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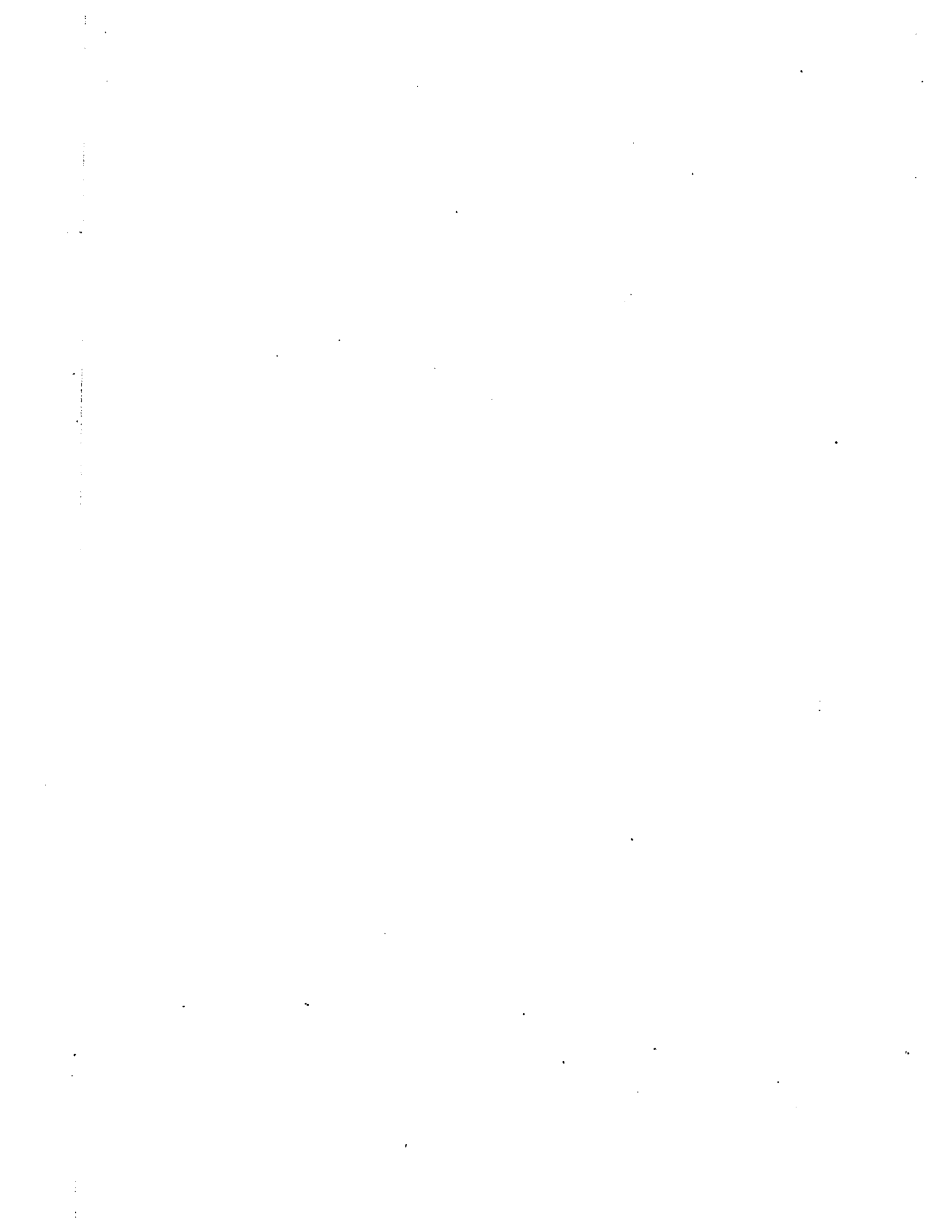
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LATTICE DYNAMICS OF DIAMOND ON THE
BASIS OF COCHRAN'S MODEL

by

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Submitted in partial fulfillment
of the requirements for the degree of
Master of Science.

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ABSTRACT

In the present thesis we have investigated the lattice dynamics of diamond on the basis of the Cochran version of the dipole approximation model. Results have been presented for the dispersion curves, vibration spectra and Debye temperatures of diamond. We have also obtained the vibration spectra and Debye temperatures of germanium.

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To my dear wife.

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CHAPTER I

INTRODUCTION

For crystals with diamond lattice, a 2-constant theory involving a radial and a non-central force between nearest neighbours was first proposed by Born (1). Since Born's original theory employs only two force constants, it predicts a relation between the three elastic constants:

$$\frac{4 c_{11} (c_{11} - c_{44})}{(c_{11} + c_{12})^2} = 1$$

A 3-constant theory was developed by Nagendra Nath (2) and by Smith (3), which took into account a central force between next nearest neighbours. The models due to Born and to Smith have been reviewed by de Launay (4).

Smith's theory was applied to Ge and Si by Hsieh (5) and compared with experiment, Hsieh's calculations have been corrected by Dayal and Singh (6).

A model due to Harrison (7) employs nearest neighbour central forces and restoring forces maintaining the tetrahedral bond angles. This model implicitly introduces forces between second nearest neighbours in a plausible way.

Experimental studies of the inelastic scattering of slow

neutrons by crystals have recently made it possible to determine directly the relation between frequency and wave number of the normal modes of a crystal. Germanium was one of the first substances to be investigated by this technique by Brockhouse and Iyengar (8) and by Ghose et al (9).

A detailed analysis of these results by Herman (10) and by Pope (11) showed that to fit all the data concerned it was necessary to include interactions out to fifth neighbours in the general force model.

Cole and Kineke (12) calculated the vibrational spectrum of Ge using the force constants of Herman (10) and that of Si using a set of three-neighbour force constants derived by Learn (13) from x-ray scattering experiments.

Cochran (14) applied a simple shell model to germanium. Each atom was regarded as composed of a core of charge Z coupled to an oppositely charged shell by means of an isotropic spring of constant k . He assumes three types of nearest neighbour interactions, the core-core, core-shell and shell-shell interactions. Two force constants specify each type. One is associated with the radial force and the other with the angular force. The formation of dipoles by the lattice wave gives rise to electrostatic forces throughout the crystal. This interaction includes all neighbours and requires no extra parameter. Therefore the shell model involves a total of eight parameters. One of them is shown to be redundant and is eliminated by specifying the polarizability β in terms of Z and k . Then Cochran reduces the number to five by setting the ratio γ of the angular force constant to the radial

Force constant equal for the three types of short range interactions. Under these restrictions the Born identity is satisfied. Two of the remaining five parameters are fixed by fitting them with the elastic constant data. The polarizability β is then calculated from the experimental value of the dielectric constant. The two remaining parameters are chosen by trial (along with a 5% adjustment in β) to fit the Neutron Scattering data. The agreement is reasonably good except for the longitudinal acoustic mode in the (111) direction, where, for the point $q = q_{\max}$ the observed and calculated frequency differ by 14%.

Cochran has also provided some theoretical justification for his work by showing its equivalence to the results of Maskevich and Tolpygo (15), who used a quantum mechanical approach. It is now generally recognized that both models are essentially dipole approximations. Cochran also showed that the short range parameters determine a long range force.

With the aid of the adiabatic approximation, the potential energy of lattices of the diamond type was found by Mashkevich and Tolpygo (15) in the form of a quadratic form in the displacements and dipole moments of the electronic shells of all atoms. In an extension of this work, Tolpygo (16) showed that Cochran's procedure of introducing mixed terms corresponding to the dipole moments of the immediate neighbours into the potential energy is justified. This theory, while formally equivalent to that of Cochran, was based not on a model representation but only on the concept of a weak distortion of electron wave functions

due to atomic vibrations. It has nine parameters. Tolpygo's theory was applied to germanium by Demidenko, Kucher and Tolpygo (17,18) and to silicon by Kucher (19).

Recently Warren, Wenzel and Yarnell (21,22) have measured the dispersion curves for phonons propagating in the (100) and (111) directions.

In the present thesis we have investigated the lattice dynamics of diamond on the basis of the Cochran version of the dipole approximation model. Results have been presented for the dispersion curves, vibration spectra and Debye temperatures of diamond. We have also obtained the vibration spectra and Debye temperatures of germanium.

While the present work was essentially complete, a paper by Dolling and Cowley (25) has appeared in which they have applied a dipole approximation model to diamond. This model includes second-nearest-neighbour interactions and has 11 parameters.

Recently Kucher and Nechiporuk (20) have calculated the dispersion curves of diamond using Tolpygo's theory. The results are in fair agreement with the experimental results of Warren et al except for the LO and TO branches in the (111) direction.

CHAPTER II

THE SECULAR EQUATION FOR THE SHELL MODEL OF THE DIAMOND LATTICE

Following Cochran we shall divide the interaction in two parts

A) Mechanical part

B) Electrostatic part

The physical picture is quite simple. Nearest neighbours are connected by radial and angular forces. The shell and core are coupled to one another by an isotropic force constant and a dipole moment may be generated by their relative displacement. The electrostatic interaction is taken to be between the component dipoles throughout the crystal.

The equivalent of the adiabatic approximation is achieved by taking the mass of each shell to be negligible.

Throughout the thesis the term "rigid ion model" will be used when the polarizability is taken to be zero.

We now derive the MECHANICAL PART of the secular equation.

1. The One-dimensional Shell Model

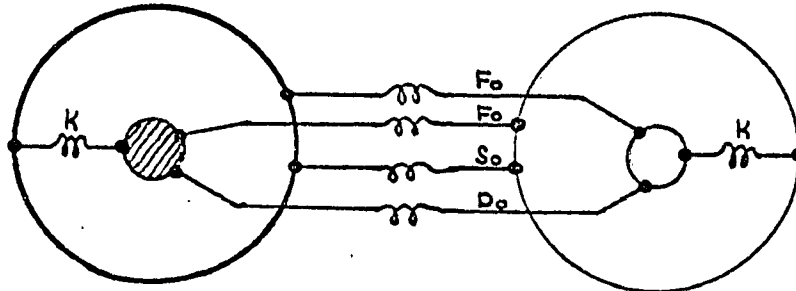


fig.(2.1)

Before we set up the formalism of the shell model we shall treat the one-dimensional case. We assume two interpenetrating lattices of particles each composed of a core and shell. For simplicity we shall consider them as being connected by springs only, which is equivalent to radial forces.

Let K denote the force constant between a core and its shell,

D_o represent the force constant for the interaction of a core with its nearest neighbour core,

S_o that of a shell with its nearest neighbour shell,

F_o that of a core with its nearest neighbour shell or vice versa.

We shall neglect all other interactions. To make the physical picture simpler, we shall call the particles of the first Bravais lattice the black particles and those of the second Bravais lattice the white particles. Let $u(1)$ be the displacement of the black core, $u(2)$ that of the white one, while

$v(1)$ and $v(2)$ represent those of the black shell and white shell respectively.

To set up the equations of motion for a black core we must find the total force acting on it. We do this by adding the respective contributions of each component. The relative displacement of a black core and its own shell is $u(1)-v(1)$ when we take the equilibrium position of the black core as origin. This contributes a force $-K(u(1)-v(1))$, since K is the force constant connecting these two components. Similarly the relative displacement of a black core and a white shell is $u(1)-v(2)$. This gives a contribution $-F_o(u(1)-v(2))$ to the total force. Proceeding thus we finally get

$$F = m\ddot{u}(1) = -(K+2D_o+2F_o)u(1) + D_o u(2) + Kv(1) + F_o v(2) \quad (2.1)$$

and similarly for $v(1)$, $u(2)$ and $v(2)$,

$$m'\ddot{v}(1) = Ku(1) + F_o u(2) - (K+2D_o+2F_o)v(1) + S_o v(2) \quad (2.2)$$

$$m\ddot{u}(2) = D_o u(2) - (K+2D_o+2F_o)u(2) + F_o v(1) + Kv(2) \quad (2.3)$$

$$m'\ddot{v}(2) = F_o u(1) + Ku(2) + S_o v(1) - (K+2F_o+2S_o)v(2) \quad (2.4)$$

Equations (2.1) and (2.2) were written using a black particle as origin. Equations (2.3) and (2.4) using a white particle as origin.

We assume four plane waves going through the cores and shells. For equation (2.1) and (2.2) they are:

$$u(1) = U(1)\exp(i\omega t) \quad u(2) = U(2)\exp(i(-kb+\omega t))$$

$$v(1) = V(1)\exp(i\omega t) \quad v(2) = V(2)\exp(i(-kb+\omega t))$$

We make the substitution, perform the differentiation and cancel the term $\exp(i\omega t)$ to get

$$-m \omega^2 U(1) = -(K+2D_0+2F_0)U(1) + D_0 e^{-ikb} U(2) + KV(1) + F_0 e^{-ikb} V(2)$$

$$-m' \omega^2 V(1) = KU(1) + F_0 e^{-ikb} U(2) - (K+2D_0+2S_0)V(1) + S_0 e^{-ikb} V(2)$$

The plane waves for equation (2.3) and (2.4) are

$$u(1) = U(1)\exp(i(kb+\omega t)) \quad u(2) = U(2)\exp(i\omega t)$$

$$v(1) = V(1)\exp(i(kb+\omega t)) \quad v(2) = V(2)\exp(i\omega t)$$

and we get

$$-m \omega^2 U(2) = D_0 e^{ikb} U(1) - (K+2D_0+2F_0)U(2) + F_0 e^{ikb} V(1) + KV(2)$$

$$-m' \omega^2 V(2) = F_0 e^{ikb} U(1) + KU(2) + S_0 e^{ikb} V(1) - (K+2D_0+2S_0)V(2)$$

This is a homogeneous linear system which can be written in matrix form.

$$\omega^2 \begin{pmatrix} m U(1) \\ m U(2) \\ m' V(1) \\ m' V(2) \end{pmatrix} = \begin{pmatrix} K+2D_0+2F_0 & D & -K & F \\ D^* & K+2D_0+2F_0 & F^* & -K \\ -K & F & K+2D_0+2S_0 & S \\ F^* & -K & S^* & K+2D_0+2S_0 \end{pmatrix} \begin{pmatrix} U(1) \\ U(2) \\ V(1) \\ V(2) \end{pmatrix} \quad (2.5)$$

where $D = -D_0 \exp(ikb)$, $F = -F_0 \exp(ikb)$, etc...

For a non-trivial solution the associated determinant must vanish. We get

$$\begin{vmatrix} K+2D_0+2F_0-\lambda & D & -K & F \\ D^* & K+2D_0+2F_0-\lambda & F^* & -K \\ -K & F & K+2D_0+2S_0-\lambda' & S \\ F^* & K & S^* & K+2D_0+2S_0-\lambda' \end{vmatrix} = 0 \quad (2.6)$$

where $\lambda = m\omega^2$ and $\lambda' = m'\omega^2$,

m denotes the mass of a core,

m' that of a shell.

Cochran puts $m' = 0$, which is equivalent to the adiabatic approximation. Determinant (2.6) now gives two solutions for ω (the optical and acoustical branch).

2. The Diamond Lattice

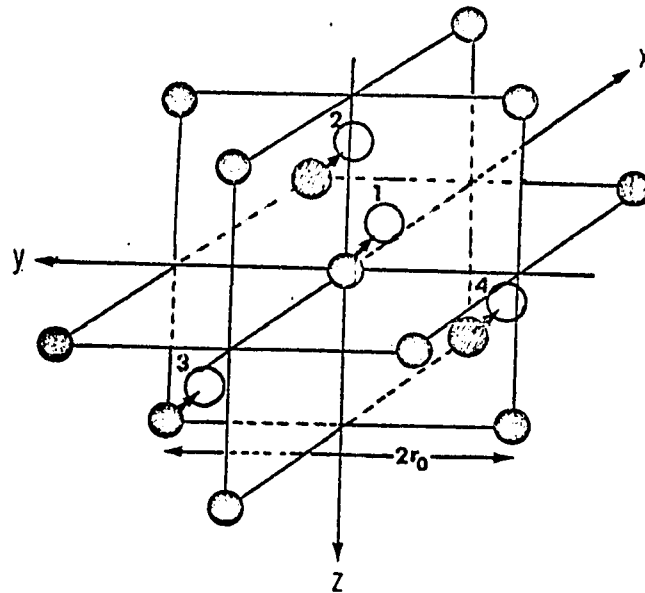


fig.(2.2)

Fig.(2.2) The black circles represent atoms of lattice I. The white circles represent the four nearest neighbours of 0 and are in lattice II.

The diamond structure is a lattice with a basis. It can be represented by two interpenetrating face-centered Bravais lattices, each of cube edge $2r_0$. Let us call the simple Bravais lattice in which the atom 0 is located "lattice I" (black circles). The atoms of lattice I are located by the vector

$$\vec{r}_I(n) = [(n_1+n_3)\vec{e}_1 + (n_1+n_2)\vec{e}_2 + (n_2+n_3)\vec{e}_3] r_0$$

The quantities n_1 , n_2 and n_3 are integers and the quantities \vec{e}_1 , \vec{e}_2 and \vec{e}_3 are unit vectors parallel to the x, y and z axes respectively.

The second simple Bravais lattice, lattice II, can be generated by displacing the entire lattice I through a distance $\vec{r}_{1,2}$

$$\vec{r}_{1,2} = -(r_0/2)(\vec{e}_1 + \vec{e}_2 + \vec{e}_3).$$

Thus the location of the atoms in lattice II is given by

$$\begin{aligned} \vec{r}_{II}(n) &= \vec{r}_I(n) + \vec{r}_{1,2} \\ &= \left[(n_1 + n_3 - 1/2)\vec{e}_1 + (n_1 + n_2 - 1/2)\vec{e}_2 + (n_2 + n_3 - 1/2)\vec{e}_3 \right] r_0 \end{aligned}$$

Remark We have chosen $\vec{r}_{1,2} = -(r_0/2)(\vec{e}_1 + \vec{e}_2 + \vec{e}_3)$ to conform with Kellermann (23) and Cochran (14), while de Launay (4) defines it with an opposite sign.

3. The Shell Model for the Diamond Lattice

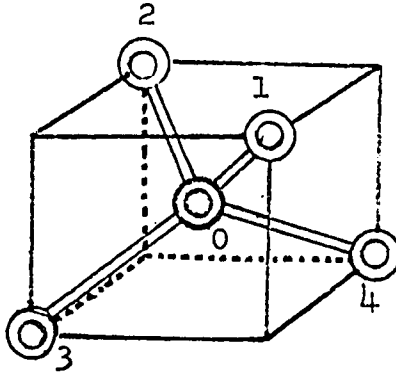


fig.(2.3)

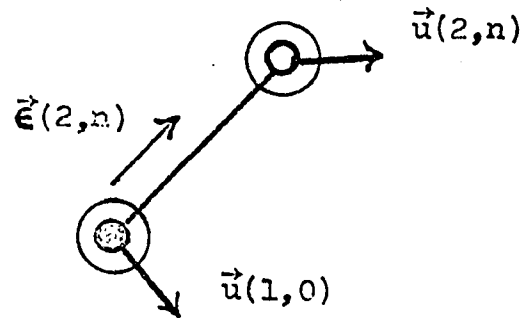


fig.(2.4)

Cochran(14) considers each particle as being composed of a core and a shell. Fig.(2.3) shows the four nearest neighbours of the particle 0. These four atoms have the same numbering as in fig.(2.2).

To make the physical picture simpler we shall use the terms "black cores" and "black shells" for the particles of lattice I, "white cores" and "white shells" for those of lattice II.

Let $\vec{e}(2,n) = (\lambda_n, \mu_n, \nu_n)$ be the unit vector which indicates the direction of the equilibrium line joining the particles. In our notations the first index is equal to one if the vector is pointing towards a particle of lattice I and it will be equal to two if it is pointing towards a particle of lattice II. The second index represents the label assigned to the particle according to the scheme of fig.(2.2). The quantities λ_n , μ_n and ν_n are the direction cosines of the particle whose position vector is $\vec{r}_{II}(n) = (x_n, y_n, z_n)$.

We now give a table of the coordinates and direction cosines for the nearest neighbours of the black central atom labeled zero.

particle no.	x_n	y_n	z_n	λ_n	μ_n	ν_n
1	$-r_0/2$	$-r_0/2$	$-r_0/2$	$-1/\sqrt{3}$	$-1/\sqrt{3}$	$-1/\sqrt{3}$
2	$r_0/2$	$r_0/2$	$-r_0/2$	$1/\sqrt{3}$	$1/\sqrt{3}$	$-1/\sqrt{3}$
3	$-r_0/2$	$r_0/2$	$r_0/2$	$-1/\sqrt{3}$	$1/\sqrt{3}$	$1/\sqrt{3}$
4	$-r_0/2$	$-r_0/2$	$r_0/2$	$1/\sqrt{3}$	$-1/\sqrt{3}$	$1/\sqrt{3}$

Before we set up the complete set of equations for the shell model we shall work out the special case of core-core interaction, i.e. let us assume for the moment that there are no shells. This formulation is parallel to de Launay's treatment (4) of the rigid ion model.

