LATTICE SPECTRUM OF THE FACE-CENTERED CUBIC LATTICE

by

RAYMOND O. SCHELGUNOV, B.S.

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CHAPTER I

INTRODUCTION

This paper is concerned with the problem of determining the vibrational frequency spectrum of the face-centered cubic lattice. Before the advent of the high speed digital computer, a problem of this complexity could yield, with a considerable amount of effort, only a vague analysis of the theory. A more complete analysis is necessary for a comparison of the accumulated empirical data.

There are, in this problem, certain parameters which when handled in any of the previous attempts merely multiply the complexity of the problem. The freedom of adjustment of these parameters is necessary for a completely general analysis. The purpose of the work reported here was to devise a digital computer program for determining the vibrational frequency spectrum for arbitrary values of the parameters arising in the problem. This permits a detailed analysis of many special cases. The flexibility of this device may prove useful in the evaluation of many peripheral theories and assumptions, such as the specific heat theory and the form of certain assumed interatomic forces.

CHAPTER II

THEORY

THE DYNAMICS OF A SPACE LATTICE

The development of the theory follows primarily that of Ziman[1]. The theory will be developed, for the most part, for an arbitrary lattice, with a few modifications which will be made where necessary to develop the problem in the most straightforward manner.

In the solid form most matter arranges itself in some crystal form. This paper is concerned primarily with the face-centered cubic lattice. Adaptation of this specific case to the general development will be made later.

A single face-centered cubic crystal may be described as follows: consider a cube with an atom located at each of its eight corners and with atoms located in the center of each of its six faces (Fig. 1). A lattice is constructed by stacking such compound "cells" one on top of the other. An atom located at the corner of a single compound cell is shared by eight single compound cells. An atom in the center of a face of a compound cell is shared by one other cell.

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[1] J. M. Ziman, Electrons and Phonons (Oxford University Press, Amen House, London E. C. 4, 1960)

