i(k_x a+k_y a+k_z a)\}+\exp\{i(k_x a+k_y a+k_z a)\}\right]$$

from atoms 2 and 6:

$$-\tfrac{1}{3}\gamma\left[\exp\{-i(-k_x a+k_y a+k_z a)\}+\exp\{i(-k_x a+k_y a+k_z a)\}\right]$$

from atoms 3 and 7:

$$-\tfrac{1}{3}\gamma\left[\exp\{-i(k_x a-k_y a+k_z a)\}+\exp\{i(k_x a-k_y a+k_z a)\}\right]$$

from atoms 4 and 8:

$$-\tfrac{1}{3}\gamma\left[\exp\{-i(k_x a+k_y a-k_z a)\}+\exp\{i(k_x a+k_y a-k_z a)\}\right]$$

Therefore

$$D_{xz} = \frac{2}{3}\gamma\left[\cos\left(k_x a + k_y a + k_z a\right) - \cos\left(-k_x a + k_y a + k_z a\right)\right] +$$

$$\frac{2}{3}\gamma\left[\cos\left(k_x a - k_y a + k_z a\right) - \cos\left(k_x a + k_y a - k_z a\right)\right]$$

$$= \frac{2}{3}\gamma\left[-2\sin\left(k_y a + k_z a\right)\sin k_x a - 2\sin k_x a \sin\left(-k_y a + k_z a\right)\right]$$

$$= -\frac{4}{3}\gamma \sin k_x a\left[\sin\left(k_y a + k_z a\right) - \sin\left(k_y a - k_z a\right)\right)$$

$$= -\frac{4}{3}\gamma \sin k_x a\left[2\cos k_y a \sin k_z a\right]$$

$$= -\frac{8}{3}\gamma \sin k_x a \cos k_y a \sin k_z a$$

Hence

$$D_{xz} = D_{zx} = +{}^{8}\!/_{3}\, \gamma Sink_x a \cos k_y a \sin k_z a \qquad (4.27)$$

The contributions to mD_{yy} are:

from atoms 1 and 5:

$$-{}^{1}\!/_{3}\,\gamma\left[\exp\left\{-i\left(k_x a + k_y a + k_z a\right)\right\} + \exp\left\{i\left(k_x a + k_y a + k_z a\right)\right\}\right],$$

from atoms 2 and 6:

$$-{}^{1}\!/_{3}\,\gamma\left[\exp\left\{-i\left(-k_x a + k_y a + k_z a\right)\right\} + \exp\left\{i\left(-k_x a + k_y a + k_z a\right)\right\}\right],$$

from atoms 3 and 7:

$$-{}^{1}\!/_{3}\,\gamma\left[\exp\left\{-i\left(k_x a - k_y a + k_z a\right)\right\} + \exp\left\{i\left(k_x a - k_y a + k_z a\right)\right\}\right],$$

from atoms 4 and 8:

$$-{}^{1}\!/_{3}\,\gamma\left[\exp\left\{-i\left(k_x a + k_y a - k_z a\right)\right\} + \exp\left\{i\left(k_x a + k_y a - k_z a\right)\right\}\right],$$

from atoms 10 and 13:

$$-R\gamma\left[\exp\left\{-i\left(k_y 2a\right)\right\} + \exp\left\{i\left(k_y 2a\right)\right\}\right] = 2R\gamma \cos 2k_y a$$

and from atom O

$$+2\gamma\left(\tfrac{4}{3}+R\right)$$

Therefore

$$D_{yy}=-\frac{2}{3}\gamma\left[\cos\left(k_xa+k_ya+k_za\right)+\cos\left(-k_xa+k_ya+k_za\right)\right]$$

$$-\frac{2}{3}\gamma\left[\cos\left(k_xa-k_ya+k_za\right)+\cos\left(k_xa+k_ya-k_za\right)\right]$$

$$=-\frac{2}{3}\gamma\left[2\cos\left(k_ya+k_za\right)\cos k_xa+2\cos k_xa\cos\left(k_ya-k_za\right)\right]$$

$$=-\frac{4}{3}\gamma\left[\cos k_xa\left\{\cos\left(k_ya+k_za\right)+\cos\left(k_ya-k_za\right)\right\}\right]$$

$$=-\frac{4}{3}\gamma\cos k_xa\left[2\cos k_ya\cos k_za\right]$$

Hence

$$D_{yy}=\frac{2\gamma}{m}\left(-\tfrac{4}{3}Cosk_xaCosk_yaCosk_za-RCos2k_xa+\tfrac{4}{3}+R\right)\tag{4.28}$$

The contributions to mD_{yz} are:

from atoms 1 and 5:

$$-\tfrac{1}{3}\gamma\left[\exp\left\{-i\left(k_xa+k_ya+k_za\right)\right\}+\exp\left\{i\left(k_xa+k_ya+k_za\right)\right\}\right],$$

from atoms 2 and 6:

$$-\tfrac{1}{3}\gamma\left[\exp\left\{-i\left(-k_xa+k_ya+k_za\right)\right\}+\exp\left\{i\left(-k_xa+k_ya+k_za\right)\right\}\right],$$

from atoms 3 and 7:

$$-\tfrac{1}{3}\gamma\left[\exp\left\{-i\left(k_xa-k_ya+k_za\right)\right\}+\exp\left\{i\left(k_xa-k_ya+k_za\right)\right\}\right],$$

from atoms 4 and 8:

$$-\tfrac{1}{3}\gamma\left[\exp\left\{-i\left(k_xa+k_ya-k_za\right)\right\}+\exp\left\{i\left(k_xa+k_ya-k_za\right)\right\}\right],$$

Therefore

$$D_{yz}=\frac{2}{3}\gamma\left[\cos\left(k_xa+k_ya+k_za\right)+\cos\left(-k_xa+k_ya+k_za\right)\right]$$

$$-\frac{2}{3}\gamma\left[\cos\left(k_x a - k_y a + k_z a\right) + \cos\left(k_x a + k_y a - k_z a\right)\right]$$

$$= \frac{2}{3}\gamma\left[2\cos\left(k_y a + k_z a\right)\sin k_x a - 2\cos k_x a\cos\left(k_y a - k_z a\right)\right]$$

$$= \frac{4}{3}\gamma\cos k_x a\left[\cos\left(k_y a + k_z a\right) - \cos\left(k_y a - k_z a\right)\right]$$

$$= \frac{4}{3}\gamma\cos k_x a\left[-2\sin k_y a\sin k_z a\right]$$

$$= -\frac{8}{3}\gamma\cos k_x a\sin k_y a\sin k_z a$$

Hence

$$D_{yz} = D_{zy} = +{}^{8}\!/_{3}\,\gamma\cos k_x a\sin k_y a\sin k_z a \tag{4.29}$$

The contributions to mD_{zz} are:

from atoms 1 and 5:

$$-{}^{1}\!/_{3}\,\gamma\left[\exp\left\{-i\left(k_x a + k_y a + k_z a\right)\right\} + \exp\left\{i\left(k_x a + k_y a + k_z a\right)\right\}\right],$$

from atoms 2 and 6:

$$-{}^{1}\!/_{3}\,\gamma\left[\exp\left\{-i\left(-k_x a + k_y a + k_z a\right)\right\} + \exp\left\{i\left(-k_x a + k_y a + k_z a\right)\right\}\right],$$

from atoms 3 and 7:

$$-{}^{1}\!/_{3}\,\gamma\left[\exp\left\{-i\left(k_x a - k_y a + k_z a\right)\right\} + \exp\left\{i\left(k_x a - k_y a + k_z a\right)\right\}\right],$$

from atoms 4 and 8:

$$-{}^{1}\!/_{3}\,\gamma\left[\exp\left\{-i\left(k_x a + k_y a - k_z a\right)\right\} + \exp\left\{i\left(k_x a + k_y a - k_z a\right)\right\}\right],$$

from atoms 11 and 14:

$$-R\gamma\left[\exp\left\{-i\left(k_z 2a\right)\right\} + \exp\left\{i\left(k_z 2a\right)\right\}\right] = 2R\gamma\cos 2k_z a$$

and

from atom O

$$+2\gamma\left({}^{4}\!/_{3} + R\right)$$

Therefore

$$D_{zz} = -\frac{2}{3}\gamma\left[\cos(k_x a + k_y a + k_z a) + \cos(-k_x a + k_y a + k_z a)\right]$$

$$-\frac{2}{3}\gamma\left[\cos(k_x a - k_y a + k_z a) + \cos(k_x a + k_y a - k_z a)\right]$$

$$= -\frac{2}{3}\gamma\left[2\cos(k_y a + k_z a)\cos k_x a + 2\cos k_x a\cos(k_y a - k_z a)\right]$$

$$= -\frac{4}{3}\gamma\left[\cos k_x a\left\{\cos(k_y a + k_z a) + \cos(k_y a - k_z a)\right\}\right]$$

$$= -\frac{4}{3}\gamma\cos k_x a\left[2\cos k_y a\cos k_z a\right]$$

Hence

$$D_{zz} = \frac{2\gamma}{m}\left(-\tfrac{4}{3}Cosk_x aCosk_y aCosk_z a - RCos2k_x a + \tfrac{4}{3} + R\right) \tag{4.30}$$

Using definitions such as

$$C_x = Cosk_x a, S_x = Sink_x a, C_{2x} = Cos2k_x a, \delta = 1 + \tfrac{3}{4}R - C_x C_y C_z,$$

$$C_y = Cosk_y a, S_y = Sink_y a, C_{2y} = Cos2k_y a, \tag{4.31}$$

$$C_z = Cosk_z a, S_z = Sink_z a, C_{2z} = Cos2k_z a,$$

The elements of D can be considerably simplified. The final result is

$$D(k) = \frac{8\gamma}{3m}\begin{pmatrix} \delta - \tfrac{3}{4}RC_{2x} & S_x S_y C_z & S_x C_y S_z \\ S_x S_y C_z & \delta - \tfrac{3}{4}RC_{2y} & C_x S_y S_z \\ S_x C_y S_z & C_x S_y S_z & \delta - \tfrac{3}{4}RC_{2z} \end{pmatrix} \tag{4.32}$$

4.3 calculation of dynamical matrix for a BCC latice with two atom unit cell.

In the case of more than one atom per unit cell is that there are three equations of motion for each of the atoms. If l is allowed to label all the atoms, then the force constant matrices will have the same form as before, but it will be necessary to lebel Φ and D, and of course the masses m and the amplitudes B, with the type of atom.

The reason for introducing B and D originally is that they must now take the form;

$$B(k) = m_k^{\frac{1}{2}} A(k), D(k,k') = (m_k m_{k'})^{-\frac{1}{2}} \sum_l \Phi_l(k,k') \exp(-ik \cdot r_l), \tag{4.33}$$

where k and k' label the n different atoms in the unit cell. The equation of motion are

$$\omega^2 B(k) = D(k,k') \cdot B(k) + \sum_{k' \neq k} D(k,k') \cdot B(k') \tag{4.34}$$

Equation (4.34) can be written more compactly as

$$\omega^2 B = D' \cdot B \tag{4.35}$$

where D' is a 3n x3n matrix and B is a column vector whose elements are $B_x(1)$, $B_y(1)$, $B_z(1)$, $B_x(2)$, $B_y(2)$, and $B_z(2)$.

Again we need to specify the type of lattice before proceeding any further. One of the simplest types of crystal structure having two atoms per unit cell is the CsCl structure, whose atoms froma BCC lattice having one type of atom at the cube centre and the other type on the corners of the cube, as shown in Figure (4.2). We shall assume as before that all the forces are radial and also that the force constants are the same for the two species of atom, so that we need consider only the difference in masses for the two types of atom.

The matrices Φ will have exactly the same form as before, except that now they must also be labelled with the species of atom, and the first eight will couple different types, whereas the next six couple identical atoms. Thus some matrices will now be zero as follows: $\Phi_l(1,1)=\Phi_l(2,2)=0$, $l=1$ to 8; $\Phi_l(1,2)=\Phi_l(2,1)=0$, $l=9$ to 14; and of course $\Phi_0(1,2)=\Phi_0(2,1)=0$ by defination, and $\Phi_0(1,1)=\Phi_0(2,2)=\left(\frac{8}{3}\gamma + 2\gamma R\right)I$, as before. Also the ratio of masses is $\rho=m_1/m_2$.

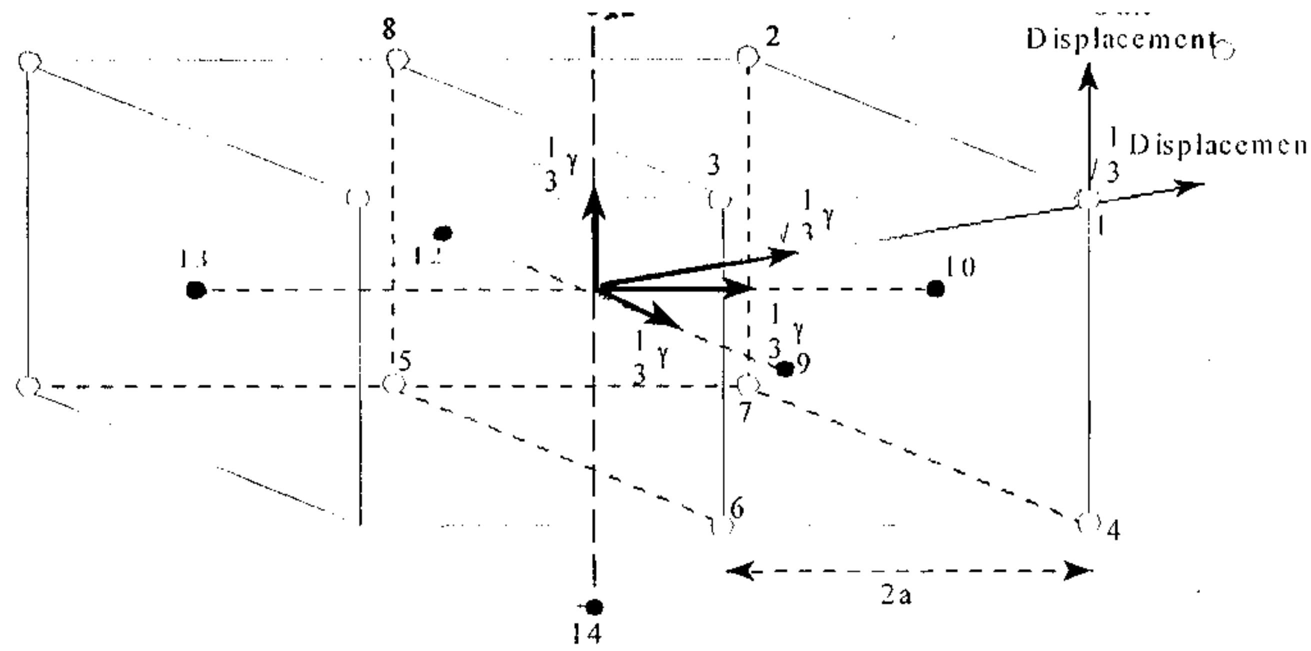

Figure 4.2 : This is the two-atom CsCl struture, where the two species are represented by the solid and open circles respectively.