Let $\vec{u}(1,0)$ denote the displacement of the central black core and $\vec{u}(2,n)$ that of the n^{th} white one. We denote by $\vec{F}_u(2,n)$ the combined radial and angular force due to the relative displacement $\vec{u}(1,0) - \vec{u}(2,n)$. (see fig.(2.4)). We have

$$\vec{F}_u(2,n) = -\alpha'_D(\vec{u}(1,0) - \vec{u}(2,n)) - (\alpha_D - \alpha'_D) \left[\vec{e}(2,n) \cdot (\vec{u}(1,0) - \vec{u}(2,n)) \right] \vec{e}(2,n)$$

where α_D and α'_D denote the radial and angular force constants for the core-core interaction.

The summation over the four nearest neighbours gives us the total force, therefore we can write

$$m \ddot{\vec{u}}(1,0) = \sum_{n=1}^4 \vec{F}_u(2,n)$$

$$\text{i.e. } m \ddot{\vec{u}}(1,0) = -\alpha'_D \sum_{n=1}^4 (\vec{u}(1,0) - \vec{u}(2,n))$$

$$-(\alpha_D - \alpha'_D) \sum_{n=1}^4 [\vec{e}(2,n) \cdot (\vec{u}(1,0) - \vec{u}(2,n))] \vec{e}(2,n)$$

Using our table we can write out explicitly the three cartesian components of this equation. After some rearrangements we get the three first equations of page 15. To solve these equations we assume that two plane waves are passing through the cores. The wave passing through the black cores has the form $\vec{U}(1) \exp i(\omega t + \vec{k} \cdot \vec{r}_I(n))$ and that passing through the white cores has the form $\vec{U}(2) \exp i(\omega t + \vec{k} \cdot \vec{r}_{II}(n))$. The result of substituting these plane waves into the equations of motion of the central black core is a set of three simultaneous homogeneous equations [(2.7), (2.8) and (2.9) written on page 16] in the six unknown amplitudes $U_x(1), \dots, U_z(2)$. These equations were obtained by making the substitutions

$$\vec{u}(1,0) = \vec{U}(1) \exp(i\omega t), \quad \vec{u}(2,n) = \vec{U}(2) \exp i(\omega t + \vec{k} \cdot \vec{r}_{II}(n)),$$

performing the differentiation $\ddot{\vec{u}}(1,0)$, cancelling the term $\exp(i\omega t)$ and defining new constants D_0 and D'_0 in terms of α_D and α'_D as follows $D_0 = 4(\alpha_D + 2\alpha'_D)/3$ and $D'_0 = 4(\alpha_D - \alpha'_D)/3$. To obtain three more equations one may develop the equations of motion for a white core such as core 1 in fig.(2.3). We get equations (2.10), (2.11) and (2.12).

$$\begin{aligned}
 m \ddot{u}_x(1,0) &= -4\beta u_x(1,0) + \beta \sum_{n=1}^4 u_x(2,n) - \beta' [2u_y(2,3) + 2u_y(2,4) - \sum_{n=1}^4 u_y(2,n)] \\
 &\quad - \beta' [2u_z(2,2) + 2u_z(2,3) - \sum_{n=1}^4 u_z(2,n)]
 \end{aligned}$$

$$\begin{aligned}
 m \ddot{u}_y(1,0) &= -4\beta u_y(1,0) + \beta \sum_{n=1}^4 u_y(2,n) - \beta' [2u_x(2,3) + 2u_x(2,4) - \sum_{n=1}^4 u_x(2,n)] \\
 &\quad - \beta' [2u_z(2,2) + 2u_z(2,4) - \sum_{n=1}^4 u_z(2,n)]
 \end{aligned}$$

$$\begin{aligned}
 m \ddot{u}_z(1,0) &= -4\beta u_z(1,0) + \beta \sum_{n=1}^4 u_z(2,n) - \beta' [2u_x(2,2) + 2u_x(2,3) - \sum_{n=1}^4 u_x(2,n)] \\
 &\quad - \beta' [2u_y(2,2) + 2u_y(2,4) - \sum_{n=1}^4 u_y(2,n)]
 \end{aligned}$$

$$m \omega^2 U_x(1) = D_{0x} U_x(1) - D_{01} a_1 U_x(2) + D_{02} a_2 U_y(2) + D_{03} a_3 U_z(2) \quad (2.7)$$

$$m \omega^2 U_y(1) = D_{0y} U_y(1) + D_{02} a_2 U_x(2) - D_{01} a_1 U_y(2) + D_{04} a_4 U_z(2) \quad (2.8)$$

$$m \omega^2 U_z(1) = D_{0z} U_z(1) + D_{03} a_3 U_x(2) + D_{04} a_4 U_y(2) - D_{01} a_1 U_z(2) \quad (2.9)$$

$$m' \omega^2 U_x(2) = -D_{01} a_1^* U_x(1) + D_{02} a_2^* U_y(1) + D_{03} a_3^* U_z(1) + D_{0x} U_x(2) \quad (2.10)$$

$$m' \omega^2 U_y(2) = D_{02} a_2^* U_x(1) - D_{01} a_1^* U_y(1) + D_{04} a_4^* U_z(1) + D_{0y} U_y(2) \quad (2.11)$$

$$m' \omega^2 U_z(2) = D_{03} a_3^* U_x(1) + D_{04} a_4^* U_y(1) - D_{01} a_1^* U_z(1) + D_{0z} U_z(2) \quad (2.12)$$

where: $a_1 = C_1 C_2 C_3 + i S_1 S_2 S_3$ $a_3 = S_1 C_1 S_3 + i C_1 S_2 C_3$ $S_n = \sin(q_n r_0/2)$

$a_2 = S_1 S_2 C_3 + i C_1 C_2 S_3$ $a_4 = C_1 S_2 S_3 + i S_1 C_2 C_3$ $C_n = \cos(q_n r_0/2)$

The condition that both waves exist leads to the vanishing of the 6x6 determinant shown below.

$$\begin{vmatrix}
 D_0 - \lambda & & & -D'_0 a_1 & D'_0 a_2 & D'_0 a_3 \\
 & D_0 - \lambda & & D'_0 a_2 & -D'_0 a_1 & D'_0 a_4 \\
 & & D_0 - \lambda & D'_0 a_3 & D'_0 a_4 & -D'_0 a_1 \\
 -D_0 a_1^* & D'_0 a_2^* & D'_0 a_3^* & D_0 - \lambda & & \\
 D'_0 a_2^* & -D_0 a_1^* & D'_0 a_4^* & & D_0 - \lambda & \\
 D'_0 a_3^* & D'_0 a_4^* & -D_0 a_1^* & & & D_0 - \lambda
 \end{vmatrix} = 0$$

where $\lambda = m \omega^2$ $m = \text{mass of a core.}$

We are now prepared to set up the complete set of equations describing the mechanical part of the shell model. Let $\vec{v}(1,n)$ denote the displacement of the n^{th} black shell and $\vec{v}(2,n)$ that of the n^{th} white shell. Let k denote the isotropic force constant connecting a core to its own shell. Let α_F and α_S denote the radial force constants for the core shell and shell-shell interactions respectively. If α'_F and α'_S represent the corresponding angular force constants, the equations of motion will be

$$m \vec{u}(1,0) = -k\vec{v}(1,0) - \alpha'_D \sum_{n=1}^4 (\vec{u}(1,0) - \vec{u}(2,n)) - (\alpha_D - \alpha'_D) \sum_{n=1}^4 [\vec{e}(2,n) \cdot (\vec{u}(1,0) - \vec{u}(2,n))] \vec{e}(2,n) \quad (2.13)$$

$$- \alpha'_F \sum_{n=1}^4 (\vec{u}(1,0) - \vec{v}(2,n)) - (\alpha_F - \alpha'_F) \sum_{n=1}^4 [\vec{e}(2,n) \cdot (\vec{u}(1,0) - \vec{v}(2,n))] \vec{e}(2,n)$$

$$m \vec{u}(2,0) = -k\vec{v}(2,0) - \alpha'_D \sum_{n=1}^4 (\vec{u}(2,0) - \vec{u}(1,n)) - (\alpha_D - \alpha'_D) \sum_{n=1}^4 [\vec{e}(1,n) \cdot (\vec{u}(2,0) - \vec{u}(1,n))] \vec{e}(1,n) \quad (2.14)$$

$$- \alpha'_F \sum_{n=1}^4 (\vec{u}(2,0) - \vec{v}(1,n)) - (\alpha_F - \alpha'_F) \sum_{n=1}^4 [\vec{e}(1,n) \cdot (\vec{u}(2,0) - \vec{v}(1,n))] \vec{e}(1,n)$$

$$m \vec{v}(1,0) = -k\vec{u}(1,0) - \alpha'_S \sum_{n=1}^4 (\vec{v}(1,0) - \vec{v}(2,n)) - (\alpha_S - \alpha'_S) \sum_{n=1}^4 [\vec{e}(2,n) \cdot (\vec{v}(1,0) - \vec{v}(2,n))] \vec{e}(2,n) \quad (2.15)$$

$$- \alpha'_F \sum_{n=1}^4 (\vec{v}(1,0) - \vec{u}(2,n)) - (\alpha_F - \alpha'_F) \sum_{n=1}^4 [\vec{e}(2,n) \cdot (\vec{v}(1,0) - \vec{u}(2,n))] \vec{e}(2,n)$$

$$m \vec{v}(2,0) = -k\vec{u}(2,0) - \alpha'_S \sum_{n=1}^4 (\vec{v}(2,0) - \vec{v}(1,n)) - (\alpha_S - \alpha'_S) \sum_{n=1}^4 [\vec{e}(1,n) \cdot (\vec{v}(2,0) - \vec{v}(1,n))] \vec{e}(1,n) \quad (2.16)$$

$$- \alpha'_F \sum_{n=1}^4 (\vec{v}(2,0) - \vec{u}(1,n)) - (\alpha_F - \alpha'_F) \sum_{n=1}^4 [\vec{e}(1,n) \cdot (\vec{v}(2,0) - \vec{u}(1,n))] \vec{e}(1,n)$$

where equation (2.13) is for a central black core (2.14) for a central white core

(2.15) for a central black shell (2.16) for a central white shell

To solve these equations we assume that four plane waves are propagated through the diamond lattice. The wave passing through the black shells has the form $\vec{V}(1)\exp i(\omega t + \vec{k} \cdot \vec{r}_I(n))$ and that passing through the white shells has the form $\vec{V}(2)\exp i(\omega t + \vec{k} \cdot \vec{r}_{II}(n))$. The result of substituting the four plane waves into the equations of motion is a set of twelve simultaneous homogeneous equations in the twelve amplitude components $U_x(1), \dots, U_x(2), \dots, V_x(1), \dots, V_z(2)$. The condition for a solution leads to the vanishing of the 12×12 determinant shown on page 20.

The system of 12 equations is given on page 33. We label it SYSTEM (1).

$k+D_0+F_0-\lambda$	$-D_{0a1}$	D_{0YD2}	D_{0YD3}	$-k$	$-F_{0a1}$	F_{0YFa2}	F_{0YFa3}
$k+D_0+F_0-\lambda$	D_{0YD2}	$-D_{0a1}$	D_{0YD4}	$-k$	F_{0YFa2}	$-F_{0a1}$	F_{0YFa4}
$k+D_0+F_0-\lambda$	D_{0YD3}	D_{0YD4}	$-D_{0a1}$	$-k$	F_{0YFa3}	F_{0YFa4}	$-F_{0a1}$
$-D_{0a1}^*$	D_{0YD2}^*	D_{0YD3}^*	$k+D_0+F_0-\lambda$	$-F_{0a1}^*$	F_{0YFa2}^*	F_{0YFa3}^*	$-k$
D_{0YD2}^*	$-D_{0a1}^*$	D_{0YD4}^*	$k+D_0+F_0-\lambda$	F_{0YFa2}^*	$-F_{0a1}^*$	F_{0YFa4}^*	$-k$
D_{0YD3}^*	D_{0YD4}^*	$-D_{0a1}^*$	$k+D_0+F_0-\lambda$	F_{0YFa3}^*	F_{0YFa4}^*	$-F_{0a1}^*$	$-k$
$-k$	$-F_{0a1}$	F_{0YFa2}	F_{0YFa3}	$k+F_0+S_0$	$-S_{0a1}$	S_{0YSa2}	S_{0YSa3}
$-k$	F_{0YFa2}	$-F_{0a1}$	F_{0YFa4}	$k+F_0+S_0$	S_{0YSa2}	$-S_{0a1}$	S_{0YSa4}
$-k$	F_{0YFa3}	F_{0YFa4}	$-F_{0a1}$	$k+F_0+S_0$	S_{0YSa3}	S_{0YSa4}	$-S_{0a1}$
$-F_{0a1}^*$	F_{0YFa2}^*	F_{0YFa3}^*	$-k$	$-S_{0a1}^*$	S_{0YSa2}^*	S_{0YSa3}^*	$k+F_0+S_0$
F_{0YFa2}^*	$-F_{0a1}^*$	F_{0YFa4}^*	$-k$	S_{0YSa2}^*	$-S_{0a1}^*$	S_{0YSa4}^*	$k+F_0+S_0$
F_{0YFa3}^*	F_{0YFa4}^*	$-F_{0a1}^*$	$-k$	S_{0YSa3}^*	S_{0YSa4}^*	$-S_{0a1}^*$	$k+F_0+S_0$

B) COULOMB PART

We now include the terms which arise from the electrostatic interaction of units within the crystal. As previously stated the shell model is essentially a dipole-approximation model, i.e. the relative displacement of a core and shell produces a dipole which in turn exerts some influence on the other units of the crystal. We now give a simple example.

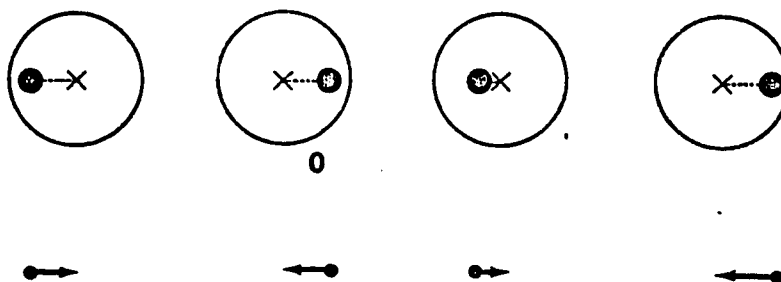
4. A One-Dimensional Array of Dipoles

fig.(2.5)

Consider a linear array of dipoles as shown. Let r_0 denote the distance separating two neighbouring particles at their equilibrium positions. Let u_n denote the displacement of the n^{th} dipole situated at a distance nr_0 from the particle labeled 0.

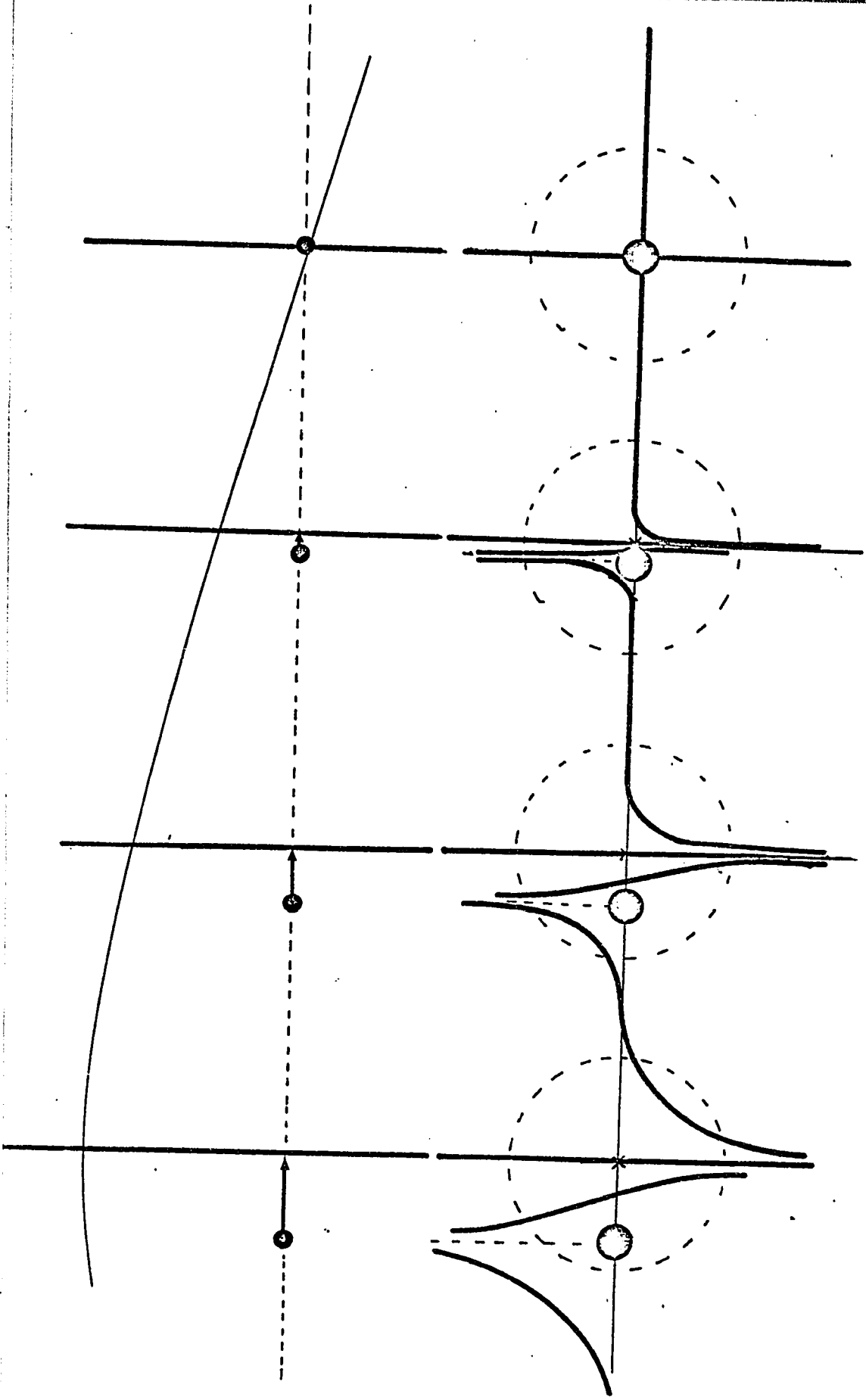


fig.(2.6)

The potential of the n^{th} dipole is given by

$$\begin{aligned}
 V_n &= \frac{Ze}{|x-nr_0|} - \frac{Ze}{|x-nr_0-u_n|} \\
 &= \frac{Ze u_n}{|x-nr_0||x-nr_0-u_n|} \\
 &= \frac{Ze u_n}{|x-nr_0|^2} \quad \text{since } u_n \ll nr_0
 \end{aligned}$$

which can be written as

$$V_n = -Ze \frac{\partial}{\partial x} \frac{u_n}{|x-nr_0|} \quad (2.17)$$

The force exerted on a core of charge Ze situated at $x = 0$ is given by

$$F_n = -Ze \left(\frac{\partial V_n}{\partial x} \right)_{x=0}$$

Substituting V_n as given by equation (2.17) we get

$$F_n = Z^2 e^2 \lim_{x \rightarrow 0} \left[\frac{\partial^2}{\partial x^2} \frac{u_n}{|x-nr_0|} \right] \quad (2.18)$$

So the equation of motion for this core is given by

$$m \ddot{u}_0 = \sum'_n F_n \quad \text{the prime means exclude } n = 0$$

Substituting F_n as given by equation (2.18) we get

$$m \ddot{u}_0 = Z^2 e^2 \lim_{x \rightarrow 0} \left[\sum'_n \frac{\partial^2}{\partial x^2} \frac{u_n}{|x - nr_0|} \right] \quad (2.19)$$

Since we have a lattice wave creating a dipole at each lattice site the displacement u_n is of the form

$$u_n = U \exp(i\omega t + knr_0) \quad (2.20)$$

We substitute this plane wave into equation (2.19). After some simplification we get

$$m \omega^2 = Z^2 e^2 \lim_{x \rightarrow 0} \left[\sum'_n \frac{\partial^2}{\partial x^2} \frac{\exp(iknr_0)}{|x - nr_0|} \right] \quad (2.21)$$

Equation (2.21) shows us that the concept of a force constant does not appear in this problem. The expression on the right hand side is called a bonding coefficient, in this case it is a Coulomb coefficient. We designate it by the symbol C_1^{xx} .