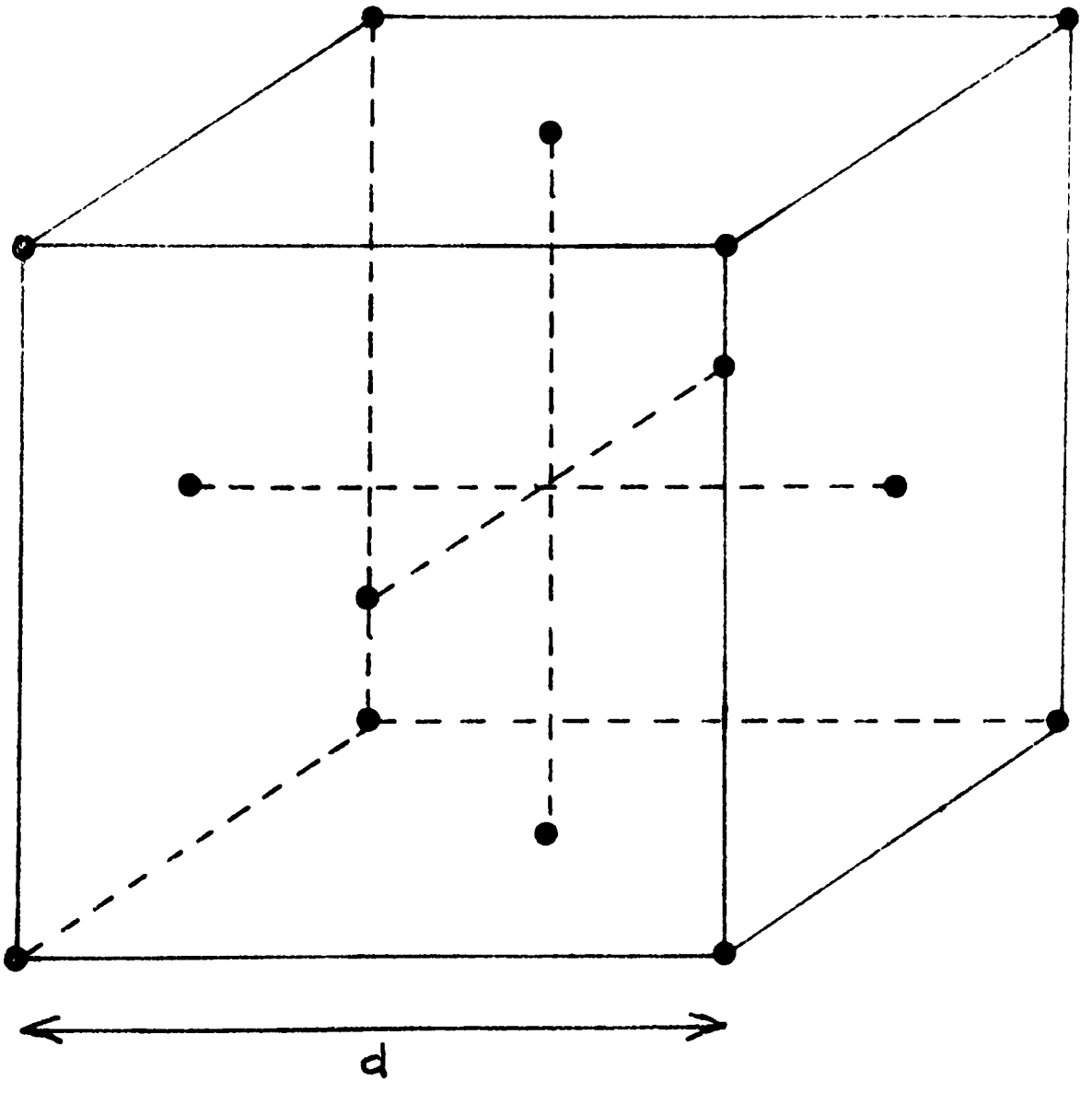

Fig. 1 Face-centered Cubic Compound Cell

The atoms in the described array are held in the general vicinity of their respective lattice sites by an interatomic force. We shall assume that this force is a central force, that is, a function of distance only between any two atoms.

The theory is concerned with the vibrational frequency of the atoms about their respective equilibrium positions. Let us locate the N equilibrium sites by the position vectors $\vec{\ell}$. The actual location of the atoms will be given by the N position vectors $\vec{X}_{\vec{\ell}}$. This notation refers to the position of the atom which belongs to the particular site $\vec{\ell}$. As we are primarily concerned with the motion of the atoms about their equilibrium positions, we can benefit most by referring to the displacement vector $\vec{S}_{\vec{\ell}}$, where

$$\vec{S}_{\vec{\ell}} = \vec{X}_{\vec{\ell}} - \vec{\ell} \ .$$

The total lattice potential energy $V(s_{\vec{\ell}})$ can be expanded about the equilibrium positions in a Taylor's series:

$$V(s_{\vec{\ell}}) = V_0 + \sum_{\ell} \frac{\partial V}{\partial \vec{S}_{\vec{\ell}}}\Big]_0 \cdot \vec{S}_{\vec{\ell}} + \frac{1}{2} \sum_{\vec{\ell},\vec{\ell}'} \vec{S}_{\vec{\ell}} \cdot \left[\frac{\partial^2 V}{\partial \vec{S}_{\vec{\ell}} \partial \vec{S}_{\vec{\ell}'}}\right]_0 \cdot \vec{S}_{\vec{\ell}} + \cdots$$

where $\left[\dfrac{\partial^2 V}{\partial \vec{S}_{\vec{\ell}} \partial \vec{S}_{\vec{\ell}'}}\right]$ is of the dyadic form.

We make the harmonic approximation which drops all terms

in the series higher than the quadratic term. The constant term V_0 is arbitrary and we shall ignore it. Since the configuration in which the atoms occupy the lattice sites is the equilibrium state, the second term in the expansion is zero:

$$\frac{\partial V}{\partial \vec{S}_{\vec{\ell}}}\Big]_0 = 0 .$$

This leaves

$$V(S_{\vec{\ell}}) = \frac{1}{2} \sum_{\vec{\ell},\vec{\ell}'} \vec{S}_{\vec{\ell}} \cdot \frac{\partial^2 V}{\partial \vec{S}_{\vec{\ell}} \partial \vec{S}_{\vec{\ell}'}}\Big]_0 \cdot \vec{S}_{\vec{\ell}'} .$$

In order to simplify the notation let

$$\overleftrightarrow{G} = \frac{\partial^2 V}{\partial \vec{S}_{\vec{\ell}} \partial \vec{S}_{\vec{\ell}'}}\Big]_0 .$$