We should now calculate D from equation(4.33) ie

$$D(k,k') = (m_k, m_{k'})^{-1/2} \sum_l \Phi(k,k') \exp\left(-\vec{k} \bullet \vec{r}_l\right) \tag{4.36}$$

The contribution to D(x,x') are using Figure 4.2, we know initially that the matrices $\Phi_l(1,1)= \Phi_l(2,2)=0$ for l=1 to 8. Therefore, from atom O:

$$-\Phi_{0,xx} = 2\gamma\left(4/3 + R\right) - \Phi_{0,xy} = -\Phi_{0,xz} = 0 \tag{4.37}$$

and from atoms 9 and 12

$$-R\gamma\left[\exp(-ik_x \cdot 2a) + \exp(ik_x \cdot 2a)\right] = -2R\gamma Cos 2k_x a$$

therefore

$$D_{(x,x')} = (m_1 m_2)^{-1/2}\left\{\rho^{-1/2}\left[2\gamma\left(4/3 + R\right) - 2R\gamma Cos 2k_x a\right]\right\} = 8/3\,\gamma(m_1 m_2)^{-1/2}\left[\rho^{-1/2}\left(1 + r_x\right)\right] \tag{4.38}$$

where $r_x = 3/4\, R\left(1 - Cos 2k_x a\right)$ and $D_{x,y} = D_{y,z} = 0$.

The contribution to D(y,y') are:

from atom O:

$$-\Phi_{0,yy} = 2\gamma\left(4/3 + R\right) - \Phi_{0,yx} = -\Phi_{0,yz} = 0 \tag{4.39}$$

and from atoms 10 and 13

$$-R\gamma\left[\exp\left(-ik_y\cdot 2a\right)+\exp\left(ik_y\cdot 2a\right)\right]=-2R\gamma Cos2k_ya$$

therefore

$$D_{(y,y')}=\left(m_1m_2\right)^{-\frac{1}{2}}\left\{\rho^{-\frac{1}{2}}\left[2\gamma\left(\tfrac{4}{3}+R\right)-2R\gamma Cos2k_ya\right]\right\}=\tfrac{8}{3}\gamma\left(m_1m_2\right)^{-\frac{1}{2}}\left[\rho^{-\frac{1}{2}}\left(1+r_y\right)\right] \quad (4.40)$$

where $r_y=\frac{3}{4}R\left(1-Cos2k_ya\right)$ and $D_{y,x}=D_{y,z}=0$.

The contribution to D(z,z') are:

from atom O:

$$-\Phi_{0,zz}=2\gamma\left(\tfrac{4}{3}+R\right),-\Phi_{0,zx}=-\Phi_{0,zy}=0 \quad (4.41)$$

and from atoms 11 and 14

$$-R\gamma\left[\exp\left(-ik_z\cdot 2a\right)+\exp\left(ik_z\cdot 2a\right)\right]=-2R\gamma Cos2k_za$$

therefore

$$D_{(z,z')}=\left(m_1m_2\right)^{-\frac{1}{2}}\left\{\rho^{-\frac{1}{2}}\left[2\gamma\left(\tfrac{4}{3}+R\right)-2R\gamma Cos2k_za\right]\right\}=\tfrac{8}{3}\gamma\left(m_1m_2\right)^{-\frac{1}{2}}\left[\rho^{-\frac{1}{2}}\left(1+r_z\right)\right] \quad (4.42)$$

where $r_z=\frac{3}{4}R\left(1-Cos2k_za\right)$ and $D_{z,x}=D_{z,y}=0$.

Hence

$$\Phi_l(1,1)=\tfrac{8}{3}\gamma\left(m_1m_2\right)^{-\frac{1}{2}}\begin{Bmatrix}\rho^{-\frac{1}{2}}\left(1+r_x\right) & 0 & 0\\ 0 & \rho^{-\frac{1}{2}}\left(1+r_y\right) & 0\\ 0 & 0 & \rho^{-\frac{1}{2}}\left(1+r_z\right)\end{Bmatrix} \quad (4.43)$$

We are now in a position to calculate the matrix $\Phi_l(1,2)$, where $\Phi_l(1,2)=\Phi_l(2,1)=0$ for l=9 to 14.

The contribution to D(x x') are:

from atoms 1 and 5:

$$-\tfrac{1}{3}\gamma\left[\exp\left\{-i\left(k_xa+k_ya+k_za\right)\right\}+\exp\left\{i\left(k_xa+k_ya+k_za\right)\right\}\right],$$

from atoms 2 and 6:

$$-\tfrac{1}{3}\gamma\left[\exp\left\{-i\left(-k_xa+k_ya+k_za\right)\right\}+\exp\left\{i\left(-k_xa+k_ya+k_za\right)\right\}\right],$$

from atoms 3 and 7:

$$-\frac{1}{3}\gamma\left[\exp\left\{-i\left(k_x a - k_y a + k_z a\right)\right\} + \exp\left\{i\left(k_x a - k_y a + k_z a\right)\right\}\right],$$

and from atoms 4 and 8:

$$-\frac{1}{3}\gamma\left[\exp\left\{-i\left(k_x a + k_y a - k_z a\right)\right\} + \exp\left\{i\left(k_x a + k_y a - k_z a\right)\right\}\right],$$

Therefore

$$D(x,x') = -\frac{2}{3}\gamma\left[\cos\left(k_x a + k_y a + k_z a\right) + \cos\left(-k_x a + k_y a + k_z a\right)\right]$$

$$-\frac{2}{3}\gamma\left[\cos\left(k_x a - k_y a + k_z a\right) + \cos\left(k_x a + k_y a - k_z a\right)\right]$$

$$= -\frac{2}{3}\gamma\left[-2\cos\left(k_y a + k_z a\right)\cos k_x a + 2\cos k_x a\cos\left(k_y a - k_z a\right)\right]$$

$$= -\frac{4}{3}\gamma\left[\cos k_x a\left\{\cos\left(k_y a + k_z a\right) + \cos\left(k_y a - k_z a\right)\right\}\right]$$

$$= -\frac{4}{3}\gamma\cos k_x a\left[2\cos k_y a\cos k_z a\right]$$

$$= -\frac{8}{3}\gamma\cos k_x a\cos k_y\cos k_z a$$

Hence

$$D(x,x') = +\frac{8}{3}\gamma\left(m_1 m_2\right)^{\frac{-1}{2}}\left(-Cosk_x aCosk_y aCosk_z a\right) \quad (4.44)$$

The contribution to D(x y) are:

from atoms 1 and 5:

$$\frac{1}{3}\gamma\left[\exp\left\{-i\left(k_x a + k_y a + k_z a\right)\right\} + \exp\left\{i\left(k_x a + k_y a + k_z a\right)\right\}\right],$$

from atoms 2 and 6:

$$-\frac{1}{3}\gamma\left[\exp\left\{-i\left(-k_x a + k_y a + k_z a\right)\right\} + \exp\left\{i\left(-k_x a + k_y a + k_z a\right)\right\}\right],$$

from atoms 3 and 7:

$$-\frac{1}{3}\gamma\left[\exp\left\{-i\left(k_x a - k_y a + k_z a\right)\right\} + \exp\left\{i\left(k_x a - k_y a + k_z a\right)\right\}\right],$$

and from atoms 4 and 8:

$$\frac{1}{3}\gamma\left[\exp\left\{-i\left(k_x a + k_y a - k_z a\right)\right\} + \exp\left\{i\left(k_x a + k_y a - k_z a\right)\right\}\right]$$

Therefore

$$D(x,y) = \frac{2}{3}\gamma\left[\cos\left(k_x a + k_y a + k_z a\right) - \cos\left(-k_x a + k_y a + k_z a\right)\right]$$

$$-\frac{2}{3}\gamma\left[\cos\left(k_x a - k_y a + k_z a\right) + \cos\left(k_x a + k_y a - k_z a\right)\right]$$

$$= \frac{2}{3}\gamma\left[-2\sin\left(k_y a + k_z a\right)\sin k_x a - 2\sin k_x a \sin\left(k_y a - k_z a\right)\right]$$

$$= -\frac{4}{3}\gamma\left[\sin k_x a\left\{\sin\left(k_y a + k_z a\right) + \sin\left(k_y a - k_z a\right)\right\}\right]$$

$$= -\frac{4}{3}\gamma \sin k_x a\left[2\sin k_y a \cos k_z a\right]$$

$$= -\frac{8}{3}\gamma \sin k_x a \sin k_y \cos k_z a$$

Hence

$$D(x,y) = D(y,x) = +\frac{8}{3}\gamma\left(m_1 m_2\right)^{-\frac{1}{2}}\left(-Sink_x aSink_y aCosk_z a\right) \tag{4.45}$$

The contribution to D(y y') are:

from atoms 1 and 5:

$$-\frac{1}{3}\gamma\left[\exp\left\{-i\left(k_x a + k_y a + k_z a\right)\right\} + \exp\left\{i\left(k_x a + k_y a + k_z a\right)\right\}\right]$$

from atoms 2 and 6:

$$-\frac{1}{3}\gamma\left[\exp\left\{-i\left(-k_x a + k_y a + k_z a\right)\right\} + \exp\left\{i\left(-k_x a + k_y a + k_z a\right)\right\}\right]$$

from atoms 3 and 7:

$$-\frac{1}{3}\gamma\left[\exp\left\{-i\left(k_x a - k_y a + k_z a\right)\right\} + \exp\left\{i\left(k_x a - k_y a + k_z a\right)\right\}\right]$$

and from atoms 4 and 8:

$$-\frac{1}{3}\gamma\left[\exp\left\{-i\left(k_x a + k_y a - k_z a\right)\right\} + \exp\left\{i\left(k_x a + k_y a - k_z a\right)\right\}\right]$$

Therefore

$$D(y,y') = -\frac{2}{3}\gamma\left[\cos\left(k_x a + k_y a + k_z a\right) + \cos\left(-k_x a + k_y a + k_z a\right)\right]$$

$$-\frac{2}{3}\gamma\left[\cos\left(k_x a - k_y a + k_z a\right) + \cos\left(k_x a + k_y a - k_z a\right)\right]$$

$$= -\frac{2}{3}\gamma\left[-2\cos\left(k_y a + k_z a\right)\cos k_x a + 2\cos k_x a\cos\left(k_y a - k_z a\right)\right]$$

$$= -\frac{4}{3}\gamma\left[\cos k_x a\left\{\cos\left(k_y a + k_z a\right) + \cos\left(k_y a - k_z a\right)\right\}\right]$$

$$= -\frac{4}{3}\gamma\cos k_x a\left[2\cos k_y a\cos k_z a\right]$$

$$= -\frac{8}{3}\gamma\cos k_x a\cos k_y\ \cos k_z a$$

Hence

$$D(y,y') = +\frac{8}{3}\gamma\left(m_1 m_2\right)^{\frac{-1}{2}}\left(-Cosk_x aCosk_y aCosk_z a\right) \tag{4.46}$$

The contribution to D(y z) are:

from atoms 1 and 5:

$$\tfrac{1}{3}\gamma\left[\exp\left\{-i\left(k_x a + k_y a + k_z a\right)\right\} + \exp\left\{i\left(k_x a + k_y a + k_z a\right)\right\}\right],$$

from atoms 2 and 6:

$$-\tfrac{1}{3}\gamma\left[\exp\left\{-i\left(-k_x a + k_y a + k_z a\right)\right\} + \exp\left\{i\left(-k_x a + k_y a + k_z a\right)\right\}\right],$$

from atoms 3 and 7:

$$-\tfrac{1}{3}\gamma\left[\exp\left\{-i\left(k_x a - k_y a + k_z a\right)\right\} + \exp\left\{i\left(k_x a - k_y a + k_z a\right)\right\}\right],$$

and from atoms 4 and 8:

$$-\tfrac{1}{3}\gamma\left[\exp\left\{-i\left(k_x a + k_y a - k_z a\right)\right\} + \exp\left\{i\left(k_x a + k_y a - k_z a\right)\right\}\right],$$

Therefore

$$D(y,z) = \frac{2}{3}\gamma\left[\cos\left(k_x a + k_y a + k_z a\right) + \cos\left(-k_x a + k_y a + k_z a\right)\right]$$

$$-\frac{2}{3}\gamma\left[\cos\left(k_xa-k_ya+k_za\right)+\cos\left(k_xa+k_ya-k_za\right)\right]$$

$$=\frac{2}{3}\gamma\left[2\cos\left(k_ya+k_za\right)\cos k_xa-2\cos k_xa\cos\left(k_ya-k_za\right)\right]$$

$$=-\frac{4}{3}\gamma\left[\sin k_xa\left\{\sin\left(k_ya+k_za\right)+\sin\left(k_ya-k_za\right)\right\}\right]$$

$$=-\frac{4}{3}\gamma\cos k_xa\left[-2\sin k_ya\sin k_za\right]$$

$$=-\frac{8}{3}\gamma\cos k_xa\cos k_y\ \sin k_za$$

Hence

$$D(y,z)=D(z,y)=+\frac{8}{3}\gamma\left(m_1m_2\right)^{\frac{-1}{2}}\left(Cosk_xaSink_yaSink_za\right) \tag{4.47}$$

The contribution to D(z z') are:

from atoms 1 and 5:

$$-\frac{1}{3}\gamma\left[\exp\left\{-i\left(k_xa+k_ya+k_za\right)\right\}+\exp\left\{i\left(k_xa+k_ya+k_za\right)\right\}\right],$$

from atoms 2 and 6:

$$-\frac{1}{3}\gamma\left[\exp\left\{-i\left(-k_xa+k_ya+k_za\right)\right\}+\exp\left\{i\left(-k_xa+k_ya+k_za\right)\right\}\right],$$

from atoms 3 and 7:

$$\frac{1}{3}\gamma\left[\exp\left\{-i\left(k_xa-k_ya+k_za\right)\right\}+\exp\left\{i\left(k_xa-k_ya+k_za\right)\right\}\right],$$

and from atoms 4 and 8:

$$-\frac{1}{3}\gamma\left[\exp\left\{-i\left(k_xa+k_ya-k_za\right)\right\}+\exp\left\{i\left(k_xa+k_ya-k_za\right)\right\}\right],$$