By definition $C_1^{xx} = Z^2 e^2 \lim_{x \rightarrow 0} \left[\sum'_n \frac{\partial^2}{\partial x^2} \frac{\exp(iknr_0)}{|x - nr_0|} \right] \quad (2.22)$

We have given this simple example as an illustration only. We now give Kellerman's definition for the Coulomb coefficients.

5. Kellermann's Coefficients for the Diamond Lattice

Kellermann (23) has defined the Coulomb coefficients in his work on the NaCl lattice. Cochran (14) has applied this definition to the case of diamond. From Cochran's paper it follows that

$$C_{xy}(11) = -Z^2 e^2 \lim_{\vec{r} \rightarrow 0} \left[\sum' \frac{\partial^2}{\partial x \partial y} \frac{\exp(i\vec{q} \cdot \vec{r}_l)}{|\vec{r} - \vec{r}_l|} \right] \quad (2.23)$$

$$C_{xy}(12) = -Z^2 e^2 \left\{ \exp(i\vec{q} \cdot \vec{r}_{1,2}) \right\} \lim_{\vec{r} \rightarrow -\vec{r}_{1,2}} \left[\sum \frac{\partial^2}{\partial x \partial y} \frac{\exp(i\vec{q} \cdot \vec{r}_l)}{|\vec{r} - \vec{r}_l|} \right] \quad (2.24)$$

We have used a slightly different notation with the abbreviation $\vec{r}_l \equiv \vec{r}_I(l)$ (see page 10 for a definition of $\vec{r}_I(n)$).

In the following discussion we shall denote $C_{xy}(11)$ by C_1 and $C_{xy}(12)$ by C_2 .

- C_1 represents the interaction of the black core 0 with all the other black cores.
- $-C_1$ represents the interaction of the black core 0 with all the other black shells (i.e. exclude shell 0).
- C_2 represents the interaction of the black core with all the white cores.
- $-C_2$ represents the interaction of the black core with all the white shells.

Restricting ourselves to the interaction of a core of lattice I with the other cores of lattice I and all those of lattice II we would get

$$\begin{vmatrix}
 C_1^{xx-\lambda} & C_1^{xy} & C_1^{xz} & C_2^{xx} & C_2^{xy} & C_2^{xz} \\
 C_1^{xy} & C_1^{yy-\lambda} & C_1^{yz} & C_2^{xy} & C_2^{yy} & C_2^{yz} \\
 C_1^{xz} & C_1^{yx} & C_1^{zz-\lambda} & C_2^{xz} & C_2^{yz} & C_2^{zz} \\
 C_2^{xx*} & C_2^{xy*} & C_2^{xz*} & C_2^{xx-\lambda} & C_1^{xy} & C_1^{xz} \\
 C_2^{xy*} & C_2^{yy*} & C_2^{yz*} & C_1^{xy} & C_2^{yy-\lambda} & C_1^{yz} \\
 C_2^{xz*} & C_2^{yz*} & C_2^{zz*} & C_1^{xz} & C_1^{yz} & C_2^{zz-\lambda}
 \end{vmatrix} = 0$$

The determinant is of the form

$$\begin{vmatrix}
 C_1 - \lambda & C_2 \\
 C_2^* & C_1 - \lambda
 \end{vmatrix} = 0$$

We now quote the complete 12x12 array representing the Coulomb interaction. It is given on page 27.

Adding the mechanical and the Coulomb parts we get the secular equation for the shell model. To quote this equation we will refer to DET(1) page 20 and page 27.

aC_{11}^{xx}	aC_{11}^{xy}	aC_{11}^{xz}	aC_{21}^{xx}	aC_{21}^{xy}	aC_{21}^{xz}	$-aC_{11}^{xx}$	$-aC_{11}^{xy}$	$-aC_{11}^{xz}$	$-aC_{21}^{xx}$	$-aC_{21}^{xy}$	$-aC_{21}^{xz}$
aC_{11}^{xy}	aC_{11}^{yy}	aC_{11}^{yz}	aC_{21}^{xy}	aC_{21}^{yy}	aC_{21}^{yz}	$-aC_{11}^{xy}$	$-aC_{11}^{yy}$	$-aC_{11}^{yz}$	$-aC_{21}^{xy}$	$-aC_{21}^{yy}$	$-aC_{21}^{yz}$
aC_{11}^{xz}	aC_{11}^{yz}	aC_{11}^{zz}	aC_{21}^{xz}	aC_{21}^{yz}	aC_{21}^{zz}	$-aC_{11}^{xz}$	$-aC_{11}^{yz}$	$-aC_{11}^{zz}$	$-aC_{21}^{xz}$	$-aC_{21}^{yz}$	$-aC_{21}^{zz}$
aC_{22}^{xx} *	aC_{22}^{xy} *	aC_{22}^{xz} *	aC_{12}^{xx}	aC_{12}^{xy}	aC_{12}^{xz}	$-aC_{22}^{xx}$ *	$-aC_{22}^{xy}$ *	$-aC_{22}^{xz}$ *	$-aC_{12}^{xx}$	$-aC_{12}^{xy}$	$-aC_{12}^{xz}$
aC_{22}^{xy} *	aC_{22}^{yy} *	aC_{22}^{yz} *	aC_{12}^{xy}	aC_{12}^{yy}	aC_{12}^{yz}	$-aC_{22}^{xy}$ *	$-aC_{22}^{yy}$ *	$-aC_{22}^{yz}$ *	$-aC_{12}^{xy}$	$-aC_{12}^{yy}$	$-aC_{12}^{yz}$
aC_{22}^{xz} *	aC_{22}^{yz} *	aC_{22}^{zz} *	aC_{12}^{xz}	aC_{12}^{yz}	aC_{12}^{zz}	$-aC_{22}^{xz}$ *	$-aC_{22}^{yz}$ *	$-aC_{22}^{zz}$ *	$-aC_{12}^{xz}$	$-aC_{12}^{yz}$	$-aC_{12}^{zz}$
$-aC_{11}^{xx}$	$-aC_{11}^{xy}$	$-aC_{11}^{xz}$	$-aC_{21}^{xx}$	$-aC_{21}^{xy}$	$-aC_{21}^{xz}$	aC_{11}^{xx}	aC_{11}^{xy}	aC_{11}^{xz}	aC_{21}^{xx}	aC_{21}^{xy}	aC_{21}^{xz}
$-aC_{11}^{xy}$	$-aC_{11}^{yy}$	$-aC_{11}^{yz}$	$-aC_{21}^{xy}$	$-aC_{21}^{yy}$	$-aC_{21}^{yz}$	aC_{11}^{xy}	aC_{11}^{yy}	aC_{11}^{yz}	aC_{21}^{xy}	aC_{21}^{yy}	aC_{21}^{yz}
$-aC_{11}^{xz}$	$-aC_{11}^{yz}$	$-aC_{11}^{zz}$	$-aC_{21}^{xz}$	$-aC_{21}^{yz}$	$-aC_{21}^{zz}$	aC_{11}^{xz}	aC_{11}^{yz}	aC_{11}^{zz}	aC_{21}^{xz}	aC_{21}^{yz}	aC_{21}^{zz}
$-aC_{22}^{xx}$ *	$-aC_{22}^{xy}$ *	$-aC_{22}^{xz}$ *	$-aC_{12}^{xx}$	$-aC_{12}^{xy}$	$-aC_{12}^{xz}$	aC_{22}^{xx} *	aC_{22}^{xy} *	aC_{22}^{xz} *	aC_{12}^{xx}	aC_{12}^{xy}	aC_{12}^{xz}
$-aC_{22}^{xy}$ *	$-aC_{22}^{yy}$ *	$-aC_{22}^{yz}$ *	$-aC_{12}^{xy}$	$-aC_{12}^{yy}$	$-aC_{12}^{yz}$	aC_{22}^{xy} *	aC_{22}^{yy} *	aC_{22}^{yz} *	aC_{12}^{xy}	aC_{12}^{yy}	aC_{12}^{yz}
$-aC_{22}^{xz}$ *	$-aC_{22}^{yz}$ *	$-aC_{22}^{zz}$ *	$-aC_{12}^{xz}$	$-aC_{12}^{yz}$	$-aC_{12}^{zz}$	aC_{22}^{xz} *	aC_{22}^{yz} *	aC_{22}^{zz} *	aC_{12}^{xz}	aC_{12}^{yz}	aC_{12}^{zz}

DET (2)

6. Numerical Formulae for Calculating the Coefficients

The results quoted in this section are taken from Kellermann's paper with the appropriate modifications for the diamond lattice.

The cell vectors for the diamond lattice are

$$\begin{aligned} \vec{a}_1 &= r_0(0,1,1) & \vec{r}_{2,1} &= -\vec{r}_{1,2} = (r_0/2)(1,1,1) \\ \vec{a}_2 &= r_0(1,0,1) & v_a &= 2r_0^3 & (2.25) \\ \vec{a}_3 &= r_0(1,1,0) \end{aligned}$$

The lattice vector $\vec{r}_I(l)$ is therefore of the form

$$\vec{r}_I(l) = r_0(l_1+l_3, l_3+l_1, l_1+l_2) = r_0(l_x, l_y, l_z) \quad \sum l_x = 2N$$

$$\vec{r}_{II}^*(l) = r_0(l_1+l_3+1/2, l_3+l_1+1/2, l_1+l_2+1/2) = r_0(m_x, m_y, m_z) \quad \sum m_z = 2N+3/2$$

The reciprocal vectors are given by

$$\begin{aligned}\vec{b}_1 &= (1/2r_0)(-1,1,1) \\ \vec{b}_2 &= (1/2r_0)(1,-1,1) \\ \vec{b}_3 &= (1/2r_0)(1,1,-1)\end{aligned}\tag{2.26}$$

so that a vector in the reciprocal lattice is given by

$$\begin{aligned}\vec{b}_h &= (1/2r_0)(h_2+h_3-h_1, h_3+h_1-h_2, h_1+h_2-h_3) \\ &= (1/2r_0)(h_x, h_y, h_z) \quad h_x, h_y, h_z \text{ all odd or all even}\end{aligned}\tag{2.27}$$

Now

$$\begin{aligned}\vec{d} &= q_1\vec{b}_1 + q_2\vec{b}_2 + q_3\vec{b}_3 \\ &= (1/2r_0)(q_2+q_3-q_1, q_3+q_1-q_2, q_1+q_2-q_3) \\ &= (1/2r_0)(q_x, q_y, q_z)\end{aligned}\tag{2.28}$$

We now put $C_{xy}(11)$ and $C_{xy}(12)$ in dimensionless form by multiplying them by the factor (v_a/e^2)

So we redefine them as

$$\left. \begin{aligned}C_1^{xy} &= (v_a/e^2)C_{xy}(11) \\ C_2^{xy} &= (v_a/e^2)C_{xy}(12)\end{aligned}\right\}\tag{2.29}$$

We now quote Kellermann's formulae for the Coulomb coefficients (with modifications for the Diamond lattice).

$$\left. \begin{aligned} C_1^{xy} &= G_{xy}^{11} - \frac{H_{xy}}{l^{xy}} - \frac{8}{3\sqrt{\pi}} \epsilon^3 \delta_{xy} \\ C_2^{xy} &= G_{xy}^{12} - \frac{H_{xy}}{m} \end{aligned} \right\} \quad (2.30)$$

$$\left. \begin{aligned} G_{xy}^{11} &= 4\pi \sum_{\vec{h}} \frac{(h_x + q_x)(h_y + q_y)}{(\vec{h} + \vec{q})^2} \exp\left[-\frac{\pi^2}{4\epsilon^2} (\vec{h} + \vec{q})^2\right] \\ G_{xy}^{12} &= 4\pi \sum_{\vec{h}} \frac{(h_x + q_x)(h_y + q_y)}{(\vec{h} + \vec{q})^2} \exp\left[-\frac{\pi^2}{4\epsilon^2} (\vec{h} + \vec{q})^2\right] \exp\left[i\pi(h_x + h_y + h_z)\right] \\ H_{l^{xy}} &= 2 \sum_{\vec{l}} \left[-f(l) \delta_{xy} + g(l) \frac{l_x l_y}{l^2} \right] \exp(i\pi \vec{q} \cdot \vec{l}) \quad (\vec{l} = 0 \text{ excluded}) \end{aligned} \right\} \quad (2.31)$$

$$f(l) = \frac{2}{\sqrt{\pi}} \epsilon \frac{\exp(-\epsilon^2 l^2)}{l^2} + \frac{\psi(\epsilon l)}{l^3}$$

$$g(l) = \frac{4}{\sqrt{\pi}} \epsilon^3 \exp(-\epsilon^2 l^2) + \frac{6}{\sqrt{\pi}} \epsilon \frac{\exp(-\epsilon^2 l^2)}{l^2} + \frac{3\psi(\epsilon l)}{l^3}$$

$$\psi(\epsilon l) = 1 - \frac{2}{\sqrt{\pi}} \int_0^{\epsilon l} \exp(-\xi^2) d\xi$$

$$l = |\vec{l}| = \sqrt{l_x^2 + l_y^2 + l_z^2}$$

These equations only hold for $\vec{q} \neq (0,0,0)$. The arbitrary parameter ϵ can be chosen such that the two series $\sum_{\vec{h}}$ and $\sum_{\vec{l}}$ converge rapidly.

CHAPTER III

THE DISPERSION EQUATIONS FOR SPECIAL DIRECTIONS

1. The Secular Equation for Special Directions

Our starting point is the system of 12 linear equations, obtained in the last section (see SYSTEM (1) page 33).

We shall work out the case (100) Transverse. In this instance

$$q_x = q \quad q_y = q_z = 0$$

$$\text{consequently } C_1 = c \quad C_2 = C_3 = 1$$

$$S_1 = s \quad S_2 = S_3 = 0$$

$$c = \cos \theta \quad s = \sin \theta \quad \theta = qr_0/2$$

The atomic displacements are fixed by symmetry to be perpendicular to a mirror plane, which we take to be $(01\bar{1})$, so that

$$U_x(1) = 0, \quad U_y(1) = U_z(1) = U(1)$$

with similar equations for $\vec{U}(2)$, $\vec{V}(1)$ and $\vec{V}(2)$

SYSTEM (1) now reduces to the set of equations of page 34. These contain two identical sets of 4 equations.

We extract one set to get

SYSTEM (2)

$$m \omega^2 U(1) = (aC_1 + k + D_0 + F_0)U(1) + (aC_2 + D)U(2) + (-aC_1 - k)V(1) + (-aC_2 + F)V(2)$$

$$m \omega^2 U(2) = (aC_2^* + D^*)U(1) + (aC_1 + k + D_0 + F_0)U(2) + (-aC_2^* + F^*)V(1) + (-aC_1 - k)V(2)$$

$$m' \omega^2 V(1) = (-aC_1 - k)U(1) + (-aC_2 + F)U(2) + (aC_1 + k + S_0 + F_0)V(1) + (aC_2 + S)V(2)$$

$$m' \omega^2 V(2) = (-aC_2^* + F^*)U(1) + (-aC_1 - k)U(2) + (aC_2^* + S^*)V(1) + (aC_1 + k + S_0 + F_0)V(2)$$

where $D = -D_0 (\cos \theta - i\gamma_D \sin \theta)$ with similar expressions for F and S with $\theta = qr_0/2$ (see Cochran (14)). We have included the corresponding Coulomb terms $C_1 = C_1^{xx} + C_1^{xy}$ and $C_2 = C_2^{xx} + C_2^{xy}$. In general $D = -D_0 G_D$, with analogous expressions for F and S . We list C_1 and G_D for the (100) and (111) directions.

$$(100)L \quad C_1 = C_1^{xx} \quad G_D = c$$

$$(100)T \quad C_1 = C_1^{xx} + C_1^{xy} \quad G_D = c - i\gamma_D s$$

$$(111)L \quad C_1 = C_1^{xx} + 2C_1^{xy} \quad G_D = (c^3 - 2\gamma_D s^2 c) + i(s^3 - 2\gamma_D c^2 s)$$

$$(111)T \quad C_1 = C_1^{xx} - C_1^{xy} \quad G_D = (c^3 + \gamma_D s^2 c) + i(s^3 + \gamma_D c^2 s)$$

	$U_x(1)$	$U_y(1)$	$U_z(1)$	$U_x(2)$	$U_y(2)$	$U_z(2)$	$V_x(1)$	$V_y(1)$	$V_z(1)$	$V_x(2)$	$V_y(2)$	$V_z(2)$
$m \omega^2 U_x(1) =$	$k+D_0+F_0$			$-D_0 a_1$	$D_0 \gamma_D a_2$	$D_0 \gamma_D a_3$	$-k$			$-F_0 a_1$	$F_0 \gamma_F a_2$	$F_0 \gamma_F a_3$
$m \omega^2 U_y(1) =$		$k+D_0+F_0$		$D_0 \gamma_D a_2$	$-D_0 a_1$	$D_0 \gamma_D a_4$		$-k$		$F_0 \gamma_F a_2$	$-F_0 a_1$	$F_0 \gamma_F a_4$
$m \omega^2 U_z(1) =$			$k+D_0+F_0$	$D_0 \gamma_D a_3$	$D_0 \gamma_D a_4$	$-D_0 a_1$			$-k$	$F_0 \gamma_F a_3$	$F_0 \gamma_F a_4$	$-F_0 a_1$
$m \omega^2 U_x(2) =$	$-D_0 a_1$	$D_0 \gamma_D a_2$	$D_0 \gamma_D a_3$	$k+D_0+F_0$			$-F_0 a_1$	$F_0 \gamma_F a_2$	$F_0 \gamma_F a_3$	$-k$		
$m \omega^2 U_y(2) =$	$D_0 \gamma_D a_2$	$-D_0 a_1$	$D_0 \gamma_D a_4$	$k+D_0+F_0$			$F_0 \gamma_F a_2$	$-F_0 a_1$	$F_0 \gamma_F a_4$		$-k$	
$m \omega^2 U_z(2) =$	$D_0 \gamma_D a_3$	$D_0 \gamma_D a_4$	$-D_0 a_1$				$F_0 \gamma_F a_3$	$F_0 \gamma_F a_4$	$-F_0 a_1$			$-k$
$m' \omega^2 V_x(1) =$	$-k$			$-F_0 a_1$	$F_0 \gamma_F a_2$	$F_0 \gamma_F a_3$	$k+F_0+S_0$			$-S_0 a_1$	$S_0 \gamma_S a_2$	$S_0 \gamma_S a_3$
$m' \omega^2 V_y(1) =$		$-k$		$F_0 \gamma_F a_2$	$-F_0 a_1$	$F_0 \gamma_F a_4$		$k+F_0+S_0$		$S_0 \gamma_S a_2$	$-S_0 a_1$	$S_0 \gamma_S a_4$
$m' \omega^2 V_z(1) =$			$-k$	$F_0 \gamma_F a_3$	$F_0 \gamma_F a_4$	$-F_0 a_1$			$k+F_0+S_0$	$S_0 \gamma_S a_3$	$S_0 \gamma_S a_4$	$-S_0 a_1$
$m' \omega^2 V_x(2) =$	$-F_0 a_1$	$F_0 \gamma_F a_2$	$F_0 \gamma_F a_3$	$-k$			$-S_0 a_1$	$S_0 \gamma_S a_2$	$S_0 \gamma_S a_3$	$k+F_0+S_0$		
$m' \omega^2 V_y(2) =$	$F_0 \gamma_F a_2$	$-F_0 a_1$	$F_0 \gamma_F a_4$		$-k$		$S_0 \gamma_S a_2$	$-S_0 a_1$	$S_0 \gamma_S a_4$	$k+F_0+S_0$		
$m' \omega^2 V_z(2) =$	$F_0 \gamma_F a_3$	$F_0 \gamma_F a_4$	$-F_0 a_1$			$-k$	$S_0 \gamma_S a_3$	$S_0 \gamma_S a_4$	$-S_0 a_1$		$k+F_0+S_0$	

	U(1)	U(2)	V(1)	V(2)
$m \omega^2 U(1) =$	$k+D_0+S_0$	0	$-k$	0
$m \omega^2 U(2) =$	0	$k+D_0+S_0$	0	$-F_0 c$
$m \omega^2 V(1) =$	$-D_0 c$	$iD_0 \gamma_{Ds}$	$-F_0 c$	$iF_0 \gamma_{Fs}$
$m \omega^2 V(2) =$	$-iD_0 \gamma_{Ds}$	0	$iF_0 \gamma_{Fs}$	0
$m' \omega^2 V(1) =$	$-k$	0	$k+S_0+F_0$	0
$m' \omega^2 V(2) =$	0	$-k$	0	$-S_0 c$
$m' \omega^2 U(1) =$	$-F_0 c$	$-iF_0 \gamma_{Fs}$	$-S_0 c$	$iS_0 \gamma_{Ss}$
$m' \omega^2 U(2) =$	$-iF_0 \gamma_{Fs}$	$-F_0 c$	$-iS_0 \gamma_{Ss}$	0

SYSTEM (1) for (100)T

Now SYSTEM (2) has a non-trivial solution if the corresponding determinant vanishes. Putting $m' = 0$ we get

$$\begin{vmatrix} aC_1+k+D_0+F_0-\lambda & aC_2+D_0G_D & -aC_1-k & -aC_2-F_0G_T \\ aC_2^*+D_0G_D^* & aC_1+k+D_0+F_0-\lambda & -aC_2^*-F_0G_T^* & -aC_1-k \\ -aC_1-k & -aC_2-F_0G_T & aC_1+k+S_0+F_0 & aC_2+S_0G_S \\ -aC_2^*-F_0G_T^* & -aC_1-k & aC_2^*-S_0G_S^* & aC_1+k+S_0+F_0 \end{vmatrix} = 0 \quad (3.1)$$

Determinant (3.1) is not in a very convenient form (we shall see why in the next section). So we make the following transformations.