Then we have

$$V(S_{\vec{\ell}}) = \frac{1}{2} \sum_{\vec{\ell},\vec{\ell}'} \vec{S}_{\vec{\ell}} \cdot \overleftrightarrow{G} \cdot \vec{S}_{\vec{\ell}'} .$$

For further clarification let us write down in component form the various terms that have been used:

$$\frac{\partial V}{\partial \vec{S}} \longrightarrow \frac{\partial V}{\partial S_a} , \quad (a = 1,2,3) ,$$

$$\frac{\partial^2 V}{\partial \vec{S}_{\vec{\ell}} \partial \vec{S}_{\vec{\ell}'}} \longrightarrow \frac{\partial^2 V}{\partial S_a \partial S_b} , \quad (a,b = 1,2,3) ,$$

$$\vec{S} \cdot \overleftrightarrow{G} \cdot \vec{S} \longrightarrow \sum_{a,b} S_a G_{ab} S_b .$$

At this point we introduce the approximate Hamiltonian operator of the system as a whole:

$$H = \frac{1}{2} \sum_{\ell} \frac{1}{m} \vec{p}_{\ell} \cdot \vec{p}_{\ell'} + \frac{1}{2} \sum_{\ell,\ell'} \vec{s}_{\ell} \cdot \vec{G} \cdot \vec{s}_{\ell'} ,$$

where $\vec{p}_{\ell}$ denotes the momentum and m the mass of the ℓ^{th} atom. We wish now to find the eigenstates and eigenvalues belonging to this Hamiltonian operator. The solution is readily obtained by exploiting the translational symmetry that suggests the use of cyclic boundary conditions. The method can best be described by alluding to the one dimensional case.

Let N now correspond to the number of atoms in a linear chain. The cyclic boundary condition is

$$s_{N+\ell} \equiv s_{\ell} .$$

The displacement from equilibrium of an atom in the site $N+\ell$ refers cyclicly to the displacement at the atom occupying the ℓ^{th} site. Graphically, the linear chain is bent around into a large ring. The Hamiltonian is therefore invariant under a cyclic interchange of particle coordinates. Hence the eigenvalues of the Hamiltonian must exhibit an N-fold degeneracy, or the eigenstates differ only by a phase factor. The phase factor must be such that when a full cyclic interchange has been made it must equal one, i.e. $e^{iqN} |s_1, \cdots s_2\rangle = |s_{N+1}, s_{N+2} \cdots\rangle$,

therefore

$$e^{iqN} = 1 .$$

Hence, we must have

$$q = \frac{2\pi K}{N}$$

where K is an integer.

The wave number q exhibits cyclic properties in that the eigenstate is invariant under the addition of any integral multiple of 2π . We shall adopt a convenient principal value range convention for the wave number q :

$$-\pi < q \leq \pi .$$

The simplest function that is suggested is a linear combination of all the S_ℓ's .

$$S_q = N^{-\frac{1}{2}} \sum_\ell S_\ell e^{iq\ell} , \quad (\ell = 1, \cdots N)$$

It will be noted that this is the complex Fourier series. The Hamiltonian can be written as a function of the normalized coordinates. Where the orthogonality conditions are such that the sum over the ℓ's is removed[2]

$$\sum_q e^{iq\ell} = \begin{cases} 0 & (\ell \neq 0) \\ N & (\ell = 0) \end{cases}, \quad \sum_\ell e^{iq\ell} = \begin{cases} 0 & (q \neq 0) \\ N & (q = 0) \end{cases} .$$

The Hamiltonian is

$$H = \frac{1}{2} \sum_q \left\{ \frac{1}{m} P_q P_q^* + 2g(1 - \cos q) S_q S_q^* \right\} ,$$

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[2]Reference 1, p. 10

where P_q is the momentum canonically conjugate to the normal coordinates S_q and g is the second derivative of the interatomic potential function. Relative to the coordinates S_q, the expression

$$2g(1-\cos q),$$

is the one dimensional analogue of $\overleftrightarrow{G}$ in the general three dimensional Hamiltonian.