Therefore

$$D(z,z')=-\frac{2}{3}\gamma\left[\cos\left(k_xa+k_ya+k_za\right)+\cos\left(-k_xa+k_ya+k_za\right)\right]$$

$$-\frac{2}{3}\gamma\left[\cos\left(k_xa-k_ya+k_za\right)+\cos\left(k_xa+k_ya-k_za\right)\right]$$

$$= -\frac{2}{3}\gamma\left[-2\cos(k_y a + k_z a)\cos k_x a + 2\cos k_x a \cos(k_y a - k_z a)\right]$$

$$= -\frac{4}{3}\gamma\left[\cos k_x a\{\cos(k_y a + k_z a) + \cos(k_y a - k_z a)\}\right]$$

$$= -\frac{4}{3}\gamma \cos k_x a\left[2\cos k_y a \cos k_z a\right]$$

$$= -\frac{8}{3}\gamma \cos k_x a \cos k_y \cos k_z a$$

Hence

$$D(z, z') = +\frac{8}{3}\gamma(m_1 m_2)^{-\frac{1}{2}}\left(-Cosk_x a Cosk_y a Cosk_z a\right) \tag{4.48}$$

The contribution to D(z x) are:

from atoms 1 and 5:

$$\tfrac{1}{3}\gamma\left[\exp\{-i(k_x a + k_y a + k_z a)\} + \exp\{i(k_x a + k_y a + k_z a)\}\right]$$

from atoms 2 and 6:

$$-\tfrac{1}{3}\gamma\left[\exp\{-i(-k_x a + k_y a + k_z a)\} + \exp\{i(-k_x a + k_y a + k_z a)\}\right]$$

from atoms 3 and 7:

$$\tfrac{1}{3}\gamma\left[\exp\{-i(k_x a - k_y a + k_z a)\} + \exp\{i(k_x a - k_y a + k_z a)\}\right]$$

and from atoms 4 and 8:

$$-\tfrac{1}{3}\gamma\left[\exp\{-i(k_x a + k_y a - k_z a)\} + \exp\{i(k_x a + k_y a - k_z a)\}\right]$$

Therefore

$$D(z, x) = \frac{2}{3}\gamma\left[\cos(k_x a + k_y a + k_z a) - \cos(-k_x a + k_y a + k_z a)\right] +$$

$$\frac{2}{3}\gamma\left[\cos(k_x a - k_y a + k_z a) - \cos(k_x a + k_y a - k_z a)\right]$$

$$= \frac{2}{3}\gamma\left[-2\sin(k_y a + k_z a)\sin k_x a - 2\sin k_x a \sin(k_y a - k_z a)\right]$$

$$= -\frac{4}{3}\gamma\left[\sin k_x a\{\sin(k_y a + k_z a) - \sin(k_y a - k_z a)\}\right]$$

$$= -\frac{4}{3}\gamma \sin k_x a\left[2\cos k_y a \sin k_z a\right]$$

$$= -\frac{8}{3}\gamma \sin k_x a \cos k_y \sin k_z a$$

Hence

$$D(x,z) = D(z,x) = +\frac{8}{3}\gamma(m_1 m_2)^{\frac{-1}{2}}\left(Sink_x aCosk_y aSink_z a\right) \qquad (4.49)$$

Using the definition of equation (4.31) we obtain for $\Phi_1(1,2)$

$$\Phi_1(1,2) = {}^8\!/_3\,\gamma(m_1 m_2)^{\frac{-1}{2}}\begin{Bmatrix} -C_x C_y C_z & S_x S_y C_z & S_x C_y S_z \\ S_x S_y C_z & -C_x C_y C_z & C_x S_y S_z \\ S_x C_y S_z & C_x S_y S_z & -C_x C_y C_z \end{Bmatrix} \qquad (4.50)$$

Similarly for

$$\Phi_l(1,2)\,{}^8\!/_3\,\gamma(m_1 m_2)^{-\frac{1}{2}}\begin{Bmatrix} -C_x C_y C_z & S_x S_y C_z & S_x C_y S_z \\ S_x S_y C_z & -C_x C_y C_z & C_x S_y S_z \\ S_x C_y S_z & C_x S_y S_z & -C_x C_y C_z \end{Bmatrix} \qquad (4.51)$$

Also

$$\Phi_l(2,2) = {}^8\!/_3\,\gamma(m_1 m_2)^{-\frac{1}{2}}\begin{Bmatrix} \rho^{\frac{1}{2}}(1+r_x) & 0 & 0 \\ 0 & \rho^{\frac{1}{2}}(1+r_y) & 0 \\ 0 & 0 & \rho^{\frac{1}{2}}(1+r_z) \end{Bmatrix} \qquad (4.52)$$

The combined matrices of equations (4.43), (4.50), (4.51) and (4.52) becomes

$$D'(k) = {}^8\!/_3\,(m_1 m_2)^{-\frac{1}{2}}\begin{pmatrix} \rho^{-\frac{1}{2}}(1+r_x) & 0 & 0 & -C_x C_y C_z & S_x S_y C_z & S_x S_y S_z \\ 0 & \rho^{-\frac{1}{2}}(1+r_x) & 0 & S_x S_y C_z & -C_x C_y C_z & C_x S_y S_z \\ 0 & 0 & \rho^{-\frac{1}{2}}(1+r_z) & S_x C_y S_z & C_x S_y S_z & -C_x C_y C_z \\ -C_x C_y C_z & S_x S_y C_z & S_x C_y S_z & \rho^{\frac{1}{2}}(1+r_x) & 0 & 0 \\ S_x S_y C_z & -C_x C_y C_z & C_x S_y S_z & 0 & \rho^{\frac{1}{2}}(1+r_y) & 0 \\ S_x C_y S_z & C_x S_y S_z & -C_x C_y C_z & 0 & 0 & \rho^{\frac{1}{2}}(1+r_z) \end{pmatrix}$$

(4.53)

5.0 Results, Discussion and Conclusion

5.1 Computation

The program was taken from a book "Boardman Program" and modified substantially. It is designed in such a way that, it is unnecessary to specify values for the lattice spacing force constant, or atomic mass, as it is only the ratios of the force constant and masses that affect the shape of the curves.

The program is based on the two subroutines D1 and D2, which set up the dynamical matrices for the one-atom and two-atom cases respectively. Each subroutine is supposed to call a standard library subroutine to evaluate the secular determinant, whose eigenvalues are the squares of the frequencies of the normal modes of vibration. However since we have no access to these subroutine we developed our own subroutine which substitute the NAG subroutine F02AAF, and the subroutine solves the simple eigenvalue problem $\mathbf{A.x} = \lambda .x$ for a real symmetric matrix. It also returns the eigenvalues in ascending order as the NAG subroutine does.

After reading in the necessary data, the program calculates the frequencies of the three normal modes at equal intervals of k, along the three symmetry directions [100], [110], and [111]. Instead of the subroutine PRDC which outputs the disperson curves, in graphical form, on the line printer, we changed the program to output the numbers which are plotted using the "grapher" software

5.1.1 Data For the Program.

Variables to be specified as data are:

Atoms in 13 format, R in E6.2 format, for the two-atom case only

Ro in F6.2 format.

Atoms should be given the value 3 or 2 respectively to simulate the appropriate lattice one atom BCC or two-atom CsCl structure. The program will plot as many sets of curves as required and a value for ATOMS of Zero must be specified to terminate the program.

R is the ratio of the second nearest to nearest neighbour force constant, and any positive (or zero) value may be specified. Ro is any required for ATOMS = 2, and is the ratio of masses of the different species of atom only positive values are physically realistic. The program is listed in appendix I. The outputs of the program are in appendix II and the plotted curves are displayed on appendix III.

5.2 Curves of Dispersions and Density of States.

The forces between the atoms extend only to nearest neighbours, and the crystal is harmonic . So we represent the interaction between nearest neighbours by a spring of force constant, γ. We take the vibrations to be longitudinal, that is the displacement of an atom is along the length of the chain.

In general the wave number k depends on the force constants but when k is in certain symmetry directions such as [100], [110] and [111] in a cubic crystal, of simple structure, the modes are constrained by symmetry to be purely transverse or purely longitudinal. As a first step towards a three dimensional crystal, the atoms of one-dimensional crystal are displaced in any one of the three perpendicular directions.

For k in the [100] - direction, the two transverse branches have the same frequency lying some what below that of the longitudinal branch, except at the zone boundary where they coincide (Fig. A III.1). Therefore there will be three independent modes of vibration, two of which are degenerated in frequency.

For k in the [1 10] - direction, when interatomic forces extend further than to nearest neighbours, with again one-dimensional crystal containing one atom per unit cell, the situation remains the same. Only, the shape of the dispersion curve is altered, the greater the range of the interatomic force the greater the number of structure in the dispersion curve (Fig A III.2).

For k in the [1 1 1] - direction, the two transverse branches have the same frequency, except at the zone boundary where they coincide. The two patterns, that is, the transverse and longitudinal branches can however be brought into coincidence by a rotation of 90o and cannot therefore correspond to different frequencies of vibration. (Fig. A III.3).

In case of the CsCl crystal, for k in the [100]- direction, the dispersion curves shown in (Fig. A III.6), the branches distinguished by two atoms are known as the acoustic and optic branches respectively. For small values of wave vector k the frequency of the former is proportional to k while that of the latter is independent of k. The two branches are also distinguished by having different patterns of movement of the atoms. For k parallel to [1 1 1] the two transverse acoustic modes have the same frequency by symmetry, as have the two transverse optic modes. For k parallel to [1 1 0] the frequencies of the transverse acoustic and transverse optic modes which are polarized parallel to [1 1 0] were not determined.

The eigenfrequencies were used to determine histograms of the frequency of the normal modes and to locate and characterize the several critical points occuring in the various branches.

The histograms of the frequencies of the different branches are given in (Fig A III. 4,9). The "Longitudinal" high "transverse", and "low transverse" branches have been defined as containing respectively the high - middle -, and low - frequency solutions for a given wave vector. This definition was adopted so that in a given branch the frequency would be a continuous function of the wave vector. The histogram of the total frequency is given in (Fig. A III.5,10).

Van-Hove (1953) has shown that as a result of the periodicity of a crystal, its wave-vector space will show certain critical points which cause singularities in the frequency. These critical points are the points wave-vector space at which the gradient of the frequency of a given branch vanishes. Van -Hove (1953) discussed quantitatively the singularities arising from analytic critical points and derived from topological arguments a minimum number of the various types of critical points which must occur for each branch.

5.3 Conclusion and Suggestion for Further Work:

In this research, we have determined the force constants which describe the general interactions between first, second, and third neighbours in one atom and CsCl crystal of BCC lattice.

If we wish to obtain detailed information about lattice vibrations for which the value of k is any where in the zone we must study their interaction with radiation of wavelength, comparable with interatomic distances and having an energy quantum $\hbar\omega$ comparable with phonon energies.

We have concluded that this work can be extended by modifying the program to perform the same calculations for a one-atom face-centered cubic lattice (FCC). The only parts of the program which are affected are: the subroutine which calculates the dynamical matrix; the lengths of the dispersion curves; and also in consequence of the different Brillouin zone, the limits on the Do loops creating the mesh of points of calculate the densities of states.

At a deeper level to the lattice, representing real elements or compounds can be analyzed within the framework described in this project. As long as the relevant dynamical matrix can be determined, the computer code would perform the calculation.