Add the 3^d and 4th columns to the 1st and 2nd columns respectively, add the 3^d and 4th rows to the 1st and 2nd rows respectively.

Let $R_0 = D_0 + 2F_0 + S_0$ and $T_0 = F_0 + S_0$, we get

$$\begin{vmatrix} R_0-\lambda & -R_0G_R & T_0 & -T_0G_T \\ -R_0G_R^* & R_0-\lambda & -T_0G_T^* & T_0 \\ T_0 & -T_0G_T & aC_1+k+S_0+F_0 & aC_2-S_0G_S \\ -T_0G_T^* & T_0 & aC_2^*-S_0G_S^* & aC_1+k+S_0+F_0 \end{vmatrix} = 0 \quad (3.2)$$

Equation (3.2) contains one redundant parameter. To eliminate it we multiply row 1 and 2 by $1/T_0$, multiply column 1 and 2 by $1/T_0$ and define $B_1 = T_0^2/(k+F_0)$, $B_2 = S_0/(k+F_0)$, $\beta = a/(k+F_0)$ we get

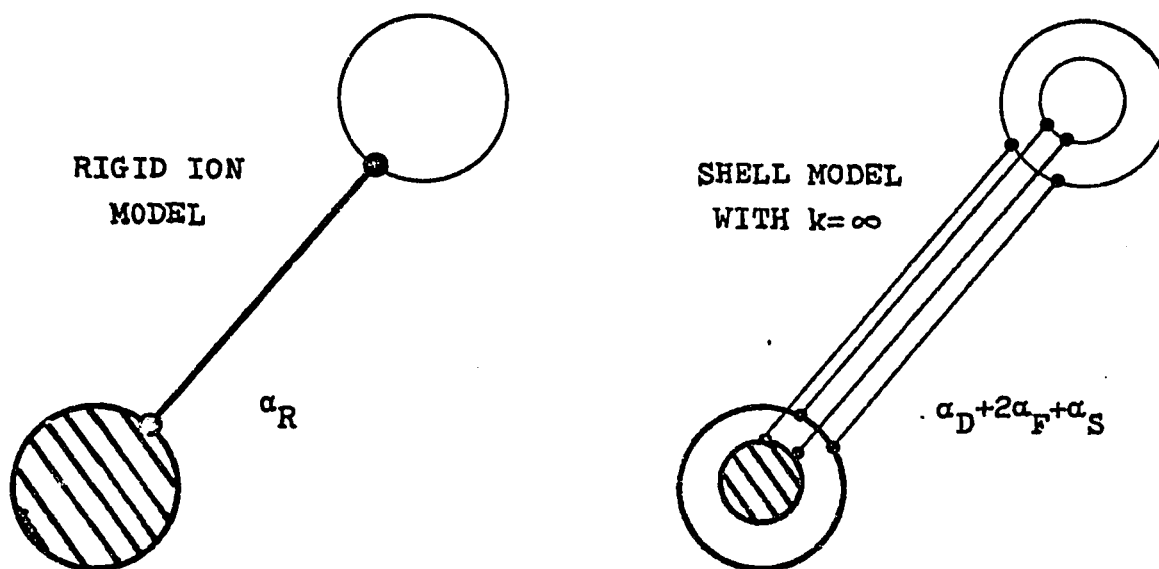
$$\begin{vmatrix}
 R_o - \lambda & -R_o G_R & 1 & -G_T \\
 -R_o G_R^* & R_o - \lambda & -G_T^* & 1 \\
 1 & -G_T & (C_1 + 1 + B_2)/B_1 & (G_2 - B_2 G)/B_1 \\
 -G_T^* & 1 & (G_2^* - B_2 G^*)/B_1 & (C_1 + 1 + B_2)/B_1
 \end{vmatrix} = 0 \quad (3.3)$$

Equation (3.3) now contains 7 parameters (R_o , B_1 , B_2 , β , γ_R , γ_S , γ_T).

2. Reduction to the Rigid Ion Model for $k = \infty$

Since k denotes the force constant between a core and its shell, the case $k = \infty$ represents a rigid ion. If we denote the corresponding force constants by α_R and α'_R then

$$\alpha_R = \alpha_D + 2\alpha_F + \alpha_S, \quad \alpha'_R = \alpha'_D + 2\alpha'_F + \alpha'_S$$



When we use R_o and R'_o instead of α_R and α'_R we get

$$R_o = D_o + 2F_o + S_o, \quad R'_o = D'_o + 2F'_o + S'_o$$

Since $\gamma_R = R'_o/R_o$ by definition we get

$$\gamma_R = \frac{D'_o + 2F'_o + S'_o}{D_o + 2F_o + S_o}$$

We now substitute $k=\infty$ into determinant (3.1). Since $B_1 = T_0^2/(k+F_0)$, $B_2 = S_0/(k+F_0)$ and $\beta = a/(k+F_0)$ by definition we get $B_1 = B_2 = \beta = 0$ when $k=\infty$. So determinant (3.1) becomes

$$\begin{vmatrix} R_0 - \lambda & -R_0 G_R & 1 & G_T \\ -R_0 G_R^* & R_0 - \lambda & G_T^* & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{vmatrix} = 0$$

Expanding we get

$$\begin{vmatrix} R_0 - \lambda & -R_0 G_R \\ -R_0 G_R^* & R_0 - \lambda \end{vmatrix} = 0$$

$$\text{i.e. } (R_0 - \lambda)^2 - R_0^2 G G^* = 0$$

$$\text{i.e. } m \omega^2 = R_0 \pm |R|$$

As expected we have obtained the dispersion equation for the rigid ion model where R_0 , R'_0 and γ_R are the corresponding rigid ion parameters.

3. Derivation of the Result $m \omega^2 = A_0 \pm |A|$

In this section we present the derivation of the dispersion curves. We use the determinant (3.3) as our starting point. Multiply rows 3 and 4 by B_1 , let $U = (1+B_2+\beta C_1)$ and $V = (\beta C_2 - B_2 G_S)$.

We get

$$\begin{vmatrix} R_0 - \lambda & -R_0 G_R & 1 & -G_T \\ -R_0 G_R^* & R_0 - \lambda & -G_T^* & 1 \\ B_1 & -B_1 G_T & U & V \\ -B_1 G_T^* & B_1 & V^* & U \end{vmatrix} = 0 \quad (3.4)$$

By means of row and column manipulations we shall reduce this 4x4 determinant to a 2x2 determinant. Divide rows 3 and 4 by U , subtract row 3 from row 1 and row 4 from row 2. We get

$$\begin{vmatrix} R_0 - \lambda - B_1/U & -R_0 G_R + B_1 G_T/U & 0 & -(G_T + V/U) \\ -R_0 G_R^* + B_1 G_T^*/U & R_0 - \lambda - B_1/U & -(G_T^* + V^*/U) & 0 \\ B_1/U & -B_1 G_T/U & 1 & V/U \\ -B_1 G_T^*/U & B_1/U & V^*/U & 1 \end{vmatrix} = 0 \quad (3.5)$$

In this way we produce zeros in desired locations.

Now multiply row 4 by $-V/U$ and add to row 3, multiply row 3 by $-UV^*$, then divide by $\alpha = U^2 - VV^*$, add row 3 to row 4 to get

$$\begin{vmatrix} R_0 - \lambda - B_1/U & -R_0 G_R + B_1 G_T/U & 0 & -(G_T + V/U) \\ -R_0 G_R^* + B_1 G_T^*/U & R_0 - \lambda - B_1/U & -(G_T^* + V^*/U) & 0 \\ B_1(U + G_T^*V)/\alpha & -B_1(G_T U + V)/\alpha & 1 & 0 \\ -B_1(G_T^*U + V^*)/\alpha & B_1(U + G_T V^*)/\alpha & 0 & 1 \end{vmatrix} = 0 \quad (3.6)$$

Now multiply row 3 by $G^* + V^*/U$, then add it to row 2, multiply row 4 by $G + V/U$, then add it to row 1.

$$\begin{vmatrix} R_0 - \lambda - B_1[U(1 + G_T G_T^*) + G_T V^* + G_T^* V]/\alpha & -R_0 G_R + B_1[2G_T U + V + V^* G_T^2]/\alpha & 0 & 0 \\ -R_0 G_R^* + B_1[2G_T^* U + V^* + V G_T^2]/\alpha & R_0 - \lambda - B_1[U(1 + G_T G_T^*) + G V^* + V^* G_T]/\alpha & 0 & 0 \\ B_1(U + G_T^* V)/\alpha & -B_1(G_T U + V)/\alpha & 1 & 0 \\ -B_1(G_T^* U + V^*)/\alpha & B_1(U + G_T V^*)/\alpha & 0 & 1 \end{vmatrix} = 0 \quad (3.7)$$

Expanding determinant (3.7) we get

$$\begin{vmatrix} R_0 - \lambda - B_1[U(1 + G_T G_T^*) + G_T V^* + G_T^* V]/\alpha & -R_0 G_R + B_1[2G_T U + V + V^* G_T^2]/\alpha \\ -R_0 G_R^* + B_1[2G_T^* U + V^* + V G_T^2]/\alpha & R_0 - \lambda - B_1[U(1 + G_T G_T^*) + G V^* + V^* G_T]/\alpha \end{vmatrix} = 0 \quad (3.8)$$

Determinant (3.8) is of the form

$$\begin{vmatrix} A_0 - \lambda & A \\ A^* & A_0 - \lambda \end{vmatrix} = 0 \quad (3.9)$$

where

$$A_o = R_o - B_1 [U(1+G_T G_T^*) + V^* G_T + V G_T^*] / \alpha$$

$$A = -R_o G_R + B_1 [2U G_T + V + V^* G_T^2] / \alpha$$

Rewriting in terms of the original quantities

$$A_o = R_o - B_1 \left[\frac{(1+B_2+\beta C_1)(1+G_T G_T^*) + (\beta C_2^* - B_2 G_T^*) G_T + (\beta C_2 - B_2 G_T) G_T^*}{(1+B_2+\beta C_1)^2 - (\beta C_2 - B_2 G_S)(\beta C_2^* - B_2 G_S^*)} \right] \quad (3.10)$$

$$A = -R_o G_R + B_1 \left[\frac{2(1+B_2+\beta C_1) G_T + (\beta C_2 - B_2 G_T) + (\beta C_2^* - B_2 G_T^*) G_T^2}{(1+B_2+\beta C_1)^2 - (\beta C_2 - B_2 G_S)(\beta C_2^* - B_2 G_S^*)} \right] \quad (3.11)$$

$$m \omega^2 = A_o \pm |A| \quad (3.12)$$

the + sign referring to optic modes and
the - sign referring to acoustic modes.

CHAPTER IV

ANOLOGOUS DISCUSSION FOR THE SECULAR DETERMINANT

Chapter III sets the pattern for the discussion of the 12x12 determinant, so our first section is called

1. Transformation of the 12x12 Determinant

We start with DET(1) from page 20. and 27.

Firstly we add the 7th column to the 1st column,
8th column to the 2nd column,
9th column to the 3rd column,
.....
12th column to the 6th column.

Secondly we add the 7th row to the 1st row,
.....
12th row to the 6th row.

Again let $R_0 = D_0 + 2F_0 + S_0$, $T_0 = F_0 + S_0$.

We get DET(2) shown on page 43. and 44.

Now we want to eliminate the redundant parameter, so multiply rows 7 to 12 by $1/T_0$, multiply columns 7 to 12 by $1/T_0$ and again let $B_1 = T_0^2/(k+F_0)$, $B_2 = S_0/(k+F_0)$, $\beta = a/(k+F_0)$.

We get DET(3) shown on page 45. and 46.

$R_{0-\lambda}$	$-R_{0a1}$	R_{0YR^2}	R_{0YR^3}	T_0	$-T_{0a1}$	$T_{0Y\tau^2}$	$T_{0Y\tau^3}$	$T_{0Y\tau^4}$
	R_{0YR^2}	$-R_{0a3}$	R_{0YR^4}	T_0	$T_{0Y\tau^2}$	$-T_{0a1}$	$T_{0Y\tau^4}$	$T_{0Y\tau^4}$
	$R_{0-\lambda}$	R_{0YR^3}	R_{0YR^4}	T_0	$T_{0Y\tau^3}$	$T_{0Y\tau^4}$	$-T_{0a1}$	
$-R_{0a1}^*$	$R_{0YR^2}^*$	$R_{0YR^3}^*$	$R_{0-\lambda}$	$-T_{0a1}^*$	$T_{0Y\tau^2}^*$	$T_{0Y\tau^3}^*$	T_0	
$R_{0YR^2}^*$	$-R_{0a1}^*$	$R_{0YR^4}^*$	$R_{0-\lambda}$	$T_{0Y\tau^2}^*$	$-T_{0a1}^*$	$T_{0Y\tau^4}^*$	T_0	
$R_{0YR^3}^*$	$R_{0YR^4}^*$	$-R_{0a1}^*$	$R_{0-\lambda}$	$T_{0Y\tau^3}^*$	$T_{0Y\tau^4}^*$	$-T_{0a1}^*$	T_0	
T_0	$-T_{0a1}$	$T_{0Y\tau^2}$	$T_{0Y\tau^3}$	$(k+F_0)+S_0$	$-S_{0a1}$	$S_{0Y\tau^2}$	$S_{0Y\tau^3}$	$S_{0Y\tau^4}$
	$T_{0Y\tau^2}$	$-T_{0a1}$	$T_{0Y\tau^4}$	$(k+F_0)+S_0$	$S_{0Y\tau^2}$	$-S_{0a1}$	$S_{0Y\tau^4}$	$-S_{0a1}$
	T_0	$T_{0Y\tau^3}$	$T_{0Y\tau^4}$	$(k+F_0)+S_0$	$(k+F_0)+S_0$	$S_{0Y\tau^3}$	$S_{0Y\tau^4}$	$-S_{0a1}$
$-T_{0a1}^*$	$T_{0Y\tau^2}^*$	$T_{0Y\tau^3}^*$	T_0	$-S_{0a1}^*$	$S_{0Y\tau^2}^*$	$S_{0Y\tau^3}^*$	$(k+F_0)+S_0$	
$T_{0Y\tau^2}^*$	$-T_{0a1}^*$	$T_{0Y\tau^4}^*$	T_0	$S_{0Y\tau^2}^*$	$-S_{0a1}^*$	$S_{0Y\tau^4}^*$	$(k+F_0)+S_0$	
$T_{0Y\tau^3}^*$	$T_{0Y\tau^4}^*$	$-T_{0a1}^*$	T_0	$S_{0Y\tau^3}^*$	$S_{0Y\tau^4}^*$	$-S_{0a1}^*$	$(k+F_0)+S_0$	

$R_{O-\lambda}$	$-R_{Oa1}$	R_{OYa2}	R_{OYa3}	1	$-a_1$	γ_{Ta2}	γ_{Ta3}	γ_{Ta2}	γ_{Ta3}
$R_{O-\lambda}$	R_{OYa2}	$-R_{Oa1}$	R_{OYa4}	1	γ_{Ta2}	$-a_1$	γ_{Ta4}	$-a_1$	γ_{Ta4}
$R_{O-\lambda}$	R_{OYa3}	R_{OYa4}	$-R_{Oa1}$	1	γ_{Ta3}	γ_{Ta4}	$-a_1$	γ_{Ta3}	$-a_1$
$-R_{Oa1}^*$	R_{OYa2}^*	R_{OYa3}^*	$R_{O-\lambda}$	$-a_1^*$	γ_{Ta2}^*	1	γ_{Ta3}^*	1	
R_{OYa2}^*	$-R_{Oa1}^*$	R_{OYa4}^*	$R_{O-\lambda}$	γ_{Ta2}^*	$-a_1^*$	γ_{Ta4}^*	1	1	
R_{OYa3}^*	R_{OYa4}^*	$-R_{Oa1}^*$	$R_{O-\lambda}$	γ_{Ta3}^*	γ_{Ta4}^*	$-a_1^*$		1	
1	$-a_1$	γ_{Ta2}	γ_{Ta3}	$(1+B_2)/B_1$	ba_1	$b\gamma_{Sa2}$	$b\gamma_{Sa3}$	$b\gamma_{Sa2}$	$b\gamma_{Sa3}$
	γ_{Ta2}	$-a_1$	γ_{Ta4}	$(1+B_2)/B_1$	$b\gamma_{Sa2}$	ba_1	$b\gamma_{Sa4}$	ba_1	$b\gamma_{Sa4}$
	γ_{Ta3}	γ_{Ta4}	$-a_1$	$(1+B_2)/B_1$	$(1+B_2)/B_1$	$b\gamma_{Sa3}$	$b\gamma_{Sa4}$	ba_1	ba_1
$-a_1^*$	γ_{Ta2}^*	γ_{Ta3}^*	1	ba_1	$b\gamma_{Sa2}^*$	$b\gamma_{Sa3}^*$	$(1+B_2)/B_1$		
γ_{Ta2}^*	$-a_1^*$	γ_{Ta4}^*	1	$b\gamma_{Sa2}^*$	ba_1^*	$b\gamma_{Sa4}^*$	$(1+B_2)/B_1$		
γ_{Ta3}^*	γ_{Ta4}^*	$-a_1^*$	1	$b\gamma_{Sa3}^*$	$b\gamma_{Sa4}^*$	ba_1^*	$(1+B_2)/B_1$		

where $b = B_2/B_1$

2. Reduction to the Rigid Ion Model

When $k = \infty$ DET(3) reduces to DET(4) shown on page 48. Expanding DET(4) (starting along row 12 and working our way up to row 7) we reduce it to the 6x6 portion of the top left hand corner. This 6x6 determinant is identical to the one derived for the core-core interaction (see equation of page 17) when we replace D_0 and D'_0 by R_0 and R'_0 respectively. This equation was derived by temporarily removing the shells from our discussion, i.e. it is the secular equation for the rigid ion model.

3. Summary of the Derivations

The determinant DET(1) of page 20 and 27 is of the form

$$\begin{vmatrix} D + C - \lambda I & F - C \\ F - C & S + C \end{vmatrix} = 0 \quad (4.1)$$

where the quantities D, F, S, C and I are 6×6 arrays.

For example D is defined by the top left hand corner of DET(1) page 20 and C is defined by the top left hand corner of DET(1) page 27.

We now write (in matrix form) the system of linear equations corresponding to equation (4.1). We get

$$\omega^2 \begin{pmatrix} m & O \\ O & O \end{pmatrix} \begin{pmatrix} -U \\ V \end{pmatrix} = \begin{pmatrix} D + C & F - C \\ F - C & S + C \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix} \quad (4.2)$$

where O represents a 6×6 array of zeros,

m is a 6×6 diagonal matrix with each diagonal element equal to m ,

U is a 6 element column vector, the corresponding row vector being given by

$$U = [U_x(1), U_y(1), U_z(1), U_x(2), U_y(2), U_z(2)]$$

V is defined in a similar fashion.

Remembering that equation (4.2) represents a system of linear equations, we note that the following rules are valid for the associated matrix equation: 1) rows can be added to rows, 2) columns can be added to columns.