When the preceding argument is generalized to three dimensions[3] the Hamiltonian is of the form

$$H = \frac{1}{2}\sum_{q}\left\{\frac{1}{m}\vec{P}_{\vec{q}}\cdot\vec{P}^{*}_{\vec{q}} + \vec{S}_{\vec{q}}\cdot\overleftrightarrow{E}(\vec{q})\cdot\vec{S}_{\vec{q}}\right\},$$

where

$$\overleftrightarrow{E}(\vec{q}) = \sum_{h} e^{i\vec{q}\cdot\vec{h}}\,\overleftrightarrow{G}(\vec{h}).$$

The range of the summation is determined by the number of atoms involved in the interaction, such as the number of nearest neighbors. The expression $\overleftrightarrow{G}(\vec{h})$ is a result of the fact that the interaction of the atoms is dependent only on the relative distance vector between them, that is

$$\vec{h} = \vec{\ell} - \vec{\ell}'$$

This new Hamiltonian can be interpreted as the sum over q of the terms

$$H_{\vec{q}} = \frac{1}{2m}\vec{P}_{\vec{q}}\cdot\vec{P}^{*}_{\vec{q}} + \frac{1}{2}\vec{S}_{\vec{q}}\cdot\overleftrightarrow{E}(\vec{q})\cdot\vec{S}^{*}_{\vec{q}}\ .$$

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[3]Reference 1, p. 16

When expressed in its component form, $H\vec{q}$ takes the form

$$H\vec{q} = \frac{1}{2m}\sum_{a} P^{a}_{\vec{q}} P^{a*}_{\vec{q}} + \frac{1}{2}\sum_{a,b} S^{a}_{\vec{q}}\, E^{ab}(\vec{q})\, S^{b}_{\vec{q}}\,, \quad (a,b=1,2,3).$$

The equations of motion are

$$m\ddot{S}^{a}_{\vec{q}} = -\sum_{b} E^{ab}(-q)\, S^{b}_{\vec{q}}$$

the solution of which is

$$S^{a}_{\vec{q}} = m^{-\frac{1}{2}}\, e^{a}_{\vec{q}}\, \exp(i\nu t).$$

Substitution of this solution into the equations of motion results in a set of three simultaneous equations of the form

$$\sum_{b}\left\{\frac{1}{m}E^{ab}(\vec{q}) - \nu^{2}_{q}\,\delta_{ab}\right\} e^{b}_{\vec{q}} = 0.$$

This is a three by three matrix. The determinant of the matrix in the brackets must vanish for a consistent solution.

At this point specific application of the theory can be made to the problem of the face-centered cubic lattice.

CHAPTER III

FORMULATION OF THE FACE-CENTERED CUBIC LATTICE PROBLEM

Once the theory has been established, it is necessary to apply it to an actual physical array. An assumption is made as to the relative effect of the interaction of an atom with the surrounding array. We here assume that all but the interaction resulting from the nearest and next nearest neighbors can be ignored. The effect of the other neighbors is shielded by the nearer neighbors. The relative effect of the two nearest neighboring arrays is of primary concern in this development.

In applying the theory to the face-centered cubic lattice and restricting the problem to the nearest and next nearest neighbor interaction, a secular determinant, that is the determinant of the matrix developed in the theory, is generated. An atom in the face-centered cubic lattice has twelve nearest neighbors and six next nearest neighbors (Fig. 2), (Fig. 3).

Let the following symbols and notations bear the assigned meanings:

γ = The Hooke's law central force constant resulting from the interaction with the next nearest neighbors. (This is possible because of the

harmonic approximation).

α = The Hooke's law central force constant resulting from the interaction with the nearest neighbors.

$\lambda^2 = 2\pi m \nu^2/\alpha$, where m is the mass of each particle and ν is the frequency which is the result of the vibrational mode analysis in the theory.