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APPENDIX I

```
      PROGRAM DISPERSION
   INTEGER ATOMS,INT,KX,KY,KZ,K,LIM,INT1,INT2,INT3,J,I,WINT,
  1     IFAIL,DCYSC,DCXSC,DOSXSC,CH(120)
   DOUBLE PRECISION  PI,R,RO,QX,QY,QZ,
  + n(200),NMAX,WMAX,NWMAX,WT,WFRAC,W(3,6,200),NW(6,200)
   COMMON CH
    open (2,file='abba21.dat')
    open (3,file='abba211.dat')
C
   IFAIL=0
   PI=4.d0*dATAN(1.d0)
    DATA DCXSC /25 /
C
    DATA DCYSC /75 /
C
   WRITE (6,*)'GIVE THE NO OF ATOMS'
 100 READ(5,1001)ATOMS
 1001 FORMAT(I3)
   IF (ATOMS.EQ.0) GOTO 199
   DATA INT /50 /
    WRITE (6,*)'WHAT IS R?'
   READ(5,1002)R
 1002 FORMAT(F6.2)
   WRITE(2,1003)
 1003 FORMAT(/////)
   WRITE(2,1005)
 1005 FORMAT(48H DISPERSION CURVES AND DENSITIES OF STATES FOR A)
   IF (ATOMS.EQ.2) GOTO 101
   J=3
   WRITE(2,1006)
 1006 FORMAT(33H MONATOMIC B.C.C. CRYSTAL LATTICE)
 101 CONTINUE
   IF (ATOMS.EQ.1) GOTO 102
   J=6
   WRITE (6,*)'WHAT IS RO?'
   READ(5,1002)RO
   WRITE(2,1007)
 1007 FORMAT(35H DIATOMIC CSCL TYPE CRYSTAL LATTICE)
 102 CONTINUE
   WRITE(2,1008)R
 1008 FORMAT(42H RATIO OF INTERATOMIC FORCE CONSTANTS = 1:,F8.4)
```

```
      IF (ATOMS.EQ.2) WRITE(2,1009)RO
 1009 FORMAT(28H RATIO OF ATOMIC MASSES = 1:,F8.4)
      WMAX=0.0
C
      INT1=DCXSC*2/ATOMS
      DO 103 K=1,INT1,1
      QX=dFLOAT(K)*PI/dFLOAT(INT1*ATOMS)
      QY=0.d0
      QZ=0.d0
      IF (ATOMS.EQ.1) CALL D1(1,K,QX,QY,QZ,R,W,IFAIL)
      IF (ATOMS.EQ.2) CALL D2(1,K,QX,QY,QZ,R,RO,W,IFAIL)
      IF (IFAIL.EQ.1) GOTO 199
      IF (WMAX.LT.W(1,J,K)) WMAX=W(1,J,K)
C
  103 CONTINUE
      INT2=IFIX(FLOAT(DCXSC)*SQRT(2.0))
      DO 104 K=1,INT2,1
        QX=FLOAT(K)*PI*0.5/FLOAT(INT2)
        QY=QX
        QZ=0.d0
        IF (ATOMS.EQ.1) CALL D1(2,K,QX,QY,QZ,R,W,IFAIL)
        IF (ATOMS.EQ.2) CALL D2(2,K,QX,QY,QZ,R,RO,W,IFAIL)
        IF (IFAIL.EQ.1) GOTO 199
        IF (WMAX.LT.W(2,J,K)) WMAX=W(2,J,K)
  104 CONTINUE
      INT3=IFIX(FLOAT(DCXSC)*SQRT(3.0)*2.0/FLOAT(ATOMS))
      DO 105 K=1,INT3,1
        QX=FLOAT(K)*PI/FLOAT(INT3*ATOMS)
        QY=QX
        QZ=QX
        IF (ATOMS.EQ.1) CALL D1(3,K,QX,QY,QZ,R,W,IFAIL)
        IF (ATOMS.EQ.2) CALL D2(3,K,QX,QY,QZ,R,RO,W,IFAIL)
        IF (IFAIL.EQ.1) GOTO 199
        IF (WMAX.LT.W(3,J,K)) WMAX=W(3,J,K)
  105 CONTINUE
      WRITE(2,1010)
 1010 FORMAT(////37H  DISPERSION CURVES - <100> DIRECTION)
      CALL PRDC(INT1,1,J,DCYSC,W,WMAX)
      WRITE(2,1011)
 1011 FORMAT(//37H  DISPERSION CURVES - <110> DIRECTION)
      CALL PRDC(INT2,2,J,DCYSC,W,WMAX)
      WRITE(2,1012)
 1012 FORMAT(//37H  DISPERSION CURVES - <111> DIRECTION)
```

```
      CALL PRDC(INT3,3,J,DCYSC,W,WMAX)
C
      DO 106 WINT=1,200,1
        N(WINT)=0
        DO 106 I=1,6,1
          NW(I,WINT)=0
  106 CONTINUE
      DOSXSC=0
      INT2=INT
      IF (ATOMS.EQ.2) INT2=INT/2
      DO 107 KX=1,INT2,1
        QX=FLOAT(KX)*PI/FLOAT(INT)
        LIM=KX
        IF (KX.GT.INT/2) LIM=INT-KX
C
C   SETS LIM AS THE APPROPRIATE BOUNDARY FOR KY.
C
      DO 107 KY=1,LIM,1
      QY=FLOAT(KY)*PI/FLOAT(INT)
      DO 107 KZ=1,KY,1
        QZ=(FLOAT(KZ)-0.5)*PI/FLOAT(INT)
        IF (ATOMS.EQ.1) CALL D1(1,1,QX,QY,QZ,R,W,IFAIL)
        IF (ATOMS.EQ.2) CALL D2(1,1,QX,QY,QZ,R,RO,W,IFAIL)
        IF (IFAIL.EQ.1) GOTO 199
C
C   IT IS UNNECESSARY THIS TIME TO FILL ALL ELEMENTS OF THE ARRAY
W
C   SINCE THE VALUES WILL IMMEDIATELY BE USED TO INCREMENT THE
C   APPROPRIATE ARRAY ELEMENTS OF THE DENSITY OF STATES.
C
        WT=1.0
        IF (KY.EQ.LIM.OR.KX.EQ.INT2) WT=0.5
        DO 107 I=1,J,1
          W(1,I,1)=FLOAT(DCYSC-1)*W(1,I,1)/WMAX
          WINT=IFIX(W(1,I,1))
          IF (DOSXSC.LT.WINT+2) DOSXSC=WINT+2
C
C   THE SCALE OF THE X AXIS (WHICH IS W IN THIS CASE) IS MADE THE
C   SAME AS THE AXIS (ALSO W) OF THE DISPERSION CURVES.
C   THE SCALE LENGTH OF THE X AXIS IS SET TO THE LARGEST VALUE of
C   FREQUENCY ANYWHERE IN THE BRILLOUIN ZONE IN CASE THERE ARE
C   ANY FREQUENCIES GREATER THAN WMAX, WHICH IS THE GREATEST
C   FREQUENCY IN ANY SYMMETRY DIRECTION.
```

```
C
          WFRAC=W(1,I,1)-FLOAT(WINT)
          NW(I,WINT+1)=NW(I,WINT+1)+(1.0-WFRAC)*WT
          NW(I,WINT+2)=NW(I,WINT+2)+WFRAC*WT
C
C   TO GENERATE A SMOOTHER DENSITY OF STATES, RATHER THAN PLOT A

C      SIMPLE HISTOGRAM EACH CALCULATED FREQUENCY IS DIVIDED
BETWEEN
C        THE TWO HISTIGRAM POINTS ABOVE AND BELOW, WEIGHTED
ACCORDING C    TO HOW CLOSE FREQUENCY IS TO EITHER POINT.
C
 107 CONTINUE
   NWMAX=0.0
   NMAX=0.0
   DO 108 WINT=1,200,1
     DO 109 I=1,3,1
       IF (ATOMS.EQ.2) NW(I,WINT)=NW(I,WINT)+NW(I+3,WINT)
       N(WINT)=N(WINT)+NW(I,WINT)
       IF (NWMAX.LT.NW(I,WINT)) NWMAX=NW(I,WINT)
 109   CONTINUE
     IF (NMAX.LT.N(WINT)) NMAX=N(WINT)
 108 CONTINUE
   CALL PRDOS(NW,NWMAX,N,NMAX,DCYSC,DOSXSC)
 199 STOP
   END

       SUBROUTINE D1(DIR,K,QX,QY,QZ,R,W,IFAIL)
   INTEGER DIR,K,I,J,IFAIL
   double precision QX,QY,QZ,R,DIAG,D(12,10),S(3),C(3),W2(3),
  +  W(3,6,200)
C
C   THIS SUBROUTINE SETS UP THE 3*3 DYNAMICAL MATRIX FOR THE ONE
C   ATOM UNIT CELL, AND USES A STANDARD LIBRARY SUBROUTINE F02AAF
C   TO FIND THE EIGENVALUES OF THE SECULAR DETERMINANT. ANY
C   SIMILAR SUB-ROUTINE WHICH FINDS THE EIGENVALUES OF A REAL
C   SYMMTRIC MATRIX MAY BE USED INSTEAD, AND THE EIGENVECTORS
ARE C   NOT REQUIRED.
C
   C(1)=dCOS(QX)
   C(2)=dCOS(QY)
   C(3)=dCOS(QZ)
   S(1)=dSIN(QX)
```

```
      S(2)=dSIN(QY)
      S(3)=dSIN(QZ)
      DIAG=1.d0+0.75d0*R-C(1)*C(2)*C(3)
      D(1,1)=DIAG-0.75d0*R*DCOS(2.0*QX) +.000000111
      D(2,2)=DIAG-0.75d0*R*DCOS(2.0*QY)+.00000000111
      D(3,3)=DIAG-0.75d0*R*DCOS(2.0*QZ)
      D(1,2)=S(1)*S(2)*C(3)+.0000001231
      D(2,3)=C(1)*S(2)*S(3)
      D(3,1)=S(1)*C(2)*S(3)+.0000000135
      D(2,1)=D(1,2)+.000000011234
      D(3,2)=D(2,3)
      D(1,3)=D(3,1)
      DATA (D(I,1),I=4,12)/9*0 /
      DATA (D(I,2),I=4,12)/ 9*0/
      DATA (D(I,3),I=4,12)/ 9*0/
      DATA ((D(I,J),I=1,12),J=4,10) /84*0 /
      CALL F02AAF1(D,3,W2,wmax)
C
C     THE PARAMETERS OF F02AAF(D,N,N,W2,WKSPC,IFAIL) ARE AS
C     FOLLOWS:
C     D IS THE DYNAMICAL MATRIX, OF DIMENSION NXN, W2 IS THE ARRAY
C     OF EIGENVALUES (THE SQUARES OF THE NORMAL MODE FREQENCIES),
C     WKSPC IS AN ARRAY OF DIMENSION N PROVIDED FOR WORKING SPACE
C     AND IFAIL IS AN INTEGER DETERMINING THE MODE OF ACTION IN
C     THE EVENT OF FAILURE OF THE SUBROUTINE. THE VALUE 0 CAUSES
C     TERMINATION OF THE PROGRAM  WHENEVER AN ERROR IS DETECTED.
C
      DO 501 I=1,3,1
        IF (ABS(W2(I)).LT.0.00001) W2(I)=0.0
C
C     ROUNDING ERRORS MAY PRODUCE SMALL NEGATIVE VALUES IN
C     THE EIGENVALUES WHEN THE CORRECT VALUES ARE ZERO
C
        IF(W2(I).LT.0.0) GOTO 502
        W(DIR,I,K)=SQRT(W2(I))
  501 CONTINUE
      RETURN
  502 WRITE(6,5001)
 5001 FORMAT(42H SUBROUTINE D1 PRODUCES NEGETIVE FREQUENCY)
      IFAIL=1
      RETURN
      END
```

```
      SUBROUTINE F02AAF1(A,N,W2,aw)
   double precision A(12,10), TOL ,W2(3)
   INTEGER N, I
   DATA NDIM,TOL/12,1.d-10/
   DATA MAXIT /50/
   PRINT 100
   CALL PRINTA(A, NDIM, N)
   PRINT 200
   CALL HESSN(A, NDIM, N)
   PRINT 300
   CALL PRINTA(A, NDIM, N)
   PRINT 200
   CALL QR(A, NDIM, N, MAXIT, TOL)
   PRINT 400
   CALL PRINTA(A, NDIM, N)
   PRINT 500
   AW=AMAX1(A(1,1),A(2,2),A(3,3))
   PRINT '(F14.12)', AW
   PRINT '(8F14.12)',(A(I,I),I=1,N)
   W2(1)=A(1,1)
   W2(2)=A(2,2)
   W2(3)=A(3,3)
100 FORMAT(///T10,'THE ORIGINAL MATRIX IS:'//)
200 FORMAT(///)
300 FORMAT(/// T10,'THE HESSN MATRIX IS:'//)
400 FORMAT(/// T10,'THE FINAL MATRIX IS:'//)
500 FORMAT(/// T10,'THE EIGENVALUES ARE:'//)
   return
   END
C*******

      SUBROUTINE F02AAF2(A,N,W2,aw)
   double precision A(20,20), TOL ,W2(6)
   INTEGER N, I
   DATA NDIM,TOL/20,1.d-10/
   DATA MAXIT /50/
   PRINT 100
   CALL PRINTA(A, NDIM, N)
   PRINT 200
   CALL HESSN(A, NDIM, N)
   PRINT 300
   CALL PRINTA(A, NDIM, N)
   PRINT 200
```

```
      CALL QR(A, NDIM, N, MAXIT, TOL)
      PRINT 400
      CALL PRINTA(A, NDIM, N)
      PRINT 500
      AW=AMAX1(A(1,1),A(2,2),A(3,3),A(4,4),A(5,5),A(6,6))
      PRINT '(F14.12)', AW
      PRINT '(8F14.12)',(A(I,I),I=1,N)
      W2(1)=A(1,1)
      W2(2)=A(2,2)
      W2(3)=A(3,3)
      W2(4)=A(4,4)
      W2(5)=A(5,5)
      W2(6)=A(6,6)
  100 FORMAT(///T10,'THE ORIGINAL MATRIX IS:'//)
  200 FORMAT(///)
  300 FORMAT(/// T10,'THE HESSN MATRIX IS:'//)
  400 FORMAT(/// T10,'THE FINAL MATRIX IS:'//)
  500 FORMAT(/// T10,'THE EIGENVALUES ARE:'//)
      return
      END
C*******
      SUBROUTINE PRINTA(A,NDIM,N)
      double precision  A(NDIM, N)
      INTEGER NDIM,N,I,J
       DO  10 I = 1, N
       PRINT 100,(A(I,J),J=1, N )
  10  CONTINUE
  100 FORMAT (8F14.10)
      RETURN
      END

      SUBROUTINE HESSN(A, NDIM, N)
      double precision A(NDIM, N), V(20),SIGMA,ETA,SUM,PI
      INTEGER N, NLESS1, NLESS2,K,  KPLUS1,I,J
      NLESS1 = N - 1
      NPLUS1 = N + 1
      NPLUS2 = N + 2
      NLESS2 = N - 2
      DO 10 K = 1,  NLESS2
      KPLUS1 = K + 1
      ETA = ABS(A(KPLUS1, K))
      DO 20 I = KPLUS1,  N
      IF (ETA. LT.ABS(A(I,K))) ETA=ABS(A(I,K))
```

```
20  CONTINUE
    IF (ETA.NE.0.0)  THEN
    SUM =0.0d0
    DO  30 I = KPLUS1, N
    V(I) = A(I, K) / ETA
    A(I,K)=V(I)
    SUM = SUM + V(I)**2
30  CONTINUE
    IF (V(KPLUS1).NE.0.0 ) THEN
    SIGMA = SQRT(SUM) * V(KPLUS1) / ABS(V(KPLUS1))
    END IF
    V(KPLUS1) = V(KPLUS1) + SIGMA
    PI = SIGMA * V(KPLUS1)
    A(NPLUS1, K) = PI
C*******
    DO 40 J = K + 1, N
    SUM = 0.0d0
    DO 50 I = KPLUS1, N
    SUM = SUM + V(I) * A(I, J)
50  CONTINUE
    RHO = SUM / PI
    DO 60 I= KPLUS1, N
    A(I, J) = A(I, J) - RHO * V(I)
60  CONTINUE
40  CONTINUE
C*******
    DO 80 I = 1, N
    SUM = 0.0
    DO 90 J = K + 1, N
    SUM = SUM + A(I, J) * V(J)
90  CONTINUE
    RHO=SUM/PI
    DO 100 J=KPLUS1,N
    A(I,J)=A(I,J)-RHO*V(J)
100 CONTINUE
80  CONTINUE
    A(NPLUS2, K) = V(KPLUS1)
    A(KPLUS1, K) = -ETA * SIGMA
    ELSE
    A(NPLUS1, K) = 0.0d0
    END IF
10  CONTINUE
    DO 110 J=1, NLESS2
```

```
      DO 120 I=J+2 ,N
      A(I,J)=0.0d0
120   CONTINUE
110   CONTINUE
      RETURN
      END
      SUBROUTINE QR (A,NDIM,N,MAXIT,TOL)
      double precision  A(NDIM,N),GAMMA(10),ETA,ALFA,BETA,DELTA,
     +KAPPA,SIGMA(10),tol
      INTEGER NDIM,N,NSTORE,MAXIT,KPLUS1,KLESS1,
     +I,J,K
      NSTORE=N
      DO 10 I=1,MAXIT
      KAPPA=A(N,N)
      A(1,1)=A(1,1)-KAPPA
      DO 20 K=1,N
      KPLUS1=K+1
      IF (K.NE.N) THEN
      ETA = AMAX1(ABS(A(K,K)),ABS(A(KPLUS1,K)))
      ALFA=A(K,K)/ETA
      BETA=A(KPLUS1,K)/ETA
      DELTA=SQRT(ALFA*ALFA+BETA*BETA)
      GAMMA(K)=ALFA/DELTA
      SIGMA(K)=BETA/DELTA
      XNU =ETA*DELTA
      A(K,K)=XNU
      A(KPLUS1,K)=0.0d0
      A(KPLUS1,KPLUS1)=A(KPLUS1,KPLUS1)-KAPPA
      DO 30 J=KPLUS1,N
      AKJ= A(K,J)
      A(K,J)=GAMMA(K)*A(K,J)+SIGMA(K)*A(KPLUS1,J)
      A(KPLUS1,J)=GAMMA(K)*A(KPLUS1,J)-SIGMA(K)*AKJ
30    CONTINUE
      ENDIF
      IF (K.NE.1)THEN
      DO 40 J=1,K
      KLESS1=K-1
      AIKL1 =A(J,KLESS1)
      A(J,KLESS1)=GAMMA(KLESS1)*A(J,KLESS1)
     +    +SIGMA(KLESS1)*A(J,K)
      A(J,K)=GAMMA(KLESS1)*A(J,K)-SIGMA(KLESS1)*AIKL1
40    CONTINUE
      A(KLESS1,KLESS1)=A(KLESS1,KLESS1)+KAPPA
```

```
    ENDIF
 20  CONTINUE
    A(N,N)=A(N,N)+KAPPA
    IF (ABS(A(N,N-1)).LT.TOL) N=N-1
    IF (N.EQ.1) THEN
    N =NSTORE
    RETURN
    ENDIF
    PRINT 100,I
    CALL PRINTA(A, NDIM, NSTORE)
  100 FORMAT (/// T10,'AT ITERATION',I2,4X,'THE MATRIX IS :'//)
  10  CONTINUE
     RETURN
    END


C*********
      SUBROUTINE D2(DIR,K,QX,QY,QZ,R,RO,W,IFAIL)
    INTEGER DIR,K,I,J,IFAIL
    double precision QX,QY,QZ,R,RO,ROOTRO,D(20,20),S(3),C(3),W2(6),
   + W(3,6,200)
C
C   THIS SUBROUTINE IS SIMILAR TO D1, EXCEPT THAT IT SOLVES THE 6*6
C   MATRIX FOR THE TWO ATOM UNIT CELL.
C
    C(1)=dCOS(QX)
    C(2)=dCOS(QY)
    C(3)=dCOS(QZ)
    S(1)=dSIN(QX)
    S(2)=dSIN(QY)
    S(3)=dSIN(QZ)
    ROOTRO=dSQRT(RO)
    DO 801 I=1,6,1
      DO 801 J=1,6,1
      D(I,J)=0.0d0
  801 CONTINUE
    D(1,1)=ROOTRO*(1.0+0.75d0*R-0.75d0*R*dCOS(2.0*QX))
    D(2,2)=ROOTRO*(1.0+0.75d0*R-0.75d0*R*dCOS(2.0*QY))
    D(3,3)=ROOTRO*(1.0+0.75d0*R-0.75d0*R*dCOS(2.0*QZ))
    D(4,4)=(1.0+0.75d0*R-0.75d0*R*dCOS(2.0*QX))/ROOTRO
    D(5,5)=(1.0+0.75d0*R-0.75d0*R*dCOS(2.0*QY))/ROOTRO
    D(6,6)=(1.0+0.75d0*R-0.75d0*R*dCOS(2.0*QZ))/ROOTRO
    DO 802 I=1,3,1
```

```
      D(I,I+3)=-C(1)*C(2)*C(3)
      D(I+3,I)=D(I,I+3)
 802 CONTINUE
     D(1,5)=S(1)*S(2)*C(3)+.00000011
     D(1,6)=S(1)*C(2)*S(3)+.00000021
     D(2,6)=C(1)*S(2)*S(3)+.00000011
     D(5,1)=D(1,5)+.00000011
     D(2,4)=D(1,5)+.00000011
     D(4,2)=D(1,5)+.00000021
     D(6,1)=D(1,6)+.00000011
     D(3,4)=D(1,6)+.00000011
     D(4,3)=D(1,6)+.00000011
     D(6,2)=D(2,6)+.00000011
     D(3,5)=D(2,6)+.00000021
     D(5,3)=D(2,6)+.00000011
     D(2,1)=0.0d0 +.00000011
     D(3,1)=0.0d0 +.00000011
     D(1,2)=0.0d0 +.00000011
     D(3,2)=0.0d0 +.0000001
     D(1,3)=0.0d0+.00000003
     D(2,3)=0.0d0+.00000004
     D(5,4)=0.0d0+.0000002
     D(6,4)=0.0d0+.0000003
     D(4,5)=0.0d0+.00000002
     D(6,5)=0.0d0 +.00000001
     D(4,6)=0.0d0 +.0000004
     D(5,6)=0.0d0 +.0000003
     DATA (D(I,1),I=7,20)/14*0 /
     DATA (D(I,2),I=7,20)/14*0/
     DATA (D(I,3),I=7,20)/14*0/
     DATA (D(I,4),I=7,20)/14*0/
     DATA (D(I,5),I=7,20)/14*0/
     DATA (D(I,6),I=7,20)/14*0/
     DATA ((D(I,J),I=1,20),J=7,20) /280*0/
     CALL F02AAF2(D,6,W2,wmax)
     DO 803 I=1,6,1
       IF (ABS(W2(I)).LT.0.00001) W2(I)=0.0
C
C    ROUNDING ERRORS MAY PRODUCE SMALL NEGATIVE VALUES IN
C    THE EIGENVALUES WHEN THE CORRECT VALUES ARE ZERO
C
       IF (W2(I).LT.0.0) GOTO 804
       W(DIR,I,K)=dSQRT(W2(I))
```

```
 803 CONTINUE
   RETURN
 804 WRITE(2,8001)
8001 FORMAT(42H SUBROUTINE D2 PRODUCES NEGATIVE FREQUENCY)
   IFAIL=1
   RETURN
   END
        SUBROUTINE PRDC(INT,DIR,J,DCYSC,W,WMAX)
    INTEGER INT,DIR,J,I,K,L,XAXIS,YAXIS,SPACE,CROSS,SUB,
   1      DCYSC,STAR,PT(6),CH(120),NOUGHT,ONE,TWO,THREE,
   2      FOUR,FIVE,SIX,SEVEN,EIGHT,NINE,DCYSC2,SCALE
   double precision PL(6),SUB1,WMAX,W(3,6,200)
   COMMON CH
   DATA XAXIS,YAXIS,SPACE,CROSS,STAR/1HI,1H-,1H ,1H+,1H*/
   DATA NOUGHT,ONE,TWO,THREE,FOUR/1H0,1H1,1H2,1H3,1H4/
   DATA FIVE,SIX,SEVEN,EIGHT,NINE/1H5,1H6,1H7,1H8,1H9/
C
C   THIS SUBROUTINE PRODUCES A GRAPH OF THE DISPERSION CURVES ON
C   THE LINEPRINTER.
C
   DCYSC2=DCYSC+2
   DO 601 L=1,DCYSC2,1
 601  CH(L)=SPACE
   CH(2)=NOUGHT
   CH(12)=ONE
   CH(22)=TWO
   CH(32)=THREE
   CH(42)=FOUR
   CH(52)=FIVE
   CH(62)=SIX
   CH(72)=SEVEN
   CH(82)=EIGHT
   CH(92)=NINE
   CH(102)=NOUGHT
   CH(112)=ONE
   WRITE(3,1601) (CH(K),K=1,DCYSC2)
   DO 602 L=2,DCYSC2,1
 602   CH(L)=YAXIS
   CH(1)=NOUGHT
   WRITE(3,1601) (CH(K),K=1,DCYSC2)
1601 FORMAT(1H ,120A1)
   DO 603 I=1,INT,1
     DO 604 L=1,DCYSC2,1
```

```
      CH(L)=SPACE
      IF (DIR.EQ.3.AND.J.EQ.3.AND.I.EQ.INT/2
  1       .AND.L.EQ.(L/2)*2) CH(L)=YAXIS
 604  CONTINUE
     CH(1)=XAXIS
     DO 605 L=1,J,1
      PL(L)=W(DIR,L,I)
      PT(L)=IFIX(W(DIR,L,I)*FLOAT(DCYSC-1)/WMAX+1.5)
      SUB1=PL(L)
      SUB=PT(L)
      IF (CH(SUB).EQ.CROSS.OR.CH(SUB).EQ.STAR) GOTO 606
      CH(SUB)=CROSS
      GOTO 605
 606    CH(SUB)=STAR
 605  CONTINUE
     WRITE (2,1111)i, (PL(L),l=1,j)
1111  format(1X,I3,2X,6F8.4)
    SCALE=I/10
     IF (SCALE*10.EQ.I) GOTO 607
     WRITE(3,1602) (CH(K),K=1,DCYSC2)
1602  FORMAT(2H  ,120A1)
     GOTO 603
 607  IF (SCALE.LT.10) GOTO 608
     SCALE=SCALE-10
     GOTO 607
 608  WRITE(3,1603)SCALE,  (CH(K),K=1,DCYSC2)
1603  FORMAT(1H  ,I1,120A1)
 603 CONTINUE
    RETURN
    END

    SUBROUTINE PRDOS(NW,NWMAX,N,NMAX,DCYSC,DOSXSC)
    INTEGER I,L,CH(120),DCYSC,DOSXSC,XAXIS,YAXIS,SPACE,CROSS,
   1      INT2,SUB,NOUGHT,ONE,TWO,THREE,FOUR,FIVE,
   2      SIX,SEVEN,EIGHT,NINE,DCYSC2,SCALE,K
    double precision NW(6,200),NWMAX,N(200),NMAX,sub1,pl(6)
    COMMON CH
    DATA XAXIS,YAXIS,SPACE,CROSS/1HI,1H-,1H ,1H+/
    DATA NOUGHT,ONE,TWO,THREE,FOUR/1H0,1H1,1H2,1H3,1H4/
    DATA FIVE,SIX,SEVEN,EIGHT, NINE/1H5,1H6,1H7,1H8,1H9/
C
C   THIS SUBROUTINE PRODUCES ON THE LINEPRINTER GRAPHS OF THE
C   DENSITY OF STATES FOR EACH POLARIZATION, AND THE TOTAL
```

```
C    DENSITY OF STATES.
C
      WRITE(2,1200)
 1200 FORMAT (/////41H  DENSITY OF STATES FOR EACH POLARIZATION)
     DCYSC2=DCYSC+2
     DO 201 L=1,DCYSC2,1
 201   CH(L)=SPACE
     CH(2)=NOUGHT
     CH(12)=ONE
     CH(22)=TWO
     CH(32)=THREE
     CH(42)=FOUR
     CH(52)=FIVE
     CH(62)=SIX
     CH(72)=SEVEN
     CH(82)=EIGHT
     CH(92)=NINE
     CH(102)=NOUGHT
     CH(112)=ONE
     WRITE(3,1201) (CH(K),K=1,DCYSC2)
     DO 202 L=2,DCYSC2,1
 202   CH(L)=YAXIS
     CH(1)=NOUGHT
     WRITE(3,1201) (CH(K),K=1,DCYSC2)
 1201 FORMAT(1H,120A1)
     DOSXSC=DOSXSC+2
     DO 203 I=1,DOSXSC,1
       DO 204 L=1,DCYSC2,1
 204       CH(L)=SPACE
       INT2=DCYSC/3
       DO 205 L=1,3,1
         SUB=IFIX(NW(L,I+1)*FLOAT(INT2)/NWMAX+1.5)+INT2*(L-1)
         CH(SUB)=CROSS
         SUB1=NW(L,I+1)+INT2*(L-1)
          PL(L)=SUB1
 205   CONTINUE
       write(2,2222)i,(PL(L),L=1,3)
 2222      format(2x,I3,2X,3(f8.4))
       CH(1)=XAXIS
       CH(INT2+1)=XAXIS
       INT2=2*INT2
       CH(INT2+1)=XAXIS
       SCALE=I/10
```

```
      IF (SCALE*10.EQ.I) GOTO 206
      WRITE(3,1202) (CH(K),K=1,DCYSC2)
1202  FORMAT(2H  ,120A1)
      GOTO 203
 206  IF(SCALE.LT.10) GOTO 207
      SCALE=SCALE-10
      GOTO 206
 207  WRITE(3,1203)SCALE,(CH(K),K=1,DCYSC2)
1203  FORMAT(1H ,I1,120A1)
 203 CONTINUE
    WRITE(2,1300)
1300 FORMAT(/////25H  TOTAL DENSITY OF STATES)
    DO 301 L=1,DCYSC2,1
 301  CH(L)=SPACE
    CH(2)=NOUGHT
    CH(12)=ONE
    CH(22)=TWO
    CH(32)=THREE
    CH(42)=FOUR
    CH(52)=FIVE
    CH(62)=SIX
    CH(72)=SEVEN
    CH(82)=EIGHT
    CH(92)=NINE
    CH(102)=NOUGHT
    CH(112)=ONE
    WRITE(3,1301) (CH(K),K=1,DCYSC2)
    DO 302 L=2,DCYSC2,1
 302  CH(L)=YAXIS
    CH(1)=NOUGHT
    WRITE(3,1301) (CH(K),K=1,DCYSC2)
1301 FORMAT(1H ,120A1)
    DO 303 I=1,DOSXSC,1
      DO 304 L=1,DCYSC2,1
 304    CH(L)=SPACE
      SUB1=N(I+1)
       WRITE(2,3333)I,SUB1
3333  FORMAT(2X,I3,2X,F8.4)
      SUB=IFIX(N(I+1)*FLOAT(DCYSC)/NMAX+1.5)
      CH(SUB)=CROSS
      CH(1)=XAXIS
      SCALE=I/10
      IF(SCALE*10.EQ.I) GOTO 305
```

```
      WRITE(3,1302) (CH(K),K=1,DCYSC2)
1302    FORMAT(2H ,120A1)
      GOTO 303
 305   IF (SCALE.LT.10) GOTO 306
      SCALE=SCALE-10
      GOTO 305
 306   WRITE(3,1303)SCALE, (CH(K),K=1,DCYSC2)
1303    FORMAT(1H ,I1,120A1)
 303 CONTINUE
    RETURN
    END
```