Adding the bottom row to the top row in both sides of equation (4.2) we get

$$\omega^2 \begin{pmatrix} m & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix} = \begin{pmatrix} D+F & F+S \\ F-C & S+C \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix} \quad (4.3)$$

Adding the second column to the first column in both sides of equation (4.3) we get

$$\omega^2 \begin{pmatrix} m & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix} = \begin{pmatrix} D+2F+S & F+S \\ F+S & S+C \end{pmatrix} \begin{pmatrix} U \\ W \end{pmatrix} \quad (4.4)$$

Let $D + 2F + S = R$ and $F + S = T$ we get

$$\omega^2 \begin{pmatrix} m & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix} = \begin{pmatrix} R & T \\ T & S+C \end{pmatrix} \begin{pmatrix} U \\ W \end{pmatrix} \quad (4.5)$$

where $W = U - V$

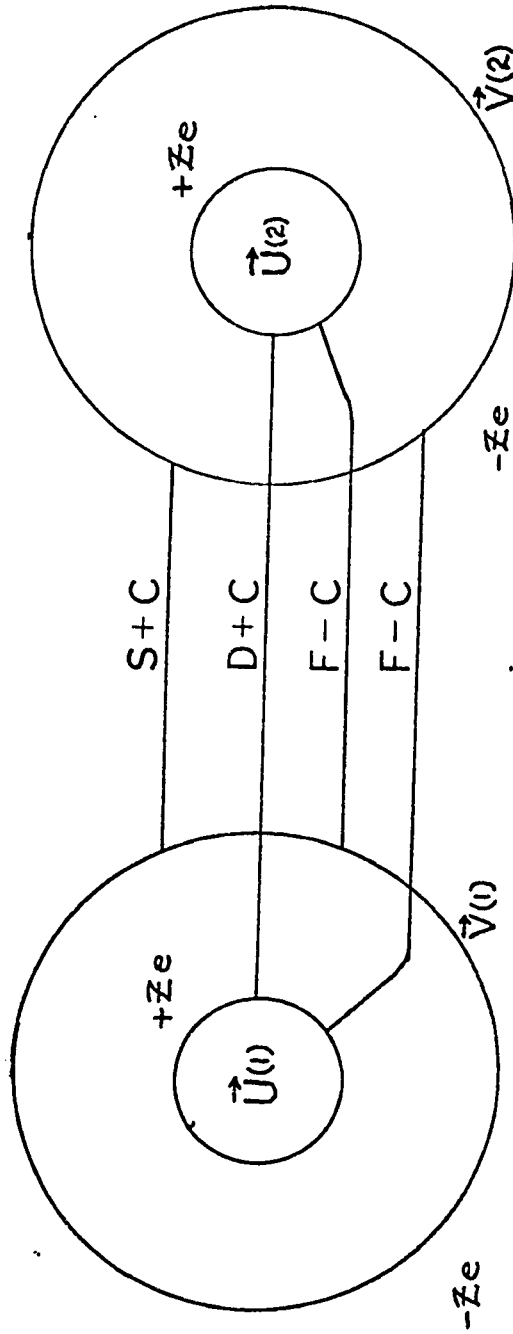


fig.(4.1)

The associated secular equation is

$$\begin{vmatrix} R - \lambda I & T \\ T & S + C \end{vmatrix} = 0 \quad (4.6)$$

We recognize equation (4.6) as being the secular equation DET(2) of page 43 and 44.

Apart from being a useful shorthand these equations help us to visualize the different types of interactions occurring in the lattice.

To illustrate the point we write equation (4.2) in the form

$$\omega^2 m \cdot U = (D + C) U + (F - C) V \quad (4.2a)$$

$$0 = (F - C) U + (S + C) V \quad (4.2b)$$

To obtain these equations we simply carried out the multiplication according to the usual rule of matrix algebra.

We now show how equations (4.2a) and (4.2b) can be visualized with the help of fig.(4.1). For example the mechanical part of the core-core interaction can be written as

$$\omega^2 m U = D U \quad (4.7)$$

Equation (4.7) is equivalent to equations (2.10) to (2.12) of page 16

with

$$U = \begin{pmatrix} \vec{U}(1) \\ \vec{U}(2) \end{pmatrix} \quad (4.8)$$

where $\vec{U}(1)$ and $\vec{U}(2)$ are the amplitudes for the vibrations of the black cores and white cores respectively.

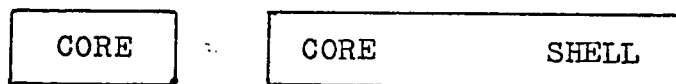
Adding the Coulomb interaction to equation (4.7) we get

$$\omega^2 m U = (D+C) U \quad (4.9)$$

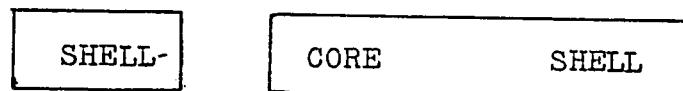
Adding the core-shell interaction terms to equation (4.9) we get

$$\omega^2 m U = (D+C) U + (F-C) V \quad (4.10)$$

Equation (4.10) can be represented as follows



To get the complete picture we need an equation of the type



i.e.

$$\omega^2 m' V = (F-C) U + (S+C) V \quad (4.11)$$

Putting $m' = 0$ in equation (4.11) we get

$$0 = (F - C)U + (S + C)V \quad (4.12)$$

Equations (4.10) and (4.12) are identical to equations (4.2a) and (4.2b).

CHAPTER V

SPECIAL ASPECTS OF THE SHELL MODEL

The purpose of this chapter is to derive certain useful formulae from the dispersion equation for special directions. Before we start we make a few remarks about the notation.

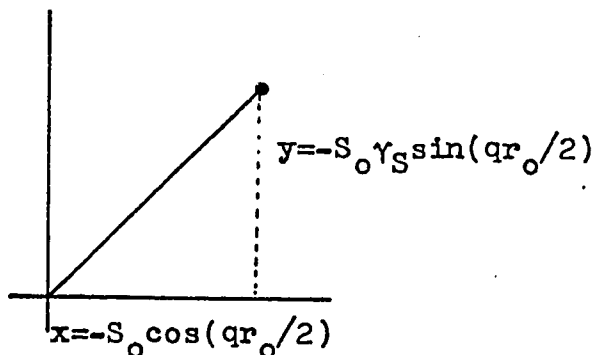
For the special case (100)T the functions R, S and T are given by $R = -R_0 (\cos \theta + i\gamma_R \sin \theta)$ with analogous expressions for S and T and where $\theta = qr_0/2$.

R, S and T are complex numbers, so they can be written either in cartesian or polar form. For example we can write S in two ways as shown below.

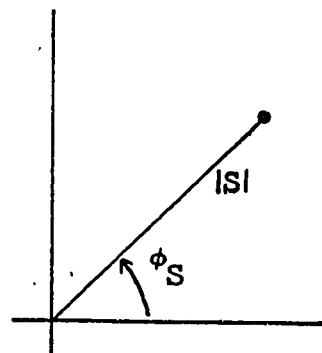
$$z = x + i y$$

$$z = |z| \exp(i\phi)$$

$$S = [-S_0 \cos(qr_0/2)] + i[-S_0 \gamma_S \sin(qr_0/2)] \quad S = |S| \exp(i\phi_S)$$



CARTESIAN FORM



POLAR FORM

1. The Case $q \rightarrow 0$ with $\gamma_R = \gamma_T$

Cochran (14) shows that for $\gamma_R = \gamma_T$ with $q \rightarrow 0$ (for acoustical waves) the dispersion equation for the shell model reduces to that of the rigid ion model.

We write $G_R = |G_R| \exp(i\phi_R)$ with analogous expressions for G_S , G_T and C_2 . Substituting into equation (3.12) and keeping only the terms of 2nd order,

the dispersion equation $m \omega^2 = A_0 - |A|$

reduces to $m \omega^2 = R_0 - |R|$

This means that when $\gamma_R = \gamma_T$ we can use the experimental values for the elastic constants to calculate R_0 and γ_R . (see Appendix A section 2) If $\gamma_R \neq \gamma_T$ this calculation can be used to get a rough estimate for these parameters.

2. The Raman Frequency

At $q = 0$ $G_R = G_S = G_T = 1$ and $C_1 = C_2$.

Substituting into the equations (3.10) and (3.11) we get

$$A_0 = R_0 + B_1 \left[\frac{-2(1+B_2+\beta C_1) - 2(\beta C_1 - B_2)}{(1+B_2+\beta C_1)^2 - (\beta C_1 + B_2)^2} \right]$$

$$A = -R_0 + B_1 \left[\frac{2(1+B_2+\beta C_1) + 2(\beta C_1 - B_2)}{(1+B_2+\beta C_1)^2 - (\beta C_1 + B_2)^2} \right]$$

with $m \omega^2 = A_0 \pm |A|$

Simplifying the expressions for A_0 and A we get

$$A_0 = R_0 - 2B_1/(1+B_2)$$

$$A = -R_0 + 2B_1/(1+B_2)$$

As expected the acoustical frequency is zero and the optical frequency is given by

$$m \omega^2 = 2R_0 - 4B_1/(1+B_2) \quad (5.1) \quad (\text{Raman frequency})$$

Equation (5.1) gives us a useful relationship between B_1 and B_2 once the parameter R_0 is determined.

3. The Zone Boundary Points ($q = q_{\max}$)

For $q = q_{\max}$ we will show that $\phi_C = \phi_R = \phi_S = \phi_T$ even when $\gamma_R \neq \gamma_S \neq \gamma_T$ (but with the restriction $\gamma_R > 1/2$, $\gamma_S > 1/2$ and $\gamma_T > 1/2$).

We shall work out the case (111)L. We have for $q = q_{\max}$

$$R = \left\{ -R_0(1-2\gamma_R)/2\sqrt{2} \right\} (1 + i)$$

$$S = \left\{ -S_0(1-2\gamma_S)/2\sqrt{2} \right\} (1 + i)$$

$$T = \left\{ -T_0(1-2\gamma_T)/2\sqrt{2} \right\} (1 + i)$$

$$C_2 = 10.67 (1 + i)$$

Writing them in the form $R = |R| \exp(i\phi_R)$ when $\gamma_R > 1/2$, $\gamma_S > 1/2$ and $\gamma_T > 1/2$ we get

$$R = \left\{ R_0(2\gamma_R-1)/2\sqrt{2} \right\} \exp(i\pi/4)$$

$$S = \left\{ R_0(2\gamma_S-1)/2\sqrt{2} \right\} \exp(i\pi/4)$$

$$T = \left\{ R_0(2\gamma_T-1)/2\sqrt{2} \right\} \exp(i\pi/4)$$

$$C_2 = 10.20 \exp(i\pi/4)$$

These expressions for R, S, T and C_2 are of the form

$$\text{positive constant} \times \exp(i\pi/4)$$

Therefore $\phi_C = \phi_R = \phi_S = \phi_T = \pi/4$ for this case.

We now list R and C_2 for the cases of interest. We get

MODE	R	C_2
(100)L	0	0
(100)T	$R_0 \gamma_R \exp(i\pi/2)$	$10.67 \exp(i\pi/2)$
(111)L	$\{R_0 (2\gamma_R - 1) / 2 \sqrt{2}\} \exp(i\pi/4)$	$10.20 \exp(i\pi/4)$
(111)T	$\{R_0 (1 + \gamma_R) / 2 \sqrt{2}\} \exp i(5\pi/4)$	$5.10 \exp(i5\pi/4)$

From the case (100)T we see that negative values of γ_R , γ_S or γ_T are excluded if we want to keep the equality

$$\phi_C = \phi_R = \phi_S = \phi_T \text{ for } q = q_{\max}$$

So we let $\phi_C = \phi_R = \phi_S = \phi_T = \phi$ for $q = q_{\max}$ and we write $C_2 = |C_2| \exp(i\phi)$, $G_R = |G_R| \exp(i\phi)$ with similar expressions for G_S and G_T substituting into equations (3.10) and (3.11) we get

$$A_o = R_o - B_1 \left[\frac{(1+B_2+\beta C_1)(1+|G_T|^2) - 2(\beta|C_2|-B_2|G_T|)|G_T|}{(1+B_2+\beta C_1)^2 - (\beta|C_2|+B_2|G_S|)^2} \right]$$

$$A = \left\{ -R_o|G_R| + B_1 \left[\frac{2(1+B_2+\beta C_1)|G_T| + 2(\beta|C_2|-B_2|G_T|)(1+|G_T|^2)}{(1+B_2+\beta C_1)^2 - (\beta|C_2|-B_2|G_S|)^2} \right] \right\} \exp(i\phi)$$

Let $X = (1+B_2+\beta C_1)$ $Y = (\beta|C_2|+B_2|G_S|)$ we get

$$\begin{aligned} A_o \pm |A| &= R_o(1 \pm |G_R|) + B_1 \left[-X(1+|G_T|^2) \pm 2|G_T| + \right. \\ &\quad \left. + Y(2|G_T| \pm 1 \pm |G_T|^2) \right] / X^2 - Y^2 \\ &= R_o(1 \pm |G_R|) - B_1(1 \pm |G_T|)^2 / (X \pm Y) \end{aligned}$$

So that at $q = q_{\max}$

$$m \omega^2 = R_o(1 \pm |G_R|) - \frac{B_1(1 \pm |G_T|)^2}{1 + \beta(C_{1 \pm} |C_2|) + B_2(1 \pm |G_S|)} \quad (5.2)$$

the + sign referring to optic modes and
the - sign referring to acoustic modes.

For (100)T $|G_R| = \gamma_R$, $|G_S| = \gamma_S$ and $|G_T| = \gamma_T$ at

$q = q_{\max}$ for $\gamma_R, \gamma_S, \gamma_T > 0$.

Equation (5.2) now becomes

$$m \omega^2 = R_0 (1 \pm \gamma_R) - \frac{B_1 (1 \pm \gamma_T)^2}{1 + \beta (C_1 \pm |C_2|) + B_2 (1 \pm \gamma_S)}$$

We list $|G_R|$ for all cases of interest.

Mode	$ G_R $ at $q = q_{\max}$
(100)L	0
(100)T	γ_R
(111)L	$(1 - 2\gamma_R)/2$
(111)T	$(1 + \gamma_R)/2$

From the table we see that the modes (100)LA and LO are degenerate at $q = q_{\max}$.

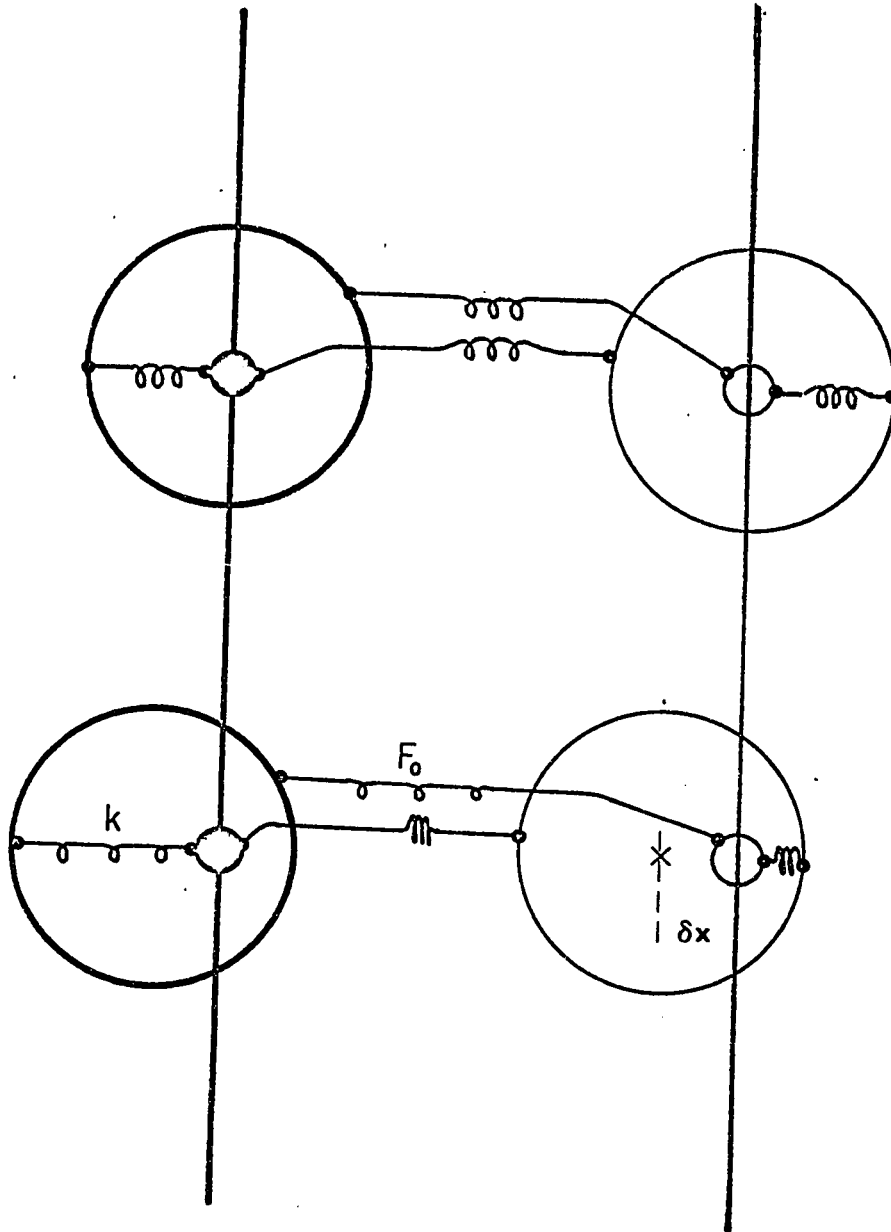


fig.(5.2)

4. The Polarizability

We apply a uniform electric field to the crystal. The dipole moment p of an atom is given by

$$p = Ze \delta x \quad (5.3)$$

To simplify the diagram we have kept the cores fixed. The force F acting on such a core is given by

$$F = Ze E \quad (5.4)$$

The polarizability of an atom is given by

$$\alpha = p/E \quad (5.5)$$

Combining equations (5.3), (5.4) and (5.5) we get

$$\alpha = Z^2 e^2 \delta x / F \quad (5.6)$$

When a uniform field is applied the cores move together and the shells move together i.e. there is no core-core and no core-shell interaction and we can write

$$F = (K + F_0) \delta x \quad (5.7)$$

Combining equations (5.6) and (5.7) we get

$$\alpha = Z^2 e^2 / (K + F_0) \quad (5.8)$$

Let $\beta = \alpha / v_a$ $v_a = \text{vol. of trigonal unit cell}$
(see page 28)

So that
$$\beta = (e^2 / v_a) \frac{Z^2}{K + F_0} \quad (5.9)$$

The polarizability as given by equation (5.9) is related to the dielectric constant ϵ by the Claussius - Mossoti formula (Cochran (14))

$$\beta = \frac{3}{8\pi} \frac{\epsilon - 1}{\epsilon + 1} \quad (5.10)$$

CHAPTER VI

NUMERICAL CALCULATIONS

1. Determination of the Parameters $R_0, B_1, B_2, \beta, \gamma_R, \gamma_S$ and γ_T

Rough values for R_0 and γ_R were used as a starting point. We now describe the procedure.

As our starting point we set $\gamma_R = \gamma_T$. Using the data of table (1) we calculated R_0 and γ_R .

$$\text{equation (A24) yields } R_0 = 15.295 \cdot 10^5 \text{ d/cm.} \quad (6.1)$$

$$\text{equation (A25) yields } \gamma_R = .682 \quad (6.2)$$

$$\text{equation (A26) yields } \gamma_R = .58 \quad (6.3)$$

Using the Neutron Scattering data of Warren et al we get another value of γ_R (curves were drawn through the experimental points and the slopes calculated from the linear portions).

$$\text{equation (A31) yields } \gamma_R = .68 \quad (6.4)$$

Equations (6.2) and (6.4) reflect the compatibility of the

Neutron Scattering data with the elastic constants measured by McSkimin and Bond. Warren (22) reached this conclusion using the linear chain model. Our observation is based on the shell model with $\gamma_R = \gamma_T$ as $q \rightarrow 0$ i.e. the rigid ion model for the diamond lattice.

Equations (6.2) and (6.3) indicate that we must set $\gamma_R \neq \gamma_S$.

We now solve for B_1 in equation (5.1) to get

$$B_1 = \{(2R_0 - m\omega_0^2)/2\}B_2 - (2R_0 - m\omega_0^2)/4 \quad (6.5)$$

Solving for β in equation (5.2) for (100)L we get

$$\beta = \frac{B_1}{C_1(R_0 - m\omega^2)} - \frac{1 + B_2}{C_1} \quad (6.6)$$

As a first approach, different values of B_2 were tried. From equation (6.5) we get B_1 , we then get β from equation (6.6). Substituting these values of B_1 , B_2 and β into equation (5.2) and setting $\gamma_R = \gamma_S = .68$ we get 6 different values for γ_T .

A program was written in which B_2 , γ_R and γ_S were scanned (our IBM 1620 was used). The 6 values of γ_T corresponding to each set were printed. The output was examined to find sets of parameters which gave compatible values for γ_T . Having found several sets we used the following method to improve them.

Substituting B_1 into equation (5.2) and rearranging we get

$$(C_{1\pm}|C_2|)\beta + \left[(1\pm|G_S|) - 1/2 \frac{2R_o - m\omega_o^2}{R_o(1\pm\gamma_R) - m\omega^2} (1\pm|G_T|)^2 \right] B_2 =$$

$$1/4 \frac{2R_o - m\omega_o^2}{R_o(1\pm\gamma_R) - m\omega^2} (1\pm|G_T|)^2 \quad (6.7)$$

Equation (6.7) yields a system of 7 linear equations in β and B_2 .