The secular determinant for the face-centered cubic lattice for the nearest and next nearest neighbor approximation may be shown to be

$$\begin{vmatrix} 2 + 2\gamma/\alpha S^2x - C_x(C_y+C_z) - \lambda^2 & S_x S_y & S_x S_z \\ S_x S_y & 2 + 2\gamma/\alpha S^2y - C_y(C_x+C_z) - \lambda^2 & S_y S_z \\ S_x S_z & S_y S_z & 2 + 2\gamma/\alpha S^2z - C_z(C_x+C_y) - \lambda^2 \end{vmatrix} = 0$$

where

$$S_x = \sin(x) \qquad C_x = \cos(x)$$
$$S_y = \sin(y) \qquad C_y = \cos(y)$$
$$S_z = \sin(z) \qquad C_z = \cos(z) \,.$$

X, Y, Z space is defined as the space which contains all the discrete permissible points which satisfy the expanded secular determinant. A line drawn from the origin of this X, Y, Z space to a permissible point is in the direction of and proportional in length to the wave

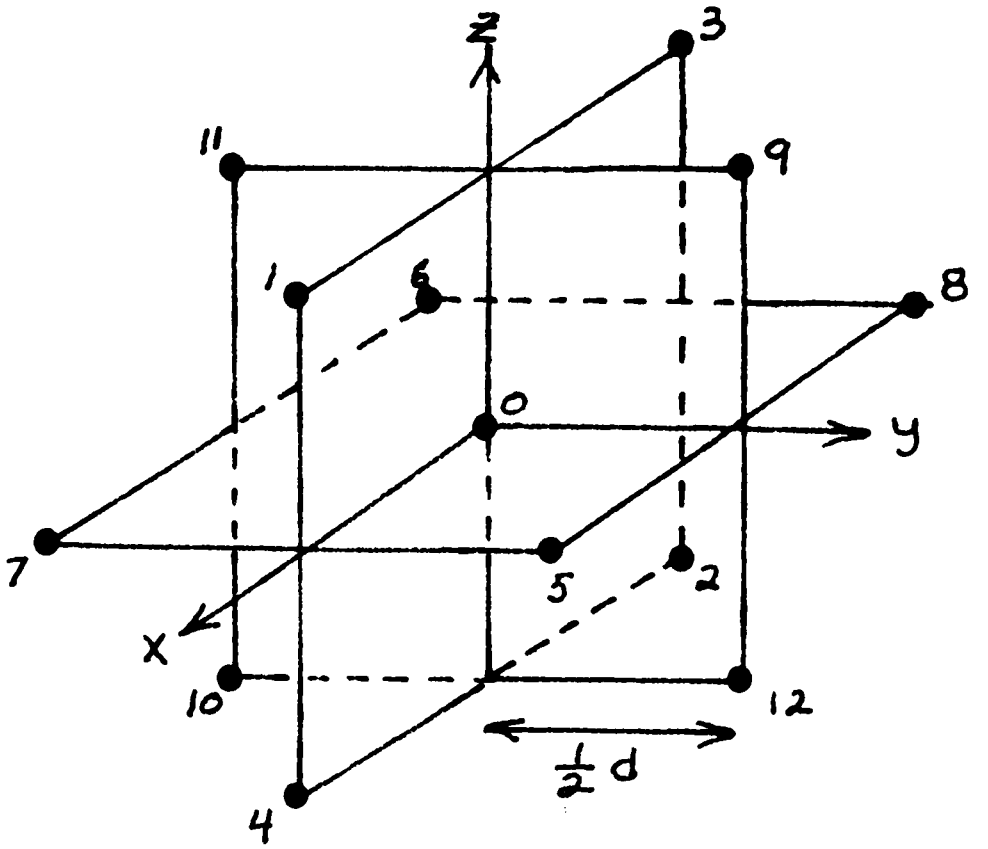

Fig. 2. The twelve nearest neighbors of the atom 0 in the face-centered cubic lattice.