APPENDIX II

Table 1:

Dispersion curves - <100> direction for a monatomic BCC crystal lattice with ratio of interatomic force constants = .5

1	.0702	.0444	.0444
2	.1402	.0888	.0888
3	.2099	.1331	.1331
4	.2789	.1772	.1772
5	.3472	.2212	.2212
6	.4146	.2650	.2650
7	.4808	.3085	.3085
8	.5457	.3517	.3517
9	.6091	.3946	.3946
10	.6709	.4370	.4370
11	.7309	.4790	.4790
12	.7890	.5206	.5206
13	.8450	.5617	.5617
14	.8988	.6021	.6021
15	.9503	.6420	.6420
16	.9994	.6813	.6813
17	1.0460	.7199	.7199
18	1.0901	.7578	.7578
19	1.1315	.7949	.7949
20	1.1702	.8313	.8313
21	1.2062	.8668	.8668
22	1.2395	.9015	.9015
23	1.2700	.9352	.9352
24	1.2978	.9681	.9681
25	1.3229	1.0000	1.0000
26	1.3453	1.0309	1.0309
27	1.3651	1.0608	1.0608
28	1.3824	1.0897	1.0897
29	1.3972	1.1174	1.1174
30	1.4098	1.1441	1.1441
31	1.4200	1.1697	1.1697
32	1.4282	1.1941	1.1941
33	1.4345	1.2173	1.2173
34	1.4389	1.2393	1.2393
35	1.4418	1.2601	1.2601
36	1.4432	1.2796	1.2796
37	1.4433	1.2979	1.2979
38	1.4424	1.3149	1.3149
39	1.4406	1.3306	1.3306
40	1.4381	1.3450	1.3450
41	1.4352	1.3581	1.3581
42	1.4319	1.3698	1.3698
43	1.4286	1.3802	1.3802
44	1.4253	1.3892	1.3892
45	1.4222	1.3968	1.3968
46	1.4195	1.4031	1.4031
47	1.4173	1.4079	1.4079
48	1.4156	1.4114	1.4114
49	1.4146	1.4135	1.4135
50	1.4142	1.4142	1.4142

Table 2.