The values previously obtained for R_o , γ_R , γ_S and γ_T were fed as data for a least square fit determining β and B_2 . B_1 was computed using equation (6.5)

A finer scanning of R_o , γ_R , γ_S and γ_T was made, and the difference between calculated and experimental frequencies were computed. Whenever the mean error δ was below a certain predetermined value, the machine would print δ , the 7 parameters, the 7 calculated frequencies and the ratios of calculated to experimental frequencies. Thousands of values were examined before a reasonably good set was obtained.

The final values for Diamond are given in Table (2) together with the values for germanium obtained by Cochran.

Table 1. Data for DiamondElastic constants ^a

$$c_{11} = 10.76 \times 10^{12} \text{ dynes/cm.}$$

$$c_{12} = 1.25 \times 10^{12} \text{ dynes/cm.}$$

$$c_{44} = 5.758 \times 10^{12} \text{ dynes/cm.}$$

$$\text{Lattice constant } ^b \quad 2r_0 = 3.567 \times 10^{-8} \text{ cm.}$$

$$\text{Raman frequency } ^c \quad \omega_R(\gamma) = 2.509 \times 10^{14} \text{ rad/sec.}$$

$$\text{Dielectric constant } ^d \quad \epsilon = 5.66$$

Table 2. Parameters

	R_0	B_1	B_2	β	γ_R	γ_S	γ_T
germanium	2.9233	4.099	3.2	.105	.6905	.6905	.6905
diamond	15.5	13.668	.982	.094	.68	.16	.96

where R_0 and B_1 are in units of 10^5 dynes/cm.

a) H.J. McSkimin and W.L. Bond, Phys. Rev., 105, 116, (1957)

b) Amer. Inst. Phys. Handbook

c) F.A. Johnson and R. Loudon, Proc. Roy. Soc., A, 281 pp. 274-289, (1964)

d) D.F. Gibbs and G.J. Hill, Phil. Mag. Vol. 9, p. 367, (1964)

FREQUENCY ω (in units of 10^{14} rad/sec)
versus REDUCED WAVE VECTOR q/q_{\max} (dimensionless)

(100) DIRECTION

q/q_{\max}	ω_{LA}	ω_{LO}	ω_{TA}	ω_{TO}
0	.00	2.50	.00	2.50
.2	.61	2.50	.39	2.46
.4	1.17	2.46	.77	2.38
.6	1.64	2.40	1.12	2.26
.8	1.99	2.33	1.42	2.12
1.0	2.21	2.21	1.57	2.02

(111) DIRECTION

q/q_{\max}	ω_{LA}	ω_{LO}	ω_{TA}	ω_{TO}
0	.00	2.50	.00	2.50
1/3	.93	2.51	.51	2.44
2/3	1.74	2.47	.93	2.30
1	2.27	2.28	1.11	2.23

Dispersion Curve data for diamond.

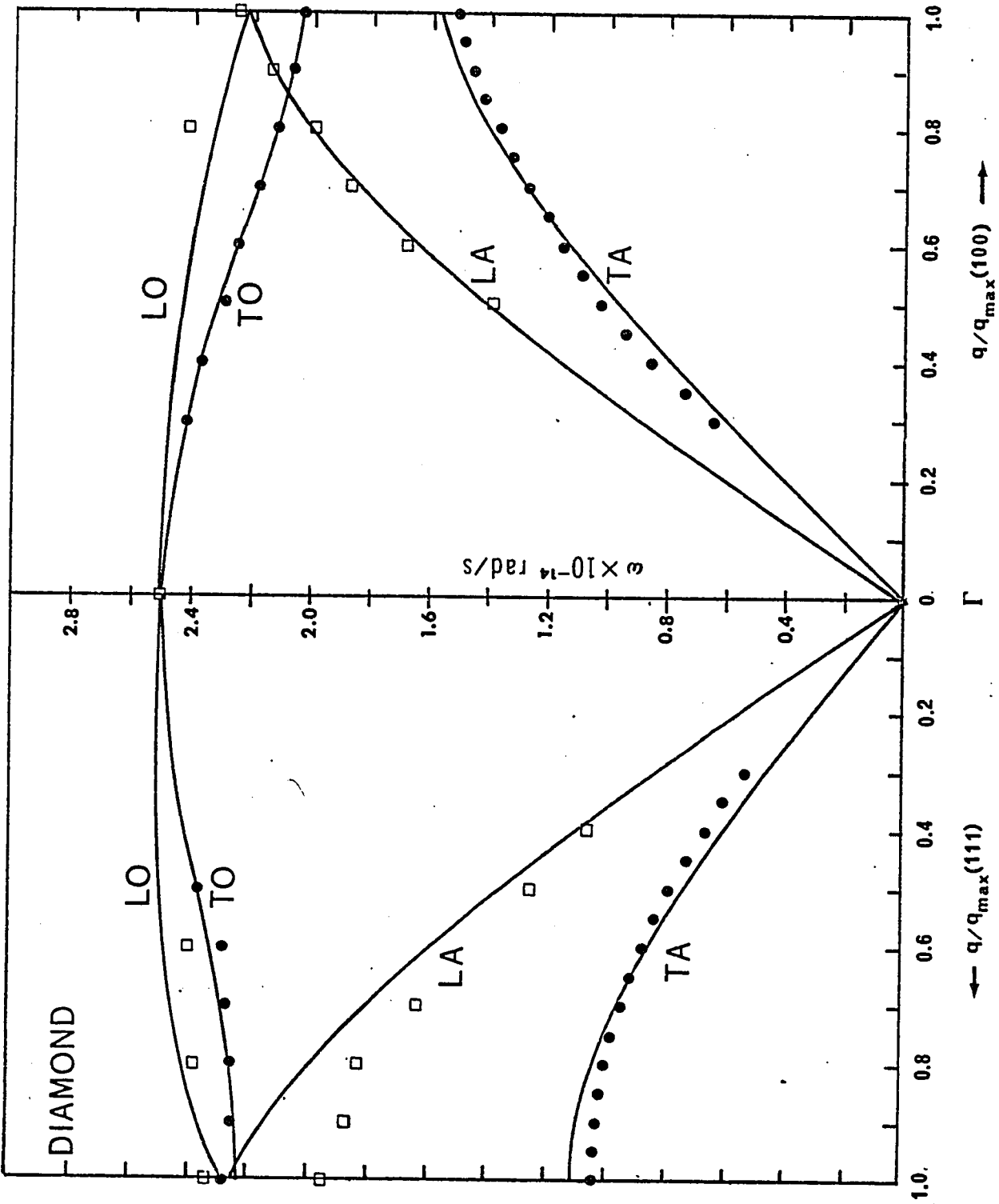


fig.(6.1)

2. Obtaining the Vibration Spectra and $\Theta_D(T)$

The following method was used to find $g(\nu)$ for germanium and diamond. The reciprocal space (f.c.c.lattice) was divided into miniature cells with axes one-fortieth of the length of the reciprocal lattice cell. Vibration frequencies were calculated from the roots of the secular determinant for $1686 - 1 = 1685$ wave vectors in the $1/48$ of the first Brillouin zone.

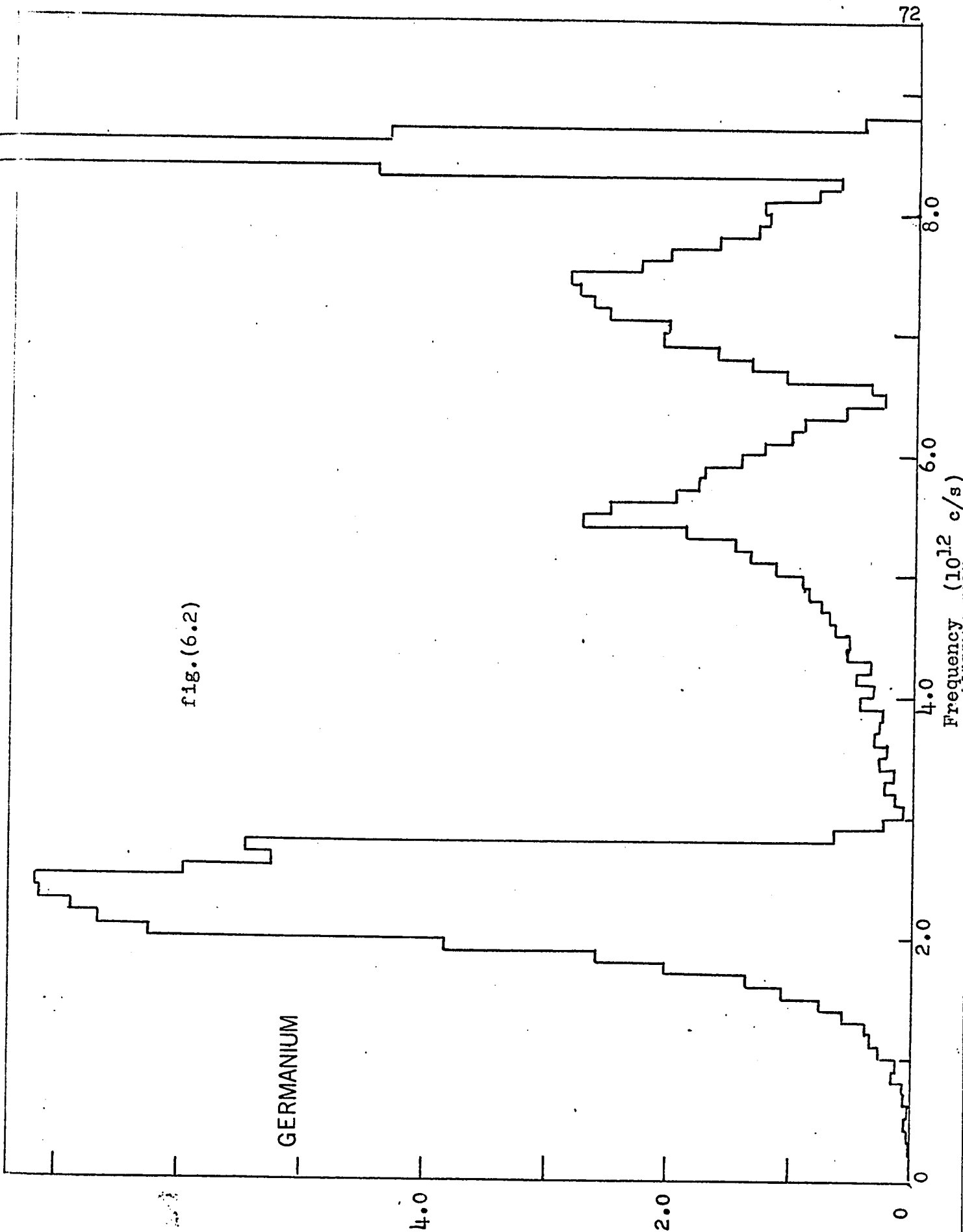
The point $\vec{q} = (0,0,0)$ was left out because of equations (2.31) page 30. Each point is weighted according to the number of points equivalent to it by symmetry. The total number of points in the whole zone was thus $40^3 - 1 = 63999$, and that of the frequencies $192000 - 6 = 191994$. The vibration spectra were then constructed using Blackman's sampling technique.

The specific heat at constant volume is given by

$$C_v = 3 R \int_0^{\nu_m} \frac{x^2 e^x}{(e^x - 1)^2} g(\nu) d\nu \quad \text{where } x = h\nu/kT$$

$$\int_0^{\nu_m} g(\nu) d\nu = 1$$

The equivalent Debye temperature Θ_D was calculated from these equations.



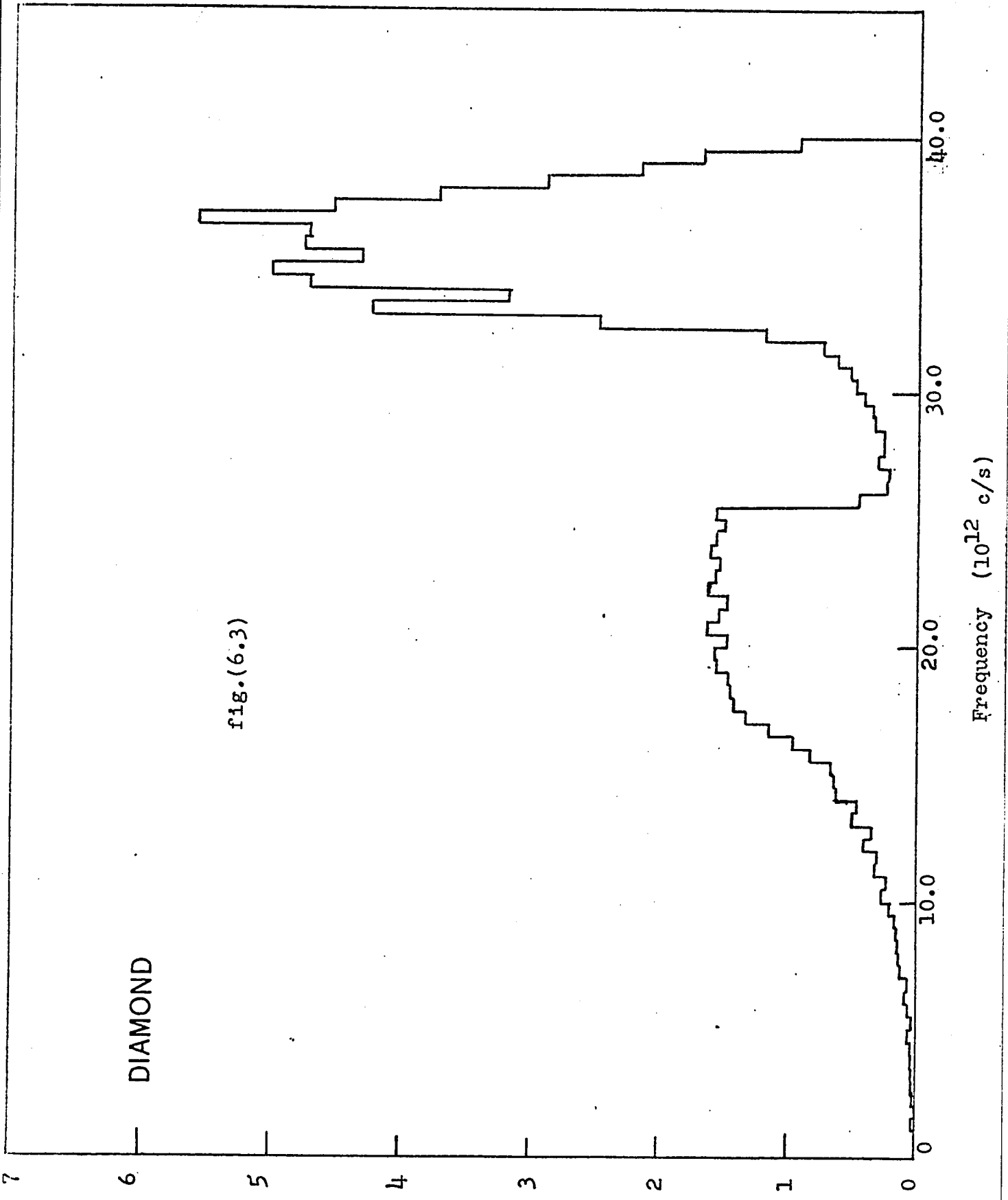
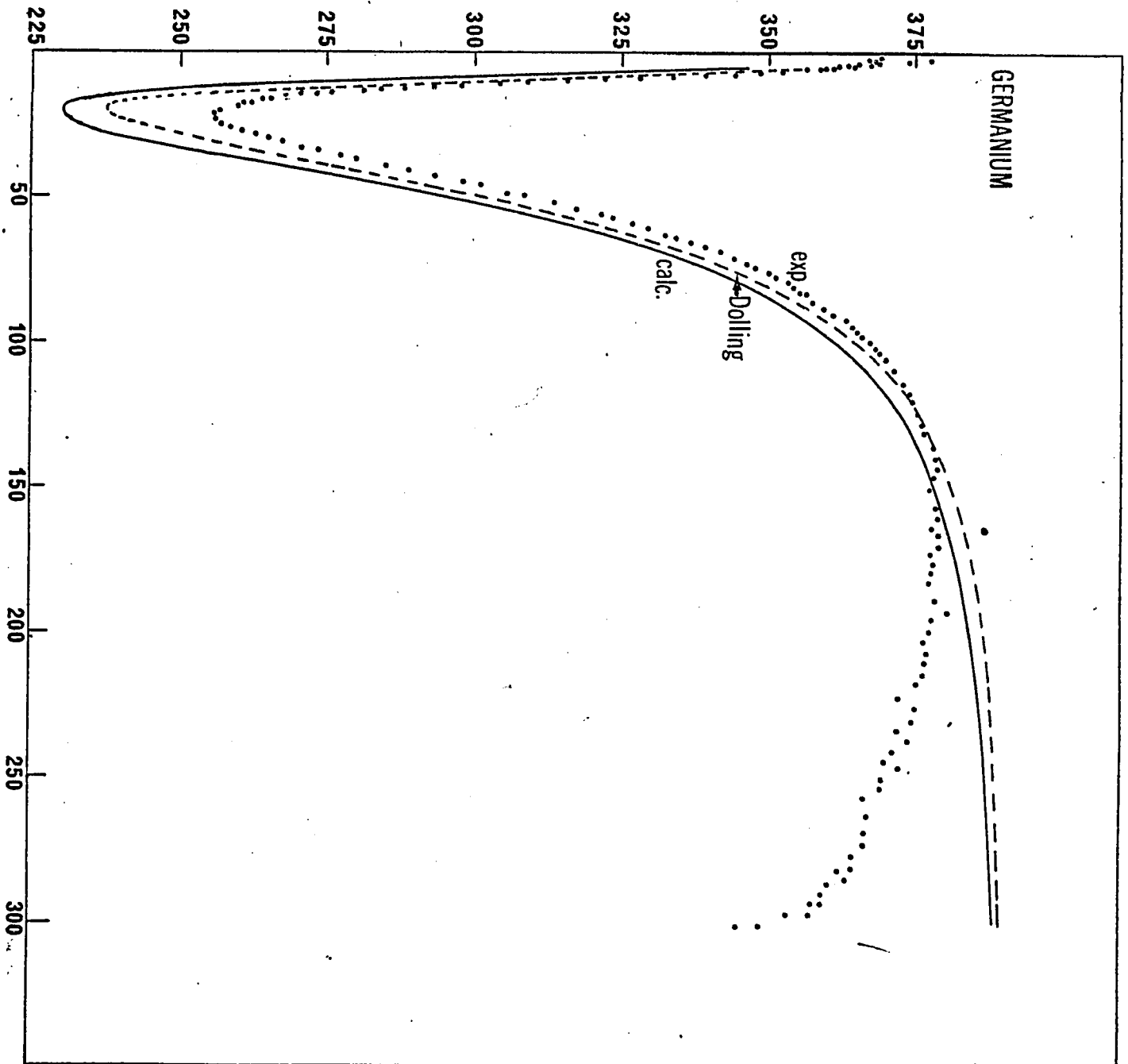


fig.(6.3)



The experimental data was taken from P. Flubacher, A. J. Leadbetter and J. A. Morrison, *Phil. Mag.*, Vol. 4, No. 39, p. 273, March 1959.