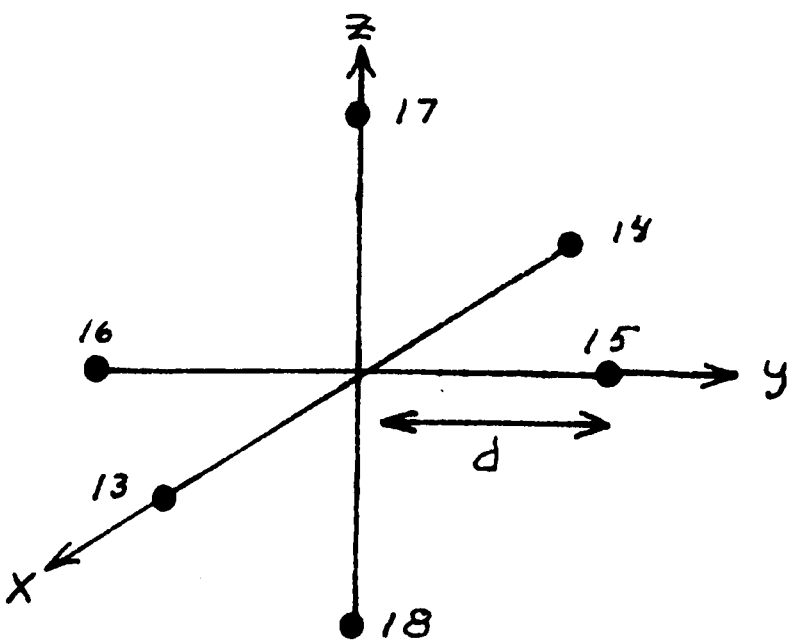

Fig. 3. The six next nearest neighbors of the atom 0 of the face-centered cubic lattice.

vector $\vec{q}$.[4] The wave vector $\vec{q}$ is restricted much the same way as the wave number q was in the linear chain. That is $-\pi < q_1, q_2, q_3 \leq \pi$ where q_1, q_2, q_3 refers to the components of the wave vector in X, Y, Z space.

When expanded the secular determinant gives a cubic equation in λ^2 . With a particular point (X, Y, Z) a solution is obtained for three different frequencies porportional to λ^2 . The same is true for any other permissible point in the X, Y, Z space. Conversely there are three points (X, Y, Z) for each value of λ^2 .

By substituting a density of points for a discrete set of points the problem reduces to one of finding the distribution function G (λ) of the frequencies. The (X, Y, Z) points will lie on a continuous surface of constant frequency in X, Y, Z space. Because the secular determinant is a cubic equation there are three surfaces of constant frequency which pass through any point.

G (λ) is defined to be proportional to the rate of change of volume, enclosed by a constant frequency surface belonging to a λ , with respect to a change in λ .

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[4]Reference 1, p. 22

$$G(\lambda) = \frac{1}{V_o} \frac{dV}{d\lambda}$$

where V_o is the volume of the space containing all the permissible points.

Because of the symmetry properties exhibited by the secular determinant only a portion of the enclosed surfaces need concern us. With this in mind, the following boundaries were established: the planes $y=o$, $x=y$, $x=z$, (symmetry planes) and $z=\pi$, $x=\frac{\pi}{2}$.[5] (Fig. 4). The three families of surfaces are called branches. The cubic equation in λ^2 is easily factored in the boundary planes. The three branches can be uniquely identified in the factored form in all the symmetry planes by finding the points of juncture along the lines of intersection of any two of the boundary planes.

As an illustration we shall present some of the factored expressions and show for one case how identification is made.

BRANCH I

Plane $y=o$:

$$\lambda^2_1 = 2 - \frac{1}{2} C_x - \frac{1}{2} C_z - C_x C_z + \frac{r}{\alpha} S^2_x + \frac{r}{\alpha} S^2_z$$
$$- \left(\left[\frac{r}{\alpha} S^2_x - \frac{r}{\alpha} S^2_z - \frac{1}{2} C_x + \frac{1}{2} C_z \right]^2 + S^2_x S^2_z \right)^{\frac{1}{2}}$$

Plane $x=y$:

$$\lambda^2_1 = 1 - C_x C_z + \frac{r}{\alpha} S^2_x$$

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[5] Robert B. Leighton, Reviews of Modern Physics, Vol. 20, No. 1, (1948), p. 165

BRANCH II

Plane $y = 0$:

$$\lambda_2^2 = 2 - C_x - C_z$$

Plane $x = y$:

$$\lambda_2^2 = \frac{3}{2}(1 - C_x C_z) + \left(1 + \frac{\pi}{\alpha}\right) S_x^2 + \frac{\pi}{\alpha} S_z^2$$

$$- \frac{1}{2}\left(\left[1 - C_x C_z - \left(2 + 2\frac{\pi}{\alpha}\right) S_x^2 + 2\frac{\pi}{\alpha} S_z^2\right]^2 + 8 S_x^2 S_z^2\right)^{\frac{1}{2}}$$