Dispersion curves - <110> direction for a monatomic BCC crystal lattice with ratio of interatomic force constants = .5

1	.0744	.0389	.0449
2	.1487	.0776	.0896
3	.2226	.1162	.1342
4	.2961	.1546	.1786
5	.3690	.1927	.2225
6	.4412	.2304	.2660
7	.5124	.2676	.3090
8	.5827	.3043	.3514
9	.6518	.3404	.3930
10	.7195	.3758	.4339
11	.7858	.4104	.4739
12	.8505	.4442	.5129
13	.9136	.4771	.5509
14	.9747	.5090	.5878
15	1.0339	.5400	.6235
16	1.0911	.5698	.6579
17	1.1460	.5985	.6911
18	1.1986	.6260	.7228
19	1.2488	.6522	.7531
20	1.2965	.6771	.7818
21	1.3416	.7006	.8090
22	1.3840	.7228	.8346
23	1.4236	.7434	.8584
24	1.4603	.7626	.8806
25	1.4941	.7803	.9010
26	1.5249	.7963	.9195
27	1.5526	.8108	.9362
28	1.5771	.8236	.9511
29	1.5986	.8348	.9640
30	1.6167	.8443	.9749
31	1.6317	.8521	.9839
32	1.6433	.8582	.9909
33	1.6516	.8625	.9960
34	1.6566	.8652	.9990
35	1.6583	.8660	1.0000

Table 3.

Dispersion curves - <110> direction for a monatomic BCC crystal lattice with ratio of interatomic force constants = .5

1	.0753	.0408	.0408	36	1.4695	1.2038	1.2038
2	.1504	.0816	.0816	37	1.4555	1.2236	1.2236
3	.2250	.1224	.1224	38	1.4389	1.2424	1.2424
4	.2991	.1630	.1630	39	1.4199	1.2604	1.2604
5	.3724	.2034	.2034	40	1.3985	1.2774	1.2774
6	.4448	.2437	.2437	41	1.3751	1.2934	1.2934
7	.5159	.2837	.2837	42	1.3498	1.3086	1.3086
8	.5857	.3235	.3235	43	1.3229	1.3229	1.3229
9	.6540	.3630	.3630	44	1.2946	1.3362	1.3362
10	.7206	.4021	.4021	45	1.2654	1.3487	1.3487
11	.7853	.4409	.4409	46	1.2354	1.3603	1.3603
12	.8480	.4792	.4792	47	1.2051	1.3710	1.3710
13	.9084	.5172	.5172	48	1.1747	1.3809	1.3809
14	.9666	.5546	.5546	49	1.1448	1.3900	1.3900
15	1.0222	.5916	.5916	50	1.1157	1.3982	1.3982
16	1.0752	.6280	.6280	51	1.0878	1.4056	1.4056
17	1.1255	.6638	.6638	52	1.0616	1.4123	1.4123
18	1.1729	.6990	.6990	53	1.0376	1.4183	1.4183
19	1.2173	.7336	.7336	54	1.0161	1.4235	1.4235
20	1.2586	.7676	.7676	55	.9977	1.4281	1.4281
21	1.2968	.8009	.8009	56	.9826	1.4319	1.4319
22	1.3318	.8334	.8334	57	.9712	1.4352	1.4352
23	1.3635	.8653	.8653	58	.9637	1.4378	1.4378
24	1.3918	.8963	.8963	59	.9603	1.4399	1.4399
25	1.4168	.9266	.9266	60	.9609	1.4415	1.4415
26	1.4383	.9561	.9561	61	.9656	1.4426	1.4426
27	1.4565	.9848	.9848	62	.9742	1.4432	1.4432
28	1.4711	1.0127	1.0127	63	.9863	1.4434	1.4434
29	1.4824	1.0397	1.0397	64	1.0018	1.4432	1.4432
30	1.4903	1.0658	1.0658	65	1.0202	1.4426	1.4426
31	1.4948	1.0911	1.0911	66	1.0410	1.4418	1.4418
32	1.4960	1.1154	1.1154	67	1.0639	1.4407	1.4407
33	1.4940	1.1389	1.1389	68	1.0884	1.4393	1.4393
34	1.4888	1.1614	1.1614	69	1.1141	1.4378	1.4378
35	1.4806	1.1831	1.1831	70	1.1404	1.4361	1.4361
71	1.1671	1.4343	1.4343	79	1.3527	1.4197	1.4197
72	1.1938	1.4324	1.4324	80	1.3686	1.4183	1.4183
73	1.2200	1.4304	1.4304	81	1.3823	1.4171	1.4171
74	1.2455	1.4285	1.4285	82	1.3937	1.4161	1.4161
75	1.2699	1.4266	1.4266	83	1.4026	1.4153	1.4153
76	1.2931	1.4247	1.4247	84	1.4090	1.4147	1.4147
77	1.3148	1.4229	1.4229	85	1.4129	1.4143	1.4143
78	1.3347	1.4212	1.4212	86	1.4142	1.4142	1.4142

Table 4:

Density of states for each Polarization for a monatomic BCC crystal lattice with ratio of interatomic force constants = .5

1	.0000	25.0000	50.0000
2	.0000	25.0000	50.0000
3	.0000	25.4942	50.3581
4	.0000	25.2462	50.1419
5	.1450	25.9195	50.8751
6	.3550	25.6840	50.5011
7	.0000	26.8844	51.4087
8	.4422	26.5763	51.5484
9	.5578	27.5885	51.5632
10	.0759	28.1172	52.9102
11	.6700	28.5368	52.3919
12	1.1529	29.5664	53.8784
13	.4706	29.7006	53.8789
14	.8778	32.1807	54.9884
15	1.6784	30.6750	55.2645
16	.9020	34.7938	56.7423
17	1.5747	32.4906	56.9386
18	1.5526	38.0670	58.0427
19	2.1805	34.8749	59.7938
20	1.7762	39.9258	59.4474
21	2.4860	39.3134	62.0467
22	2.7844	42.3453	62.4243
23	2.4527	43.4952	63.8917
24	3.2172	46.0878	65.0979
25	3.5838	48.5683	67.8035
26	3.4539	49.8204	67.7286
27	4.4865	54.2048	70.5145
28	3.8290	55.5665	71.2635
29	5.0210	59.9321	75.0064
30	5.2796	62.7145	75.0494
31	4.7804	65.8468	78.8738
32	6.9965	73.8471	80.0041
33	5.7494	70.5989	83.2075
34	6.7797	88.7890	85.7651
35	8.0881	79.8324	88.8149
36	7.1272	99.1979	91.0037
37	8.5879	98.8234	95.6898
38	9.0790	107.1139	97.9096
39	10.0822	126.1525	102.7515
40	9.4946	131.6064	106.3412
41	11.6103	144.8801	111.8468
42	11.4644	167.6271	115.0534
43	12.1310	193.3890	122.7056
44	13.8928	237.4239	126.8186
45	13.3607	284.5748	135.1632
46	15.7002	310.4953	141.7465
47	15.0656	341.7169	151.2200
48	26.0963	364.4076	162.4362
49	95.6898	302.8176	173.2571
50	77.6802	232.6997	195.0941
51	57.6278	202.1614	223.5993
52	51.9473	174.9246	244.4099
53	49.7707	158.9657	244.7697
54	45.0813	142.3865	239.6157
55	48.0066	130.4123	238.4868
56	43.3885	118.8860	237.7541
57	47.0132	110.0894	235.9496
58	45.0189	102.1989	234.2755
59	48.4030	92.5399	233.6490
60	47.4178	85.4170	232.3950
61	50.2503	80.8841	230.7153
62	51.0730	75.4482	227.5524
63	53.5280	68.4565	225.1033
64	57.5454	65.3093	221.8137
65	56.5796	60.3999	217.6819
66	66.3230	55.7662	211.3912
67	67.5409	51.8059	203.4166
68	73.1242	49.2382	190.2283
69	84.6177	45.9777	176.3338
70	87.5425	42.4961	160.8508
71	99.8500	40.2922	143.6145
72	122.0963	36.7712	119.7660
73	163.7782	44.6238	70.0472
74	236.6188	65.5537	51.8775
75	295.5443	90.4323	50.0000
76	351.1638	111.5543	50.0000
77	441.2627	125.8685	50.0000
78	479.2485	102.6203	50.0000
79	393.2909	39.8109	50.0000
80	315.6455	25.0000	50.0000
81	257.1582	25.0000	50.0000
82	207.8307	25.0000	50.0000
83	159.4439	25.0000	50.0000
84	107.1217	25.0000	50.0000
85	30.1788	25.0000	50.0000
86	.0060	25.0000	50.0000
87	.0000	25.0000	50.0000
88	.0000	25.0000	50.0000
89	.0000	25.0000	50.0000

Table 5:

Total Density of states for a monatomic BCC crystal lattice with ratio of interatomic force constants = .5

1	.0000	39	163.9861
2	.0000	40	172.4422
3	.8524	41	193.3372
4	.3880	42	219.1450
5	1.9396	43	253.2256
6	1.5401	44	303.1353
7	3.2930	45	358.0987
8	3.5670	46	392.9420
9	4.7095	47	433.0024
10	6.1033	48	477.9401
11	6.5988	49	496.7645
12	9.5976	50	430.4741
13	9.0501	51	408.3885
14	13.0468	52	396.2818
15	12.6179	53	378.5061
16	17.4382	54	352.0835
17	16.0040	55	341.9057
18	22.6623	56	325.0286
19	21.8492	57	318.0522
20	26.1494	58	306.4933
21	28.8460	59	299.5919
22	32.5530	60	290.2298
23	34.8395	61	286.8497
24	39.4029	62	279.0735
25	44.9555	63	272.0879
26	46.0029	64	269.6683
27	54.2059	65	259.6614
28	55.6591	66	258.4804
29	64.9595	67	247.7634
30	68.0435	68	237.5907
31	74.5009	69	231.9292
32	85.8477	70	215.8894
33	84.5557	71	208.7566
34	106.3338	72	203.6335
35	101.7354	73	203.4492
36	122.3288	74	279.0500
37	128.1012	75	360.9766
38	139.1024	76	437.7181
77	542.1312		
78	556.8688		
79	408.1018		
80	315.6455		
81	257.1582		
82	207.8307		
83	159.4439		
84	107.1217		
85	30.1788		

Table 6:

Dispersion curves - <100> direction for a diatomic CsCl type crystal lattice with ratio of interatomic force constants = 0.0, ratio of atomic masses = 0.8

1	.0443	.0443	.0443	1.4179	1.4179	1.4179
2	.0885	.0885	.0885	1.4158	1.4158	1.4158
3	.1327	.1327	.1327	1.4124	1.4124	1.4124
4	.1767	.1767	.1767	1.4076	1.4076	1.4076
5	.2205	.2205	.2205	1.4014	1.4014	1.4014
6	.2641	.2641	.2641	1.3938	1.3938	1.3938
7	.3074	.3074	.3074	1.3849	1.3849	1.3849
8	.3505	.3505	.3505	1.3746	1.3746	1.3746
9	.3931	.3931	.3931	1.3631	1.3631	1.3631
10	.4353	.4353	.4353	1.3502	1.3502	1.3502
11	.4771	.4771	.4771	1.3360	1.3360	1.3360
12	.5184	.5184	.5184	1.3205	1.3205	1.3205
13	.5591	.5591	.5591	1.3038	1.3038	1.3038
14	.5992	.5992	.5992	1.2858	1.2858	1.2858
15	.6387	.6387	.6387	1.2667	1.2667	1.2667
16	.6774	.6774	.6774	1.2464	1.2464	1.2464
17	.7153	.7153	.7153	1.2251	1.2251	1.2251
18	.7523	.7523	.7523	1.2027	1.2027	1.2027
19	.7884	.7884	.7884	1.1794	1.1794	1.1794
20	.8232	.8232	.8232	1.1554	1.1554	1.1554
21	.8565	.8565	.8565	1.1309	1.1309	1.1309
22	.8877	.8877	.8877	1.1065	1.1065	1.1065
23	.9156	.9156	.9156	1.0836	1.0836	1.0836
24	.9370	.9370	.9370	1.0651	1.0651	1.0651
25	.9457	.9457	.9457	1.0574	1.0574	1.0574

Table 7:

Dispersion curves - <110> direction for a diatomic CsCl type crystal lattice with ratio of interatomic force constants = 0.0, ratio of atomic masses = 0.8

1	.0000	.0633	.0447	1.4186	1.4172	1.4179
2	.0000	.0894	1.4186	1.4130	.1264	1.4158
3	.0000	.1892	1.4186	1.4059	.1338	1.4123
4	.0000	.2517	1.4186	1.3961	.1780	1.4074
5	.0000	.3136	1.4186	1.3835	.2218	1.4012
6	.0000	.3749	1.4186	1.3682	.2651	1.3936
7	.0000	.4353	1.4186	1.3502	.3080	1.3848
8	.0000	.4949	1.4186	1.3295	.3501	1.3747
9	.0000	.5533	1.4186	1.3062	.3916	1.3635
10	.0000	.6106	1.4186	1.2805	.4322	1.3512
11	.0000	.6664	1.4186	1.2523	.4720	1.3378
12	.0000	.7207	1.4186	1.2219	.5107	1.3235
13	.0000	1.4186	.7731	1.1895	.5485	1.3083
14	.0000	1.4186	.8232	1.1554	.5850	1.2924
15	.0000	1.4186	.8702	1.1204	.6203	1.2758
16	.0000	1.4186	.9119	1.0867	.6544	1.2587
17	.0000	1.4186	.9411	1.0615	.6870	1.2412
18	.0000	1.4186	.9411	1.0615	.7182	1.2234
19	.0000	1.4186	.9119	1.0867	.7478	1.2055
20	1.4186	.0000	1.1204	.8702	1.1877	.7757
21	1.4186	.0000	1.1554	.8232	1.1702	.8019
22	.0000	1.4186	.7731	1.1895	.8263	1.1531
23	.0000	1.4186	.7207	1.2219	.8488	1.1367
24	.0000	.6664	1.4186	1.2523	.8691	1.1212
25	.0000	.6106	1.4186	1.2805	.8873	1.1069
26	.0000	.5533	1.4186	1.3062	.9031	1.0940
27	.0000	.4949	1.4186	1.3295	.9163	1.0830
28	.0000	.4353	1.4186	1.3502	.9269	1.0739
29	.0000	.3749	1.4186	1.3682	.9348	1.0670
30	.0000	.3136	1.4186	1.3835	.9402	1.0623
31	.0000	.2517	1.4186	1.3961	.9434	1.0595
32	.0000	.1892	1.4186	1.4059	.9450	1.0581
33	.0000	.1264	1.4186	1.4130	.9456	1.0575
34	.0000	.0632	1.4186	1.4172	.9457	1.0574
35	.0000	.0000	1.4186	1.4186	.9457	1.0574