Experimental points, shown by closed circles, are from J.E.Desnoyers and J. A. Morrison, Phil. Mag., 3, 42 (1958)

fig.(6.5)

DIAMOND

2400

2200

2000

1800

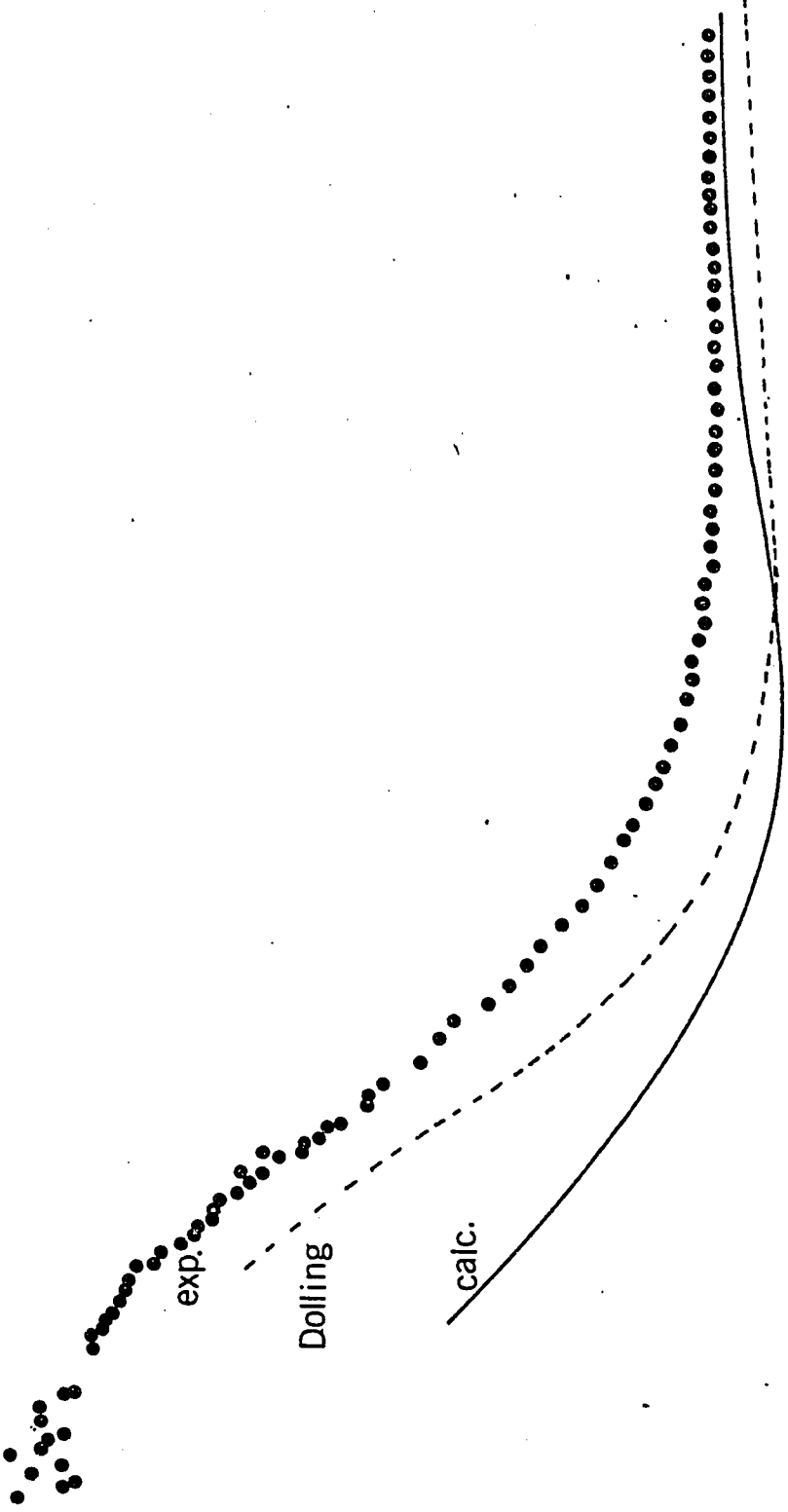
50

100

150

200

250



3. Reducing the secular equation.

Though the calculations were carried out using DET(3) of page 45 and page 46 it is easier to discuss equation (4.5)

$$\begin{vmatrix} R - \lambda I & T \\ T & S + C \end{vmatrix} = 0 \quad (4.5)$$

We note that λ 's appear in the first six diagonal elements only. Consequently, a diagonalization of the associated 12 x 12 matrix would not yield the correct roots. A simple example will show why

the equation $\begin{vmatrix} 2-\lambda & 1 \\ 1 & 2-\lambda \end{vmatrix} = 0$ yields $\lambda=1$ and $\lambda=3$

but the equation $\begin{vmatrix} 2-\lambda & 1 \\ 1 & 2 \end{vmatrix} = 0$ yields $\lambda=1.5$

To solve equation (4.5) we must reduce it to an equation of the form

$$|B - \lambda I| = 0 \quad (6.8)$$

where B is a 6 x 6 matrix,

we get 6 roots $\lambda_1, \dots, \lambda_6$ for each value of \vec{q} .

Theoretically this can be done as follows. Equation (4.5) can be written in the form

$$\omega^2 m U = R U + T V \quad (4.5a)$$

$$0 = T U + (S + C) V \quad (4.5b)$$

Solving equation (4.5b) for V we get

$$V = -(S + C)^{-1} T U$$

Substituting back into equation (4.5a) we get

$$\omega^2 m U = [R - T(S + C)^{-1} T] U$$

For a non-trivial solution the associated determinant must vanish, so we get

$$|R - T(S + C)^{-1} T - \lambda I| = 0$$

$$|B - \lambda I| = 0$$

where $B = R - T(S + C)^{-1} T$ and $\lambda = m\omega^2$

This solution requires the inversion of the matrix $S + C$

We now give a practical solution. By means of row-column manipulations we shall reduce the determinant and break off the 6x6 portion containing the λ 's.

For convenience denote the 12x12 array by A .

Firstly divide* the 12th column by $A_{12,12}$
 then multiply the 12th row by $A_{1,12}$ and subtract from the 1st row,
 12th row by $A_{2,12}$ and subtract from the 2nd row,

 12th row by $A_{11,12}$ and subtract from the 11th row.

Secondly divide the 11th column by $A_{11,11}$
 then multiply the 11th row by $A_{1,11}$ and subtract from the 1st row,
 the 11th row by $A_{2,11}$ and subtract from the 2nd row,,

 the 11th row by $A_{10,11}$ and subtract from the 10th row.

Thirdly divide the 10th column by $A_{10,10}$
 etc.

After the 1st step the determinant is of the form

$$\begin{array}{|c|} \hline \text{diagonal matrix} \\ \hline \end{array} \begin{array}{c} 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ x \end{array} = 0$$

divide by $A_{12,12}$ means multiply by $A_{12,12}^ / (A_{12,12} A_{12,12}^*)$

After the 6th step the determinant is of the form

$$= 0$$

i.e.
$$\begin{vmatrix} B-\lambda I & O \\ X & X/O \end{vmatrix} = 0 \quad (6.9)$$

Repeating the same procedure with row 12 to row 7 we further reduce it to the form

$$\begin{vmatrix} B - \lambda I & O \\ O & D \end{vmatrix} = 0 \quad (6.10)$$

where B is the same as in equation (6.9), D is diagonal. Expanding the determinant (we start with column 12 and work our way to column 7) we get

$$|B - \lambda I| = 0 \quad (6.11)$$

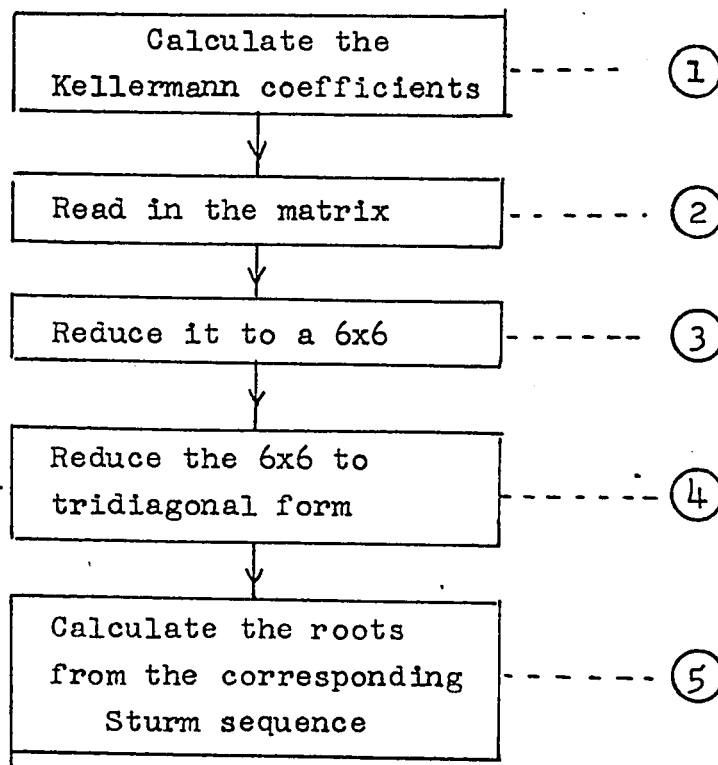
In practice we stop at equation (6.9) since the manipulation used to pass from (6.9) to (6.10) does not alter B .

4. Determining the Roots of the Secular Equation

Our first approach was to diagonalize the matrix B of equation (6.4) using the Jacobi method (29). A fortran program was made and thoroughly checked, using standard matrices of known eigenvalues (for example see the complex matrix of page 108).

We then realized we would have a time problem, i.e. we estimated that two runs, requiring approximately 33000 diagonalizations, would take about 100 hours on our IBM 1620. We scanned the literature and came across a method due to Householder (28) which was much faster (but still not fast enough on the IBM 1620). The final calculations were done on an IBM 360 (two runs of 2 1/2 hours each).

The following block diagram illustrates the calculations. Some of the more important details are given in Appendix B.



Consider the 2x2 matrix shown below.

$$B = \begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix}$$

The corresponding Sturm sequence is

$$P_0 = 1$$

$$P_1 = 1 - x$$

$$\begin{aligned} P_2 &= (1 - x)P_1 - (i)(-i)P_0 \\ &= x(x - 2) \end{aligned}$$

We wish to find the eigenvalues of B using Sturm's method.

Firstly take $x = 3$

we get

$$P_0 = 1 \quad +$$

$$P_1 = -2 \quad -$$

$$P_2 = 3 \quad +$$

The number of changes of sign is equal to two. The Sturm property says that there are two roots smaller than $x = 3$.

Now trying $x = 1/2$

we get

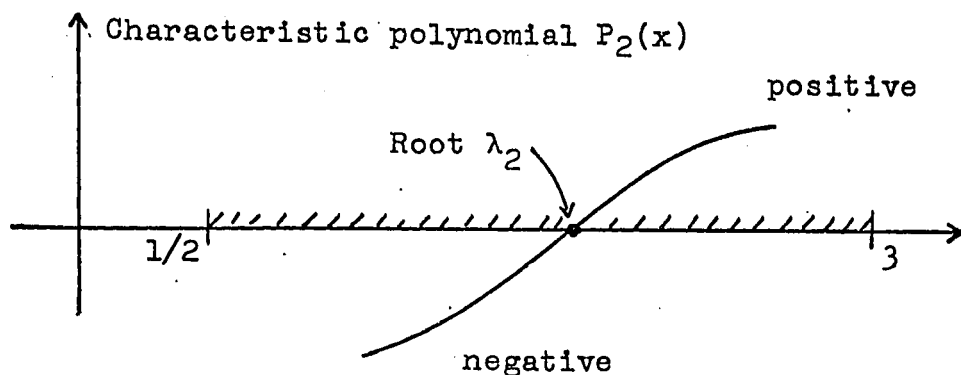
$$P_0 = 1 \quad +$$

$$P_1 = 1/2 \quad +$$

$$P_2 = -3/4 \quad -$$

There is one change in sign and consequently one root smaller than $1/2$.

So we conclude $1/2 < \lambda_2 < 3$.



We now describe the bisection method whereby we can approximate λ_2 to any desired accuracy.

Bisect the hatched interval $(A,B) = (1/2, 3)$ to get $x = 7/4$. Checking the sign of the characteristic polynomial we find that it is negative. So we let $A = 7/4$ and keep $B = 3$. Bisect again to get $x = 19/8$, the characteristic polynomial is now positive, so keep $A = 7/4$ and let $B = 19/8$. In two steps we have found

$$1.75 < \lambda_2 < 2.375 \quad (\text{we know that } \lambda_2 = 2)$$

Speed of convergence : once a root is isolated between A and B , N steps of the bisection method squeezes it within $\epsilon = (B - A)/2^N$. Taking $B - A = 1$ and solving for N we get $N = \log \epsilon / \log 2$.

Bishop (26) and Wilkinson (27) give the formulae for a real matrix only. The necessary modifications for a complex matrix are given in Appendix B page 104.

DISCUSSION

As far as possible we have attempted to keep the values of the parameters not far from the values expected for the rigid ion model and consistent with other physical data.

We quote below the rigid ion values obtained on the assumption $\gamma_R = \gamma_T$

$$R_0 = 15.295 \times 10^5 \text{ dynes/cm.}$$

$$\gamma = .682$$

which may be compared to the corresponding values in Table 2. The atomic polarizability can be calculated using the dielectric constant given in Table 1.

$$\text{Thus } \beta = \frac{3}{8\pi} \frac{\epsilon - 1}{\epsilon + 2} = .07$$

The value adopted here is larger than this value but physically quite reasonable. We may note that the results are rather sensitive to the values of β , γ_R and γ_T but not very much to the value of γ_S .

The fit of the dispersion curves in the (100) direction is quite satisfactory. The differences between experimental points and theoretical curves being of the same order as the estimated

accuracy of the experimental data, given as $\sim 3\%$ by Warren et al (22).

But in the (111) direction the theoretical LA curve deviates appreciably from the experimental points. We may note that for germanium, with this model, Cochran (14) was also not able to achieve agreement between theory and experiment for this branch. The agreement for the LO branch is also not completely satisfactory. It is of interest to note that Kucher and Nechiporuk (20) even with a nine parameter model could not obtain agreement for LO and TO branches; indeed their results are less satisfactory than ours.

The vibration spectrum for diamond obtained here, fig.(6.3), is quite similar to that obtained by Dolling and Cowley (25) from an eleven parameter model.

It is customary to express heat capacity measurements in terms of the variation of the Debye temperature θ as shown in fig.(6.5). At temperatures greater than 150° K the theoretical curve is in agreement with the experimental data within the combined experimental errors of the thermo-dynamic and neutron scattering data ($\sim 3\%$). But at low temperatures the theoretical values are too low. The theoretical curve due to Dolling and Cowley also lies below the experimental points.

Our histogram for the vibration spectrum of germanium, fig.(6.2), is in satisfactory accord with that obtained by Fray et al (24) using the same model.

The Debye temperature curve, fig.(6.4), is seen to fall slightly below the experimental values and is very close to that obtained by Dolling and Cowley (25) from a 11-parameter

model.

The behaviour of the dispersion curves of diamond and germanium shows that the two substances are not homologous (22). This is also reflected in the different shapes of the vibration spectra of the two substances.

APPENDIX A

THE RIGID ION MODEL

1. The Dispersion Relation for Special Directions

In chapter IV section 2 we obtained the secular equation (6x6 determinant) for the rigid ion model by putting $k=\infty$. We noted that it was identical with the determinant of page ... when D_0 and D'_0 were replaced by R_0 and R'_0 . To derive the dispersion equation for these special directions it is easier to use the system of 6x6 homogeneous equations rather than the determinant. These are equations (2.7) to (2.12) with R_0 and R'_0 instead of D_0 and D'_0 . We now seek the dispersion equation for special directions. We shall work out the case (100) transverse, i.e. we set

$$q_x = q \quad q_y = q_z = 0$$

consequently $C_1 = c \quad C_2 = C_3 = 1$

$$S_1 = s \quad S_2 = S_3 = 0$$

$$c = \cos\theta \quad s = \sin\theta \quad \theta = qr_0/2$$

We must also set $U_x(1) = U_y(1) = U(1)$ $U_z(1) = 0$
 $U_x(2) = U_y(2) = U(2)$ $U_z(2) = 0$

The system of 6 equations reduces to two identical sets of 2 equations of the form

$$m \omega^2 U(1) = R_0 U(1) + (-R_0 c + i R'_0 s) U(2) \quad (A1)$$

$$m \omega^2 U(2) = (-R_0 c - i R'_0 s) U(1) + R_0 U(2) \quad (A2)$$

Equations (A1) and (A2) are of the form

$$m \omega^2 U(1) = R_0 U(1) - R_0 G_R U(2) \quad (A3)$$

$$m \omega^2 U(2) = -R_0 G_R^* U(1) + R_0 U(2) \quad (A4)$$

where $G_R = c - i \gamma_R s$ and $\gamma_R = R'_0 / R_0$ by definition.

We now list all cases of interest

$$(100)L \quad G_R = c$$

$$(100)T \quad G_R = c - i \gamma_R s$$

$$(111)L \quad G_R = (c^3 - 2\gamma_R s^2 c) + i(s^3 - 2\gamma_R c^2 s)$$

$$(111)T \quad G_R = (c^3 + \gamma_R s^2 c) + i(s^3 + \gamma_R s^2 c)$$

The condition for a non-trivial solution of equations (A3) and (A4) is

$$\begin{vmatrix} R_0 - \lambda & -R_0 G_R \\ -R_0 G_R^* & R_0 - \lambda \end{vmatrix} = 0 \quad \lambda = m \omega^2$$

or

$$\begin{vmatrix} R_0 - \lambda & R \\ R^* & R_0 - \lambda \end{vmatrix} = 0 \quad R = -R_0 G_R$$

which yields $m \omega^2 = R_0 \pm |R|$ (A5)

the + sign referring to optic modes and
the - sign referring to acoustic modes.

2. The Elastic Constants

We shall derive relationships between c_{11} , c_{12} , c_{44} and the parameters R_0 and γ_R . We then show that Born's relationship is satisfied.

Our starting point is equation (A5) which can be written as

$$m \omega^2 = R_0 (1 \pm |G_R|) \quad (A6)$$

Since the elastic constants are related to the velocity of propagation of the waves in special directions, we rewrite equation (A6) in terms of this velocity U .

$$\text{We have } U^2 = \omega^2/q^2 \quad (A7)$$

Since we are comparing our lattice with a homogeneous solid we must replace the mass m by an expression involving the density ρ . From de Launay (4) (page 293) we have

$$\rho = m/r_0^3 \quad (A8)$$

Combining equations (A6), (A7) and (A8) we get

$$\rho U^2 = R_0 (1 \pm |G_R|)/r_0^3 q^2 \quad (A9)$$

To get the velocity of propagation for long waves of acoustical frequency we take the limit $q \rightarrow 0$ and select the minus sign. We get

$$\rho U^2 = (R_o/r_o^3) \lim_{q \rightarrow 0} \left[(1 - |G_R|)/q^2 \right] \quad (A10)$$

Now de Launay (4) (page 266) gives the connection between U and c_{11} , c_{12} , c_{44} . Again we are interested in the modes listed below

$$(100)L \quad \rho U_L^2 = c_{11} \quad (A11)$$

$$(100)T \quad \rho U_T^2 = c_{44} \quad (A12)$$

$$(111)L \quad \rho U_L^2 = (c_{11} + 2c_{12} + 4c_{44})/3 \quad (A13)$$

$$(111)T \quad \rho U_T^2 = (c_{11} - c_{12} + c_{44})/3 \quad (A14)$$

where the subscript L and T refers to longitudinal and transverse modes respectively.

$$\text{In general } \rho U^2 = c \quad (A15)$$

where c = linear combination of c_{11} , c_{12} and c_{44} .