BRANCH III

Plane $y = 0$:

$$\lambda_3^2 = 2 - \frac{1}{2} C_x - \frac{1}{2} C_z - C_x C_z + \frac{\pi}{\alpha}(S_x^2 + S_z^2)$$

$$+ \left(\left[\frac{\pi}{\alpha} S_x^2 - \frac{\pi}{\alpha} S_z^2 - \frac{1}{2} C_x + \frac{1}{2} C_z\right]^2 + S_x^2 S_z^2\right)^{\frac{1}{2}}$$

Plane $x = y$:

$$\lambda_3^2 = \frac{3}{2}(1 - C_x C_z) + \left(1 + \frac{\pi}{\alpha}\right) S_x^2 + \frac{\pi}{\alpha} S_z^2$$

$$+ \frac{1}{2}\left(\left[1 - C_x C_z - \left(2 + 2\frac{\pi}{\alpha}\right) S_x^2 + 2\frac{\pi}{\alpha} S_z^2\right]^2 + 8 S_x^2 S_z^2\right)^{\frac{1}{2}}$$

The line of intersection of the two planes, $y = 0$, $x = y$ is of course the Z axis.

BRANCH I

Plane $y = 0$ at $x = 0$:

$$\lambda_1^2 = 1 - C_z$$

Similarly, plane $x = y$ at $x = 0$:

$$\lambda_1^2 = 1 - C_z$$

The three factored expressions for each of the branches can be uniquely defined in a similar way in all of the boundary planes.