Table 8:

Dispersion curves - <111> direction for a diatomic CsCl type crystal lattice with ratio of interatomic force constants = 0.0, ratio of atomic masses = 0.8

1	.0681	.0257	.0257	1.4170	1.4184	1.4184
2	.1360	.0515	.0515	1.4121	1.4177	1.4177
3	.2035	.0772	.0772	1.4039	1.4165	1.4165
4	.2703	.1029	.1029	1.3926	1.4149	1.4149
5	.3364	.1286	.1286	1.3781	1.4128	1.4128
6	.4014	1.3606	.1542	.1542	1.4102	1.4102
7	.4653	.1797	.1797	1.3401	1.4072	1.4072
8	.5277	1.3168	.2052	.2052	1.4037	1.4037
9	.5884	1.2908	.2307	.2307	1.3997	1.3997
10	.6473	1.2623	.2560	.2560	1.3953	1.3953
11	.7041	1.2315	.2813	.2813	1.3904	1.3904
12	.7586	1.1988	.3064	.3064	1.3851	1.3851
13	.8102	1.1645	.3315	.3315	1.3793	1.3793
14	.8582	1.1296	.3564	.3564	1.3731	1.3731
15	.9012	1.0956	.3812	.3812	1.3664	1.3664
16	.9344	1.0674	.4059	.4059	1.3593	1.3593
17	.9454	1.0577	.4305	.4305	1.3517	1.3517
18	.9269	1.0739	.4548	.4548	1.3437	1.3437
19	.8937	1.1017	.4791	.4791	1.3353	1.3353
20	.8557	1.1315	.5031	.5031	1.3264	1.3264
21	.8166	1.1600	.5270	.5270	1.3171	1.3171
22	.7780	1.1863	.5506	.5506	1.3074	1.3074
23	.7411	1.2097	.5741	.5741	1.2972	1.2972
24	.7068	1.2300	.5974	.5974	1.2867	1.2867
25	.6762	.6204	.6204	1.2471	1.2758	1.2758
26	.6501	.6432	.6432	1.2609	1.2644	1.2644
27	.6295	.6658	.6658	1.2713	1.2527	1.2527
28	.6152	1.2783	.6881	.6881	1.2406	1.2406
29	.6076	1.2819	.7101	.7101	1.2281	1.2281
30	1.2821	.6072	.7318	.7318	1.2153	1.2153
31	.6138	1.2790	.7532	.7532	1.2022	1.2022
32	.6271	1.2725	.7742	.7742	1.1887	1.1887
33	.6464	1.2628	.7949	.7949	1.1750	1.1750
34	.6709	1.2499	.8152	.8152	1.1610	1.1610
35	.6997	1.2341	.8350	.8350	1.1468	1.1468
36	.7317	1.2153	.8542	.8542	1.1326	1.1326
37	.7662	1.1939	.8728	.8728	1.1184	1.1184
38	1.1701	.8021	1.1043	1.1043	.8905	.8905
39	1.1443	.8384	1.0908	1.0908	.9070	.9070
40	1.1173	.8741	1.0783	1.0783	.9219	.9219
41	.9073	1.0905	1.0676	1.0676	.9342	.9342
42	.9342	1.0676	1.0601	1.0601	.9427	.9427
43	.9457	.9457	.9457	1.0574	1.0574	1.0574

Table 9:

Density of states for each Polarization for a diatomic CsCl type crystal lattice with ratio of interatomic force constants =0.0, ratio of atomic masses = 0.8

1	8.8730	27.1127	50.0000
2	10.2690	27.0461	50.0772
3	17.2112	28.3977	50.4228
4	26.1972	30.4521	50.1222
5	25.6810	30.3220	51.4566
6	36.1261	31.9895	51.1958
7	41.8967	33.9303	52.3069
8	41.3065	33.8860	51.8934
9	54.3209	36.3108	53.1585
10	51.9550	36.1766	54.0504
11	61.2047	33.8912	53.7932
12	73.0593	35.0416	57.5161
13	68.7327	33.6994	56.5243
14	78.4498	37.7569	60.2896
15	80.4735	39.1568	58.8630
16	86.0097	41.9662	62.1135
17	87.4010	40.3857	61.0048
18	95.1412	42.7255	63.3359
19	96.6239	47.9629	63.7117
20	98.7161	50.9532	61.0699
21	99.8088	59.8656	65.6857
22	102.8582	55.4765	62.4950
23	101.5954	76.2921	67.5411
24	103.5928	66.6393	62.4439
25	104.1022	89.5857	69.2903
26	105.3838	79.8020	63.7333
27	92.9821	112.0040	71.1821
28	90.6338	105.0752	71.4582
29	73.9675	140.8461	77.2112
30	71.6666	133.1564	76.7105
31	84.0040	141.4496	86.5109
32	64.0429	123.0473	90.4728
33	51.7447	111.2712	108.9412
34	36.3960	101.2958	115.8852
35	38.0486	83.6577	133.7760
36	29.2889	76.2436	142.0857
37	41.4027	65.3746	144.9284
38	36.2046	63.7474	144.8711
39	53.2731	57.9548	145.9169
40	58.1139	54.8813	132.2285
41	80.5411	50.6964	138.7610
42	82.0434	43.1743	123.9997
43	99.6214	62.1721	128.8520
44	64.7937	82.6306	118.8087
45	66.5490	132.7230	112.1675
46	59.5516	150.2299	105.6440
47	64.2066	193.3244	91.0330
48	71.0180	289.4624	87.2619
49	76.3384	554.8275	114.7279
50	10.5776	124.4203	65.4706
51	.0000	25.0000	50.0000
52	.0000	25.0000	50.0000
53	.0000	25.0000	50.0000
54	.0000	25.0000	50.0000
55	.5333	40.8911	529.3948
56	2.0331	55.8958	583.7112
57	4.5030	65.4387	357.8587
58	8.3560	69.6516	301.3137
59	14.6587	69.5245	288.4616
60	18.9444	80.3852	254.0055
61	29.4179	112.4653	205.1559
62	43.2580	148.1563	158.7068
63	61.7152	168.8642	128.9699
64	86.1304	178.4115	111.7527
65	120.2897	175.2208	106.6522
66	160.5857	176.6574	108.2416
67	229.9521	169.7620	135.9917
68	269.5306	145.9760	154.8080
69	213.1239	137.0303	211.9463
70	176.3523	171.3756	217.1956
71	141.4558	234.2572	194.9916
72	129.6487	235.9006	209.5349
73	169.5207	211.9625	205.4017
74	90.9747	126.6593	127.8946
75	.0159	25.0143	50.0111
76	.0000	25.0000	50.0000
77	.0000	25.0000	50.0000
78	.0000	25.0000	50.0000

Table 10:

Total Density of states for a diatomic Cscl type crystal lattice with ratio of interatomic force constants =0.0, ratio of atomic masses = 0.8

1	10.9857
2	12.3922
3	21.0317
4	31.7714
5	32.4597
6	44.3115
7	53.1339
8	52.0858
9	68.7903
10	67.1820
11	73.8890
12	90.6170
13	83.9565
14	101.4963
15	103.4933
16	115.0893
17	113.7915
18	126.2025
19	133.2985
20	135.7392
21	150.3602
22	145.8296
23	170.4286
24	157.6760
25	187.9782
26	173.9191
27	201.1683
28	192.1672
29	217.0248
30	206.5335
31	236.9645
32	202.5630
33	196.9571
34	178.5770
35	180.4923
36	172.6182
37	176.7057
38	169.8231
39	182.1448
40	170.2237
41	194.9986
42	174.2173
43	215.6454
44	191.2330
45	236.4394
46	240.4255
47	273.5640
48	372.7424
49	670.8938
50	125.4685
51	.0000
52	.0000
53	.0000
54	.0000
55	495.8192
56	566.6401
57	352.8003
58	304.3213
59	297.6447
60	278.3350
61	272.0391
62	275.1210
63	284.5493
64	301.2945
65	327.1627
66	370.4846
67	460.7059
68	495.3146
69	487.1005
70	489.9235
71	495.7046
72	500.0842
73	511.8849
74	270.5286
75	.0413
76	.0000
77	.0000
78	.0000

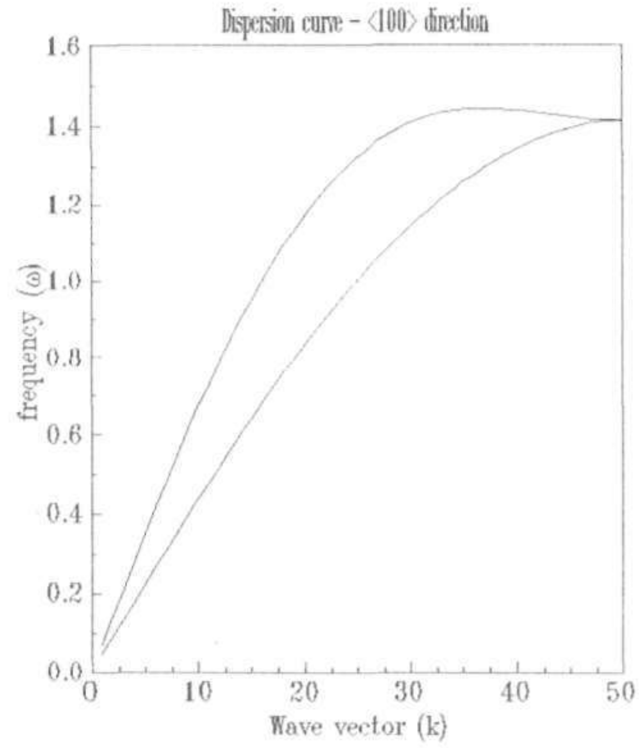

Fig. (A III.1) The [100] phonon dispersion curve for a one-atom BCC crystal lattice. Force constant ratio R = .5

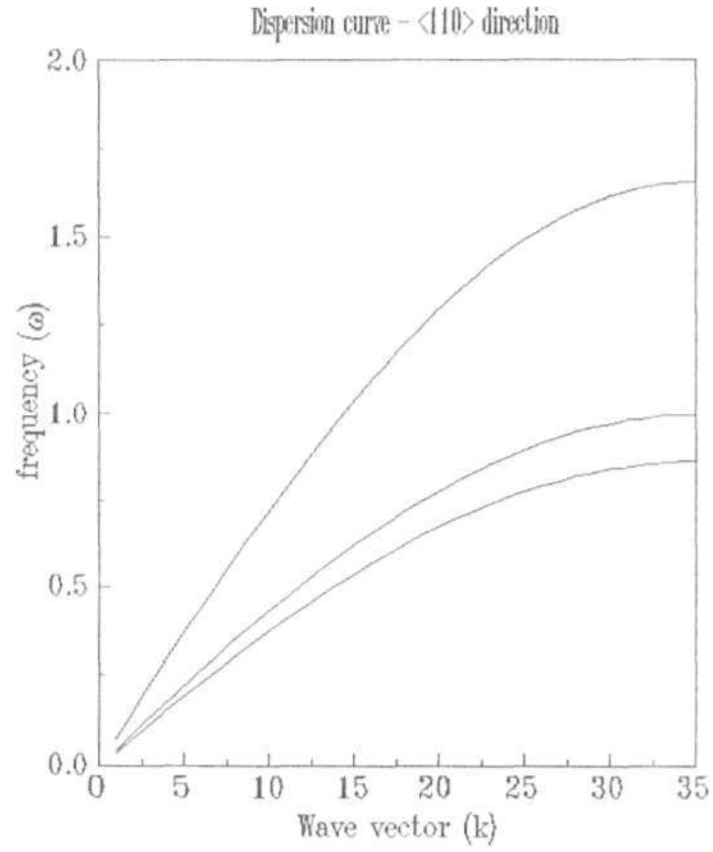

Fig. (A III .2). The [110] phonon dispersion curve for a monatomic BCC crystal lattice. Force constant ratio R = .5

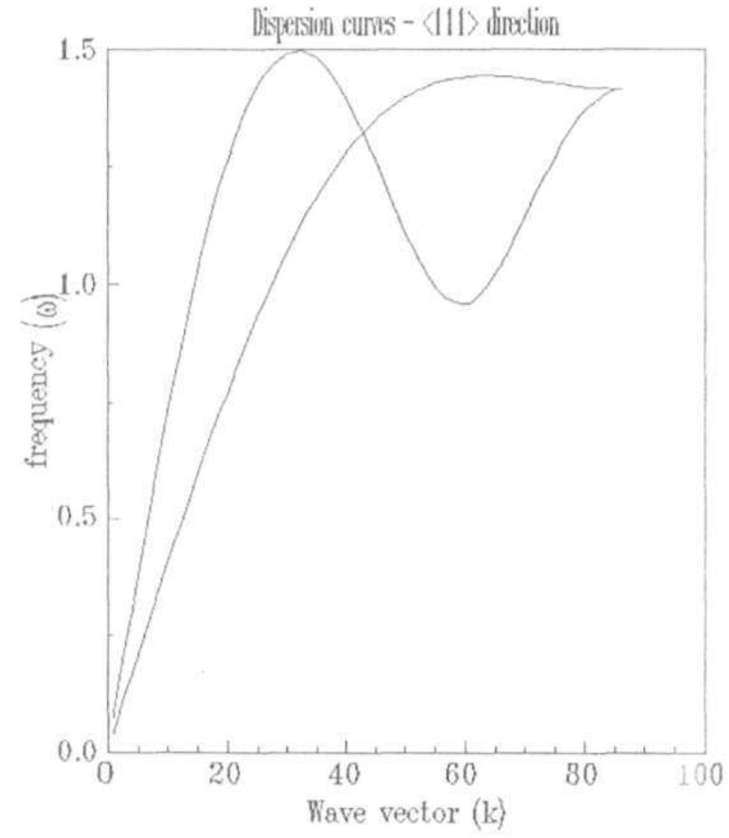

Fig. (A III). The [111] phonon dispersion curve for a monatomic BCC crystal lattice. Force constants ratio R = .5.