Combining equations (A10) and (A15) we get

$$c = (R_o/r_o^3) \lim_{q \rightarrow 0} \left[(1 - |G_R|)/q^2 \right] \quad (A16)$$

CASE I (100)L

For this case equation (A16) is

$$c_{11} = (R_o/r_o^3) \lim_{q \rightarrow 0} [(1 - |G_R|)/q^2] \quad (A17)$$

where $G_R = \cos \theta$ $\theta = qr_o/2$ for this case

as $q \rightarrow 0$ $G_R \rightarrow 1 - \theta^2/2 = 1 - q^2 r_o^2/8$

so that $\lim_{q \rightarrow 0} [(1 - |G_R|)/q^2] = r_o^2/8$ (A18)

Combining equations (A17) and (A18) we get

$$c_{11} = R_o/8r_o \quad (A19)$$

CASE II (100)T

For this case equation (A16) is

$$c_{44} = (R_o/r_o^3) \lim_{q \rightarrow 0} [(1 - |G_R|)/q^2] \quad (A20)$$

where $G_R = \cos \theta + i\gamma_R \sin \theta$

therefore $|G_R| = \sqrt{\cos^2 \theta + \gamma_R^2 \sin^2 \theta}$

as $q \rightarrow 0$ $|G_R| \rightarrow \sqrt{1 - \theta^2 + \gamma_R^2 \theta^2}$

Expanding (using the Binomial theorem) we get

$$|G_R| \rightarrow 1 - 1/2(1 - \gamma_R^2)\theta^2 = 1 - 1/2(1 - \gamma_R^2)q^2 r_o^2/4$$

so that $\lim_{q \rightarrow 0} [(1 - |G_R|)/q^2] = (r_o^2/8)(1 - \gamma_R^2)$

Using equation (A20) we get

$$c_{44} = (R_o/8r_o)(1 - \gamma_R^2)$$

Using equation (A 19) we get

$$c_{44} = c_{11}(1 - \gamma_R^2) \quad (A21)$$

CASE III (111)T

For this case equation (A16) is

$$(c_{11} - c_{12} + c_{44})/3 = (R_o/r_o^3) \lim_{q \rightarrow 0} [(1 - |G_R|)/q^2] \quad (A22)$$

where $G_R = (\cos^3\theta + \gamma_R \sin^2\theta \cos\theta) + i(\sin^3\theta + \gamma_R \cos^2\theta \sin\theta)$

with $\theta = qr_o/2\sqrt{3}$

as $q \rightarrow 0$ $G_R \rightarrow 1 - (3/2)\theta^2 + \gamma_R\theta^2 + i\gamma_R\theta$

$$|G_R| \rightarrow \sqrt{(1 - (3/2)\theta^2 + \gamma_R\theta^2)^2 + \gamma_R^2\theta^2}$$

Expanding $|G_R| \rightarrow 1 - 1/2(3 - 2\gamma_R - \gamma_R^2)\theta^2$

so $1 - |G_R| \rightarrow 1/2(3 - 2\gamma_R - \gamma_R^2)q^2r_o^2/12$

and $\lim_{q \rightarrow 0} [(1 - |G_R|)/2] = (r_o^2/24)(3 - 2\gamma_R - \gamma_R^2)$

Using equation (A22) we get

$$(c_{11} - c_{12} + c_{44})/3 = (R_o/r_o^3)(r_o^2/24)(3 - 2\gamma_R - \gamma_R^2)$$

Using equation (A21) and (A19) we get

$$c_{11} - c_{12} + c_{11}(1 - \gamma_R^2) = c_{11}(3 - 2\gamma_R - \gamma_R^2)$$

Solving for c_{12}

$$c_{12} = c_{11}(2\gamma_R - 1)$$

(A23)

We list our results

$$c_{11} = R_o/8r_o \quad (A19)$$

$$c_{44} = c_{11}(1 - \gamma_R^2) \quad (A21)$$

$$c_{12} = c_{11}(2\gamma_R - 1) \quad (A23)$$

We rewrite them as

$$R_o = 8r_o c_{11} \quad (A24)$$

$$\gamma_R = \sqrt{1 - c_{44}/c_{11}} \quad (\text{A25})$$

$$\gamma_R = (1 + c_{12}/c_{11})/2 \quad (\text{A26})$$

To get Born's identity we eliminate γ_R from equations (A23) and (A24)

We get

$$4c_{11}(c_{11} - c_{44}) = (c_{11} + c_{12})^2 \quad (\text{A 27})$$

3. Upper Bound for γ_R

For the limiting case $\vec{q} \rightarrow 0$ the parameter γ_R can be written in terms of the ratio ω_T/ω_L of the transverse and longitudinal frequencies for the acoustical branches in the (100) direction.

$$\text{For (100)L} \quad m \omega_L^2 = R_0(1 - |G_R|) \quad |G_R| = \cos\theta$$

$$\text{when } \vec{q} \rightarrow 0 \quad m \omega_L^2 \rightarrow R_0 \theta^2 / 2 \quad (\text{A28})$$

$$\text{For (100)T} \quad m \omega_T^2 = R_0(1 - |G_R|) \quad |G_R| = \sqrt{\cos^2\theta + \gamma_R^2 \sin^2\theta}$$

$$\text{when } \vec{q} \rightarrow 0 \quad m \omega_T^2 \rightarrow (1 - \gamma_R^2) \theta^2 \quad (\text{A29})$$

Dividing equation (A29) by equation (A28) we get

$$\text{for } \vec{q} \rightarrow 0 \quad \omega_T^2 / \omega_L^2 \rightarrow 1 - \gamma_R^2 \quad (\text{A30})$$

$$\text{Solving for } \gamma_R \text{ we get} \quad \gamma_R = \sqrt{1 - \omega_T^2 / \omega_L^2} \quad (\text{A31})$$

Equation (A31) yields $\gamma_R < 1$

APPENDIX B

1. Kellermann's Coefficients for the Diamond Lattice

Various tests showed that for the choice $\epsilon = 1$ the sums \sum_n , \sum_l and \sum_m had to be carried out using 15, 42, and 68 terms respectively to obtain good accuracy. A program was written in which $\psi(l) = \int_0^l e^{-\xi^2} d\xi$ was calculated by means of an approximation due to Hastings (30). To reduce the computing time, tables were made for $f(l)$, $g(l)/l^2$, $f(m)$, $g(m)/m^2$, $\cos \alpha$, and $\sin \alpha$, where $\alpha = \pi(h_x + h_y + h_z)$. This program was checked against Cochran's table. We also completely reproduced Kellermann's tables for Na Cl (execution time = 8 minutes on the IBM 1620). Practically all values were within the 1% accuracy of Kellermann's results. In the following tables we have left out the different sign combinations for l and m .

	h_x	h_y	h_z	$\cos \alpha$	$\sin \alpha$
1	0	0	0	1	0
2	0	0	2	-1	0
3	0	0	-2	-1	0
4	0	2	0	-1	0
5	0	-2	0	-1	0
6	2	0	0	-1	0
7	-2	0	0	-1	0
8	1	1	1	0	-1
9	-1	-1	-1	0	1
10	1	1	-1	0	1
11	-1	-1	1	0	-1
12	1	-1	1	0	1
13	-1	1	-1	0	-1
14	-1	1	1	0	1
15	1	-1	-1	0	-1

Number of combinations	l_x	l_y	l_z	$f(l)$	$g(l)/l^2$
$4 \times 3 = 12$	1	1	0	$.924416 \times 10^{-1}$	$.291372$
	1	0	1		
	0	1	1		
$2 \times 3 = 6$	2	0	0	$.575143 \times 10^{-2}$	$.146471 \times 10^{-1}$
	0	2	0		
	0	0	2		
$8 \times 3 = 24$	2	1	1	$.502372 \times 10^{-3}$	$.118351 \times 10^{-2}$
	1	2	1		
	1	1	2		

Number of combinations	m_x	m_y	m_z	$f(m)$	$g(m)/m^2$
$4 \times 1 = 4$	- .5	- .5	- .5	1.050424	5.623052
$4 \times 3 = 12$.5	.5	1.5	$.304008 \times 10^{-1}$	$.856262 \times 10^{-1}$
	1.5	.5	.5		
$4 \times 3 = 12$	- .5	-1.5	-1.5	$.225371 \times 10^{-2}$	$.553387 \times 10^{-2}$
	-1.5	- .5	-1.5		
$4 \times 3 = 12$	-1.5	-1.5	- .5	$.209350 \times 10^{-3}$	$.484510 \times 10^{-3}$
	1.5	1.5	1.5		
$4 \times 3 = 12$	- .5	- .5	-2.5	$.209350 \times 10^{-3}$	$.484510 \times 10^{-3}$
	- .5	-2.5	- .5		
$4 \times 3 = 12$	-2.5	- .5	- .5	$.215522 \times 10^{-4}$	$.482589 \times 10^{-4}$
	.5	1.5	2.5		
$4 \times 6 = 24$.5	2.5	1.5	$.215522 \times 10^{-4}$	$.482589 \times 10^{-4}$
	1.5	.5	2.5		
	1.5	2.5	.5		
	2.5	.5	1.5		
	2.5	1.5	.5		

2. Determinant Evaluation

Starting with a 12x12 determinant and carrying out 11 steps of the reduction procedure described on pp. 78 and 79, we reduce it to the triangular form. The product of the diagonal elements gives the numerical value of the determinant. This procedure was programed (flowchart 1) and used to reduce the secular equation. The following test was applied.

Let $J_n = J$ be of order n (see page 108)

$$\text{then } \text{Det}(J_n) = n + 1$$

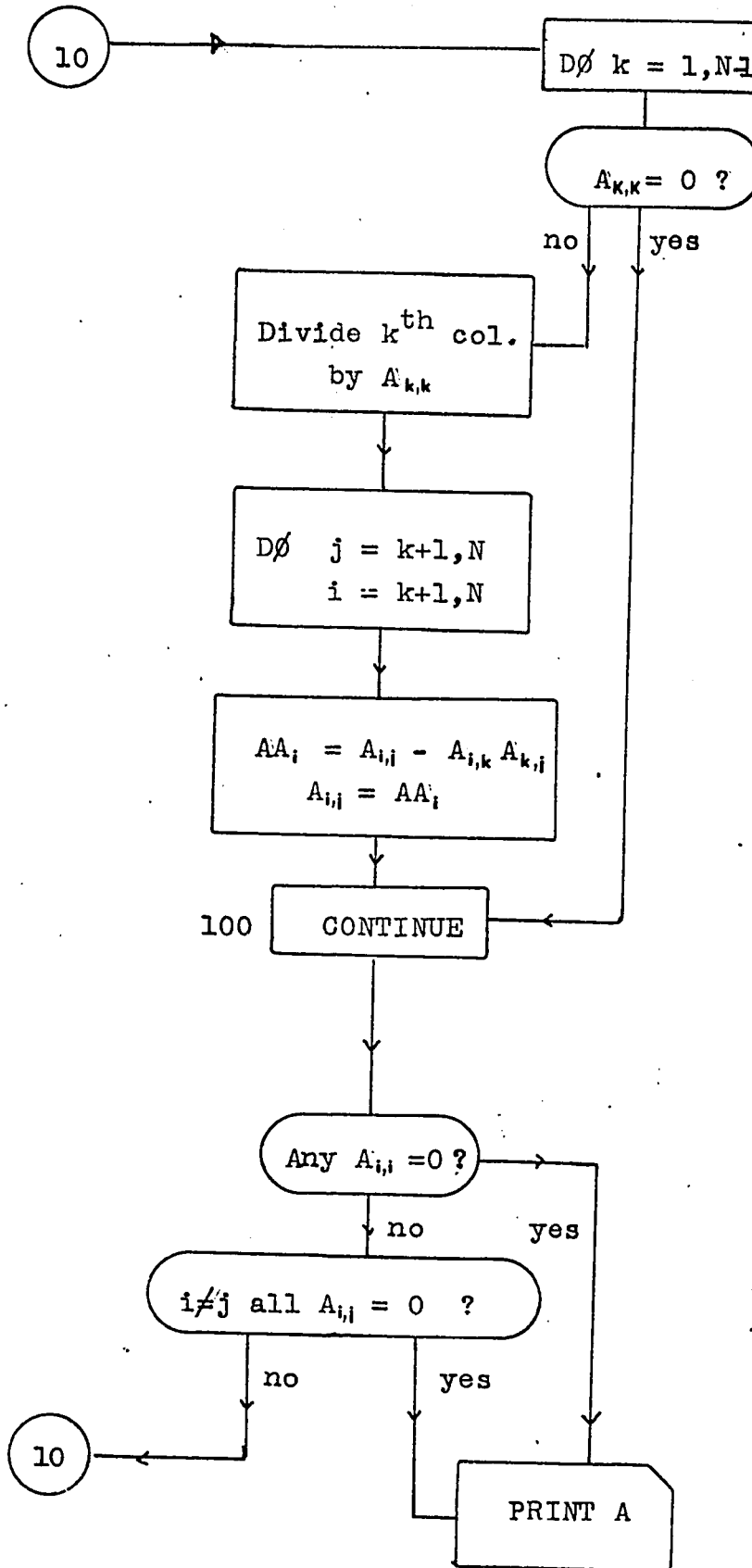
$$\text{so that } \text{Det}(A_n) = (n + 1)^3 \quad \text{where } A_n = J_n^3.$$

This result holds for arbitrary θ .

$$\text{Det}(A_6) = (7)^3 = 343 \quad \text{theoretical value}$$

$$\text{Det}(A_6) = \begin{cases} 343.008 & \theta = \pi/2 \\ 343.047 & \theta = \pi/3 \quad \text{calculated} \\ 343.032 & \theta = \pi/4 \end{cases}$$

flowchart 1.



3. Root Evaluation

As previously stated the roots were computed by reducing B to tridiagonal form (see page 104) and then isolating the roots using the Sturm sequence (see flowchart 2). Two roots are considered equal if contained within $\epsilon = 10^{-5}$. The program was tested using matrix A_6 of page 108. 20 steps of the bisection method were applied to each root, giving an accuracy $\epsilon \sim 10^{-5}$.

Theoretical Roots for A_6	Calculated Roots		
	$\theta = \pi/2$	$\theta = \pi/3$	$\theta = \pi/4$
54.95598	54.95597	54.95597	54.95597
34.23250	34.23249	34.23249	34.23249
14.61702	14.617028	14.617028	14.617007
3.75972	3.759726	3.759726	3.759725
.42699	.426990	.426990	.426990
.00776	.007766	.007768	.007766

For real symmetrical matrices Householder's method described in Bishop's book (26). We now give the necessary modifications for the case of a complex hermitian matrix.

The derivation for the real case can be modified as follows.

The rotation matrix is of the form

$$R = I - \mu ZZ'$$

where Z is a column vector, the corresponding row vector being given by

$$Z' = (z_1^*, z_2^*, \dots, z_n^*)$$

$$\text{and } \mu = 1/Z' \cdot Z \quad (\text{B1})$$

We seek z_1, z_2, \dots, z_n such that the rotation matrix R will reduce the matrix B to tridiagonal form by reducing a whole row at a time. The necessary condition is

$$1 = 2 \mu \rho\{B\} \cdot Z \quad (\text{B2})$$

where $\rho\{B\}$ denotes the first row of B

$$\text{i.e. } \rho\{B\} = (b_{1,1}, b_{1,2}, \dots, b_{1,n}).$$

$$\text{and where } Z' = (0, z_2^*, b_{1,3}, \dots, b_{1,n})$$

we seek z_2 such that equation (B2) is satisfied.

We rewrite (B2) as follows

$$2 \rho\{B\} \cdot Z = Z' \cdot Z \quad (\text{B3})$$

Equation (B3), when written in full, gives

$$2(b_{1,2}z_2 + b_{1,3}b_{1,3}^* + \dots + b_{1,n}b_{1,n}^*) = (z_2^*z_2 + b_{1,3}b_{1,3}^* + \dots + b_{1,n}b_{1,n}^*) \quad (B4)$$

Since $Z^1 \cdot Z$ is real, the left hand side of equation (B4) is real,

$$\text{therefore} \quad z_2 = c b_{1,2}^* \quad (B5)$$

where $c = \text{some real constant.}$

Using equation (B5) we substitute z_2 back into equation (B4) to get

$$2(c + \chi^2) = c^2 + \chi^2$$

$$\text{where} \quad \chi^2 = (b_{1,3}b_{1,3}^* + \dots + b_{1,n}b_{1,n}^*)/b_{1,2}b_{1,2}^*.$$

$$\text{Solving for } c \text{ we get} \quad c = 1 \pm \sqrt{1 + \chi^2} \quad (B6)$$

Since Z is now determined completely, the rotation matrix is known and we can reduce our matrix B to tridiagonal form. We now write the formulae for the r^{th} step of the process.

Let \bar{B} stand for the reduced matrix.

Since we want $c \neq 0$ we select the $+$ sign in equation (B6)

$$\chi^2 = \left(\sum_{j=r+1}^n b_{\eta_j, j+2} b_{\eta_j, j+2}^* \right) / b_{r, r+1} b_{r, r+1}^*$$

$$z_j = \begin{cases} 0 & \text{for } j < r+1 \\ b_{r, r+1}^* \left(1 + \sqrt{1 + \chi^2} \right) & \text{for } j = r+1 \\ b_{r, j}^* & \text{for } j > r+1 \end{cases}$$

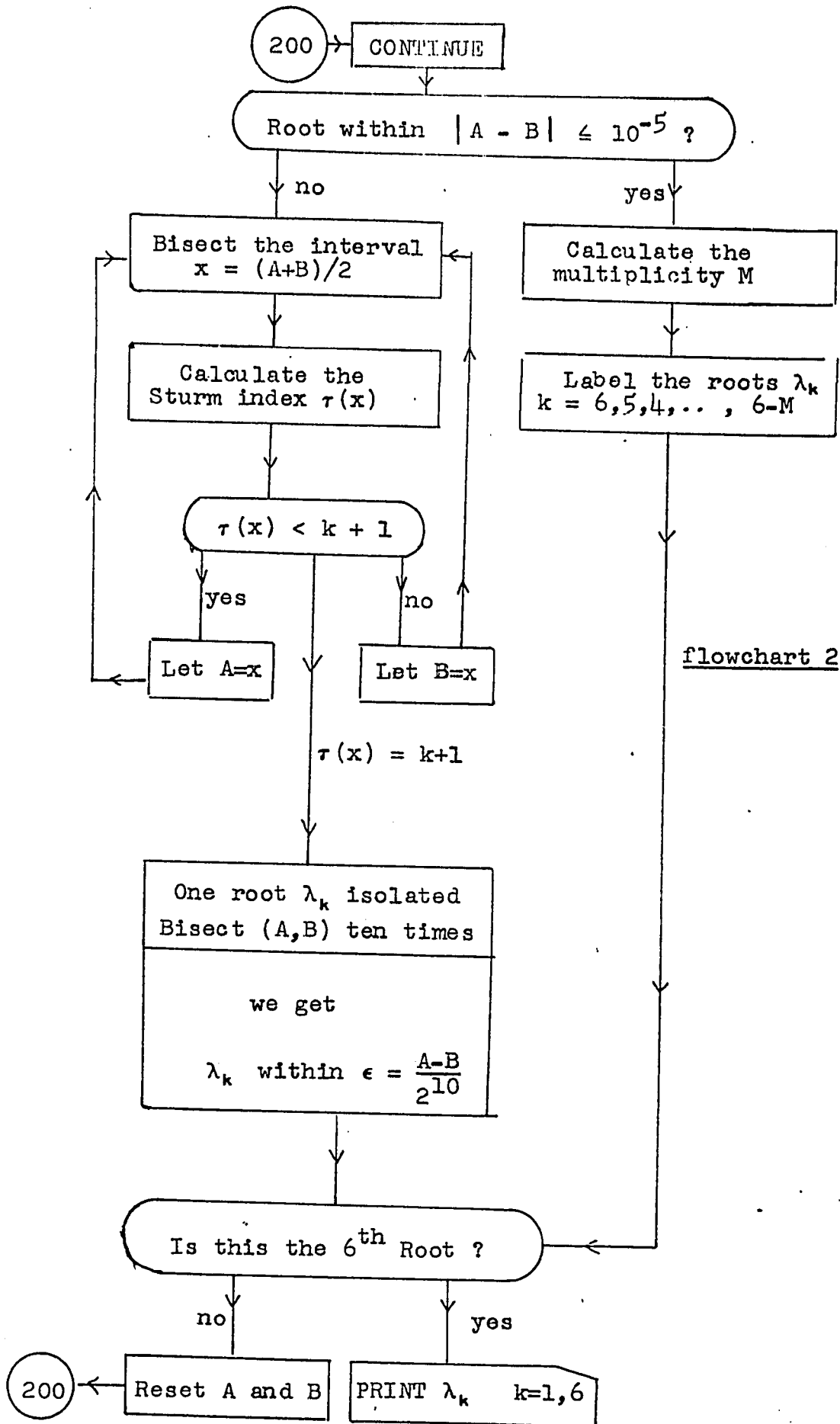
$$\mu = 1 / \left[2 b_{r, r+1} b_{r, r+1}^* \sqrt{1 + \chi^2} \left(\sqrt{1 + \chi^2} + 1 \right) \right]$$

$$Y = BZ$$

$$q = Z' \cdot Y$$

$$W = 2\mu (Y - \mu q Z)$$

$$\bar{B} = B - W Z' - Z W'$$



Complex Test Matrix

$$J = \begin{pmatrix} 2 & a & & & & & \\ a^* & 2 & a & & & & \\ & a^* & 2 & a & & & \\ & & a^* & 2 & a & & \\ & & & a^* & 2 & a & \\ & & & & a^* & 2 & a \\ & & & & & a^* & 2 \end{pmatrix} \quad a = e^{i\theta}$$

$$J^3 = A = \begin{pmatrix} 14 & 14a & 6a^2 & a^3 & 0 & 0 \\ 14a^* & 20 & 15a & 6a^2 & a^3 & 0 \\ 6a^{*2} & 15a^* & 20 & 15a & 6a^2 & a^3 \\ a^{*3} & 6a^{*2} & 15a^* & 20 & 15a & 6a^2 \\ 0 & a^3 & 6a^{*2} & 15a^* & 20 & 14a \\ 0 & 0 & a^{*3} & 6a^{*2} & 14a^* & 14 \end{pmatrix}$$

where $a = \cos\theta + i \sin\theta$

e.g. $\theta = 120^\circ$

$$a = -1/2 + \sqrt{3}/2 i$$

$$a^2 = -1/2 - \sqrt{3}/2 i$$

$$a^3 = 1$$

eigenvalues $\lambda_K = 4 \cos^2\left(\frac{\pi K}{2(N+1)}\right)$ for J $K = 1, 2, \dots, N$

eigenvalues $\lambda_K = 64 \cos^6\left(\frac{\pi K}{2(N+1)}\right)$ for A $K = 1, 2, \dots, N$

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