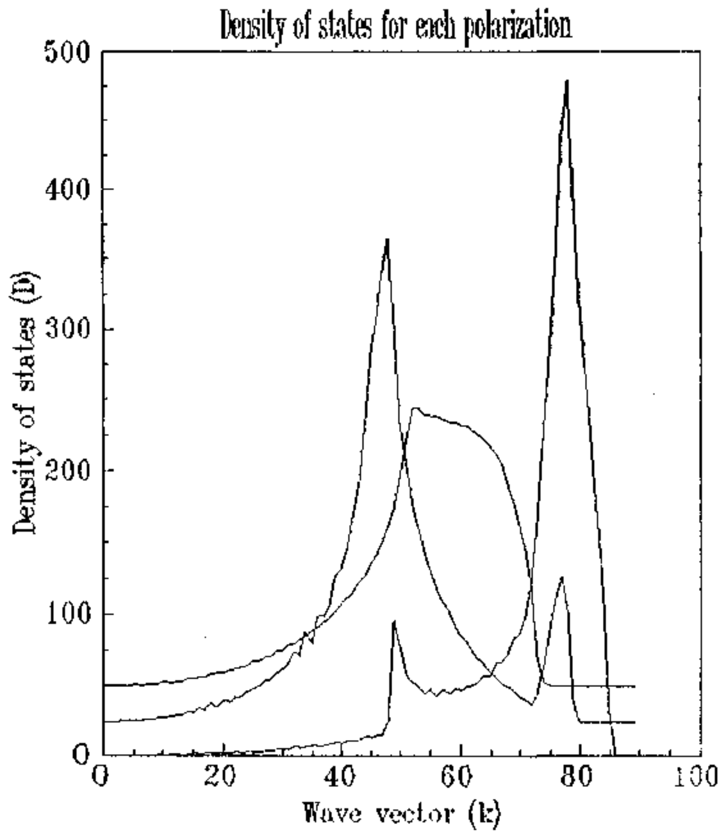

Fig. (A III). The phonon density of states for each polarization. This particular curves is for a one atom BCC latice with R = .5

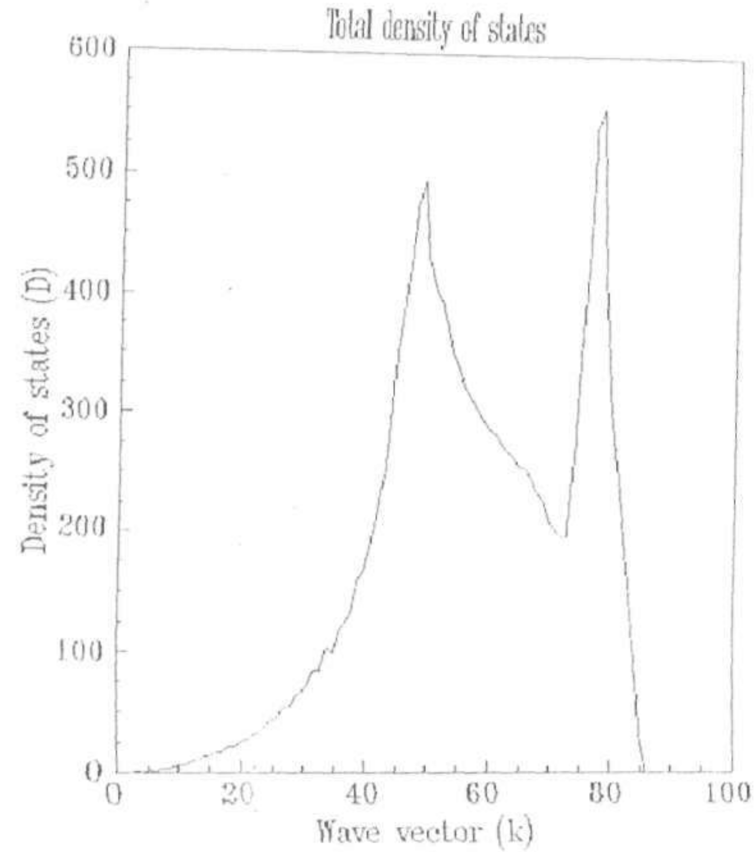

Fig. (A III.5) The phonon total density of states. This particular curve is for a monatomic BCC latice with R = .5

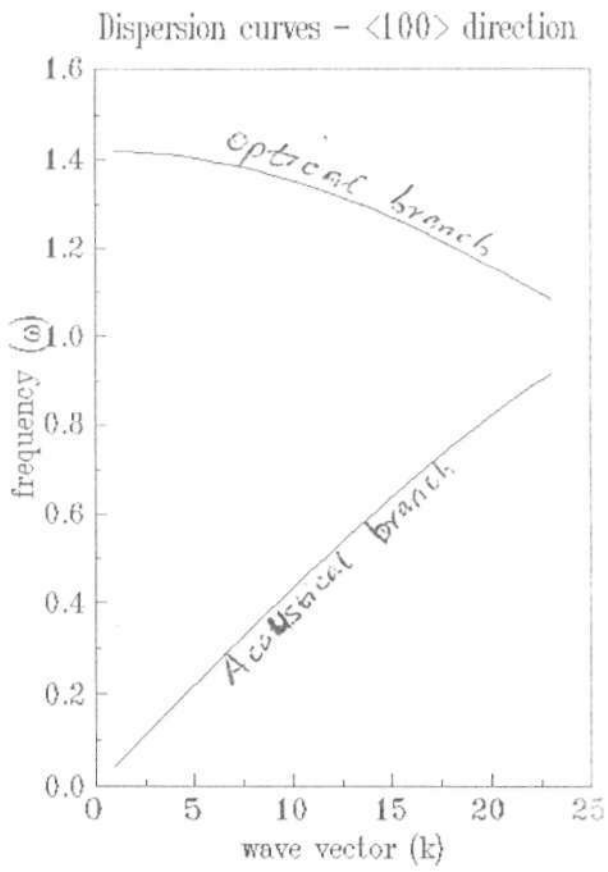

Fig. (A III). The phonon total density of states. This particular curve is for a one atom BCC latice with R = .5

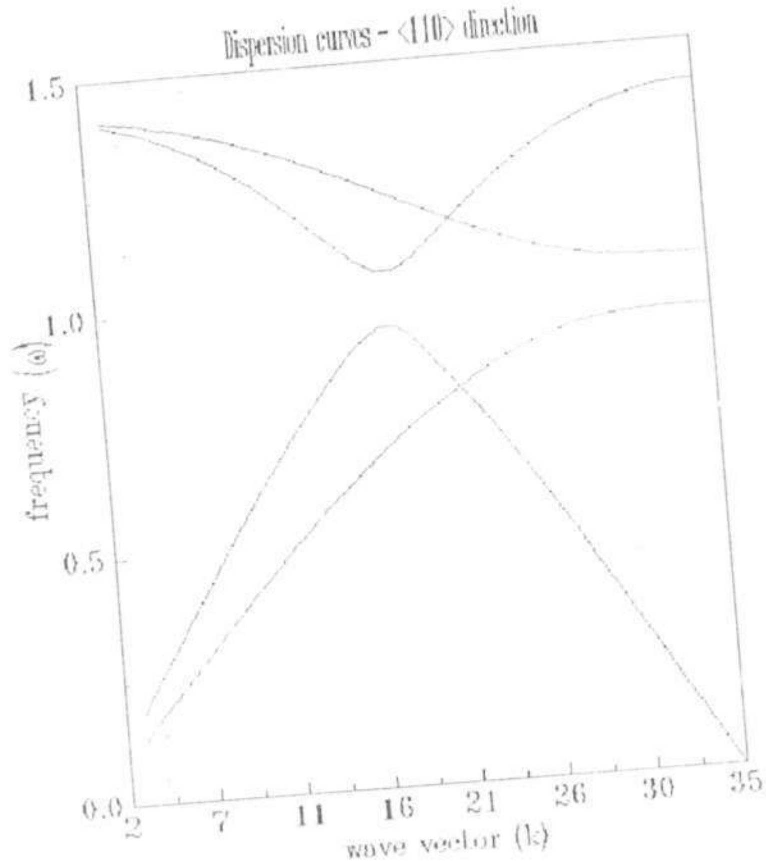

Fig.(A III.7) The [110] phonon dispersion curve for a diatomic CsCl crystal. Mass ratio ρ= .8, force constant ratio R=0.0

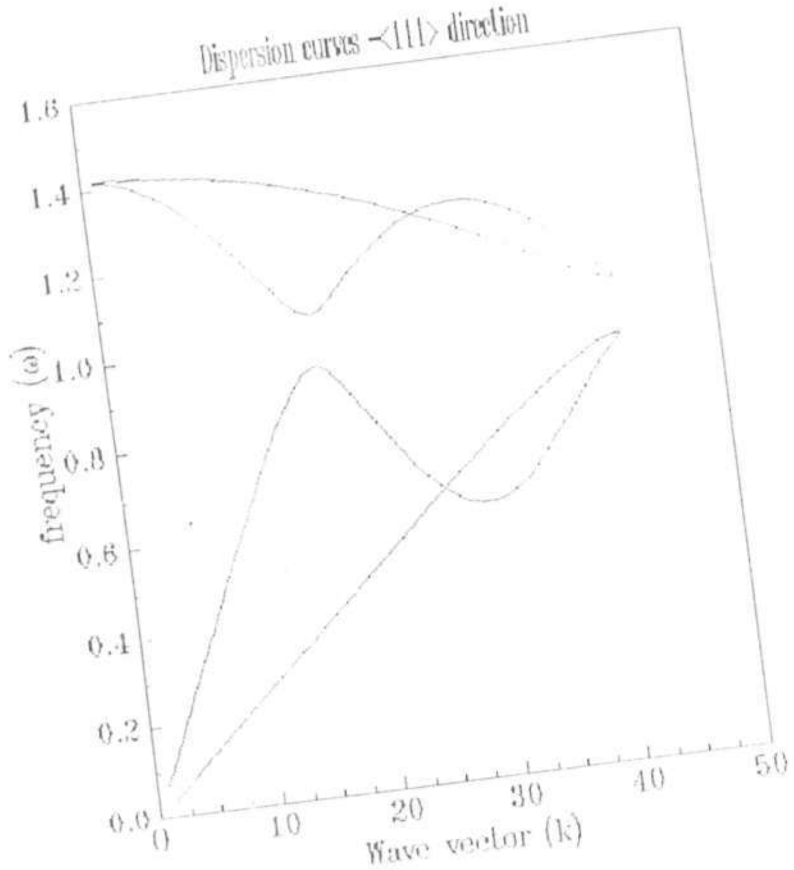

Fig.(A III.8) The [111] phonon dispersion curve for a diatomic CsCl crystal. Mass ratio ρ= .8, force constant ratio r = 0.0

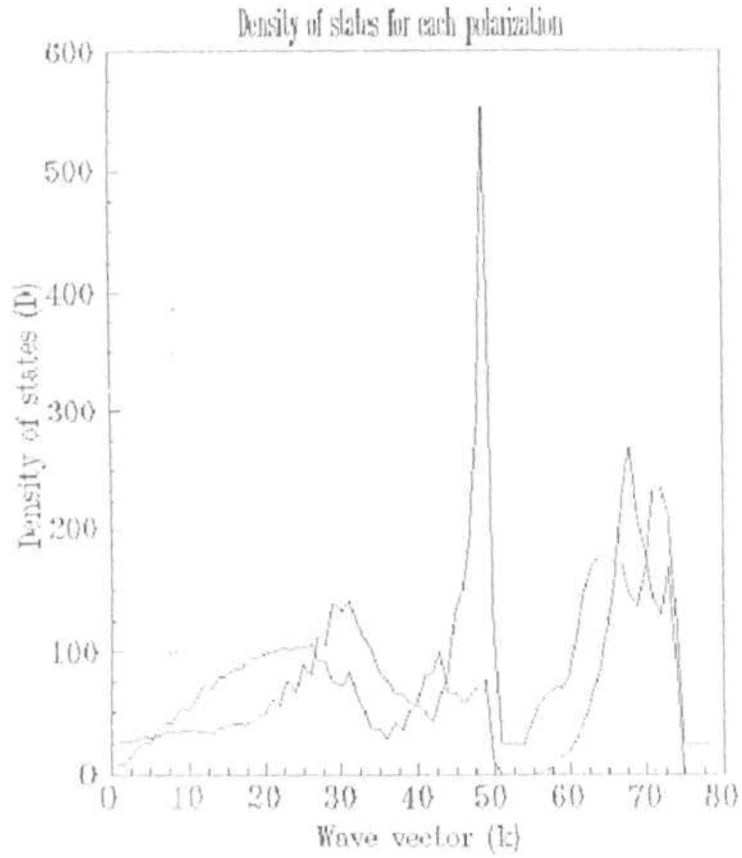

Fig.(A III.9) The phonon density of states for each polarization . This perticular curve is for a mass ratio $\rho = .8$ and force constant ratio $r = 0.0$

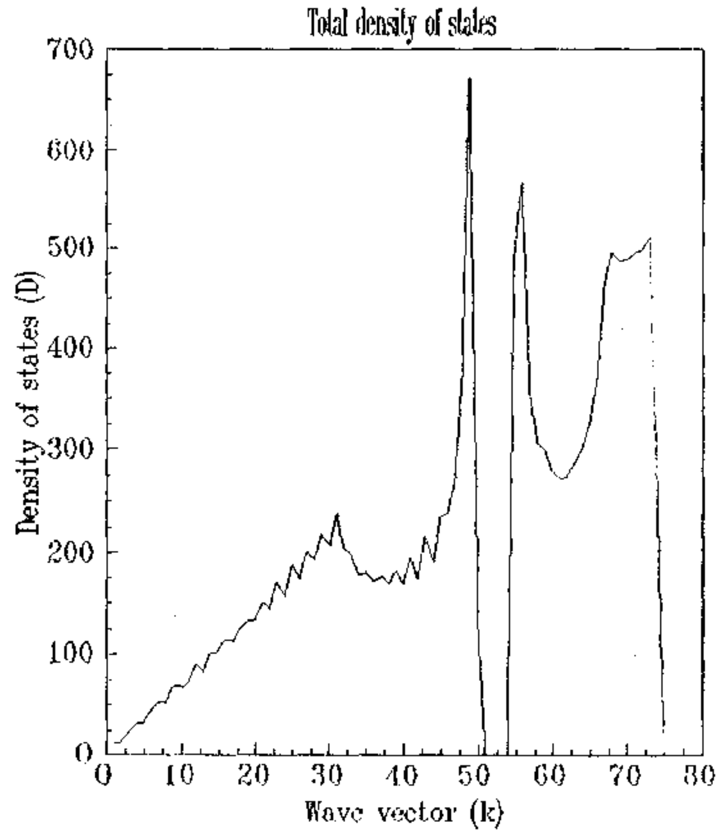

Fig. 10 The phonon tatol density of states. This perticular curve is for mass ratio p = .8 and force constant ratio r =0.0.