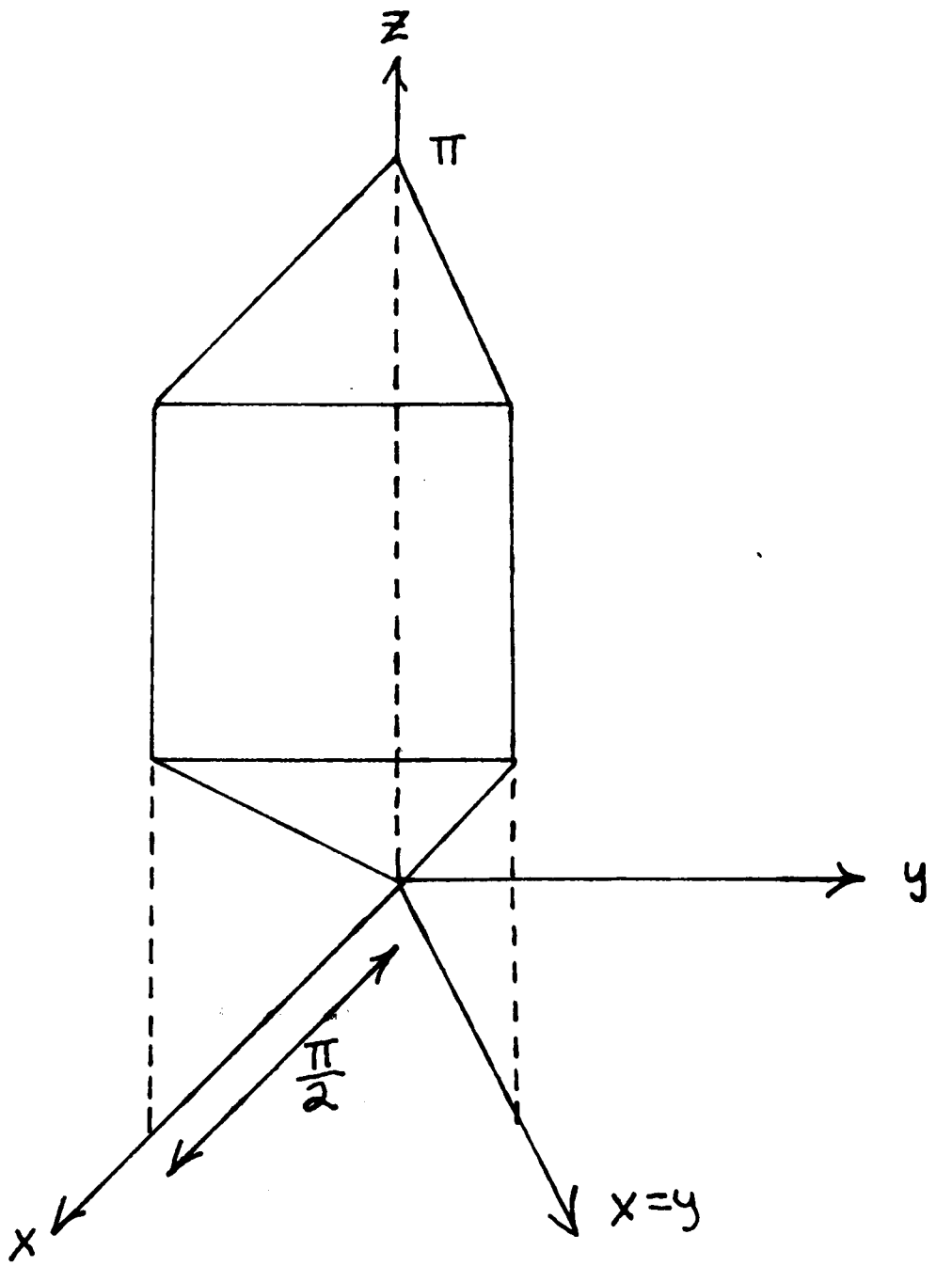

Fig. 4. Boundary of the Surfaces of Constant Frequency

CHAPTER IV

COMPLEXITIES OF THE PROBLEM

Until the advent of the high speed digital computer, only laborious approximate methods for obtaining the frequency spectrum of any lattice had been devised. It requires a great deal of arithmetical labor simply to obtain a number of constant frequency curves in the various boundary planes. In order to study in detail how $\frac{\gamma}{\alpha}$ affects these curves, a number of values of the ratio must be used. This in itself multiplies the labor involved many times. With this provided, one is still comparatively in the dark as to the shape of the surfaces for the various branches. These complexities arise due to the transcendental form of the secular equation. The numerical methods that must be used in the solution are imposing indeed. There is another complicating factor which plays an important part in the problem, that is, in order to get a clear picture of the spectrum, G (λ) must be treated as a continuous function. This means that the increment in λ affects the result of the analysis to a considerable extent. It is necessary to know to what extent, and where the limit of its influence lies.

The method for obtaining the frequency spectrum as given in this paper largely overcomes all of these complexities.

CHAPTER V

THE DIGITAL COMPUTER PROGRAM FOR DETERMINING THE FREQUENCY SPECTRUM

The method as outlined is one in programing the problem for a computer with a capacity equivalent to, or greater than the IBM 709. The problem was programed in the Fortran II system.

Use is made of the fact that the surfaces of constant frequency intercept the symmetry planes of the boundary perpendicularly.[6] The intercept of the constant frequency curves with the Z axis can be obtained easily with the computer. The Z intercept provides a unique starting point for generating the surfaces. Branches I and II for $\lambda^2 \leqslant 2$ have the same Z intercept. $\lambda^2 = 2$ is the maximum λ^2 for Branch I. For greater values of λ, Branch II no longer intercepts the Z axis; however, a factored expression for Branch II is available in the plane $Z = \pi$, which it does intercept. For $2 < \lambda^2 \leqslant 3$ this expression provides a unique starting point for Branch II. $\lambda^2 = 3$ is the maximum λ^2 for Branch II. Branch III has a Z intercept for all values of λ^2 up to its maximum which is $\lambda^2 = 4$.

We now start working with polar coordinates in X, Y, Z space. Picture a surface of constant frequency (Fig. 5).

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[6] Reference 5, p. 165

For any particular values of coordinate angles Θ and Φ within the boundary limits, the radial coordinate r, penetrates the surface at a point. What we want is a sufficiently large number of these points, belonging to a particular λ, to provide us with an accurate picture of the surface. Actually r penetrates three surfaces belonging to λ, one for each branch. The secular determinant is transcendental and numerical methods must be used to obtain the penetration points.

With a starting point along the Z axis we start systematically walking away from the Z axis. Starting with $\Phi = 0$, that is in the $y = 0$ plane, for a particular λ, values of r for increasing Θ are found. Θ is increased in steps by an increment $\Delta\Theta$ until either r or Θ reaches its respective boundary. The procedure is repeated for increased Φ. Φ is increased by steps by an increment $\Delta\Phi$ until it too reaches its boundary limit (45^{o}, the plane $x = y$). The volume under this surface of points is then determined. Now λ is increased by an increment and the above procedure is repeated until λ reaches its respective maximum value for each branch. This provides us with enough information to evaluate the frequency spectrum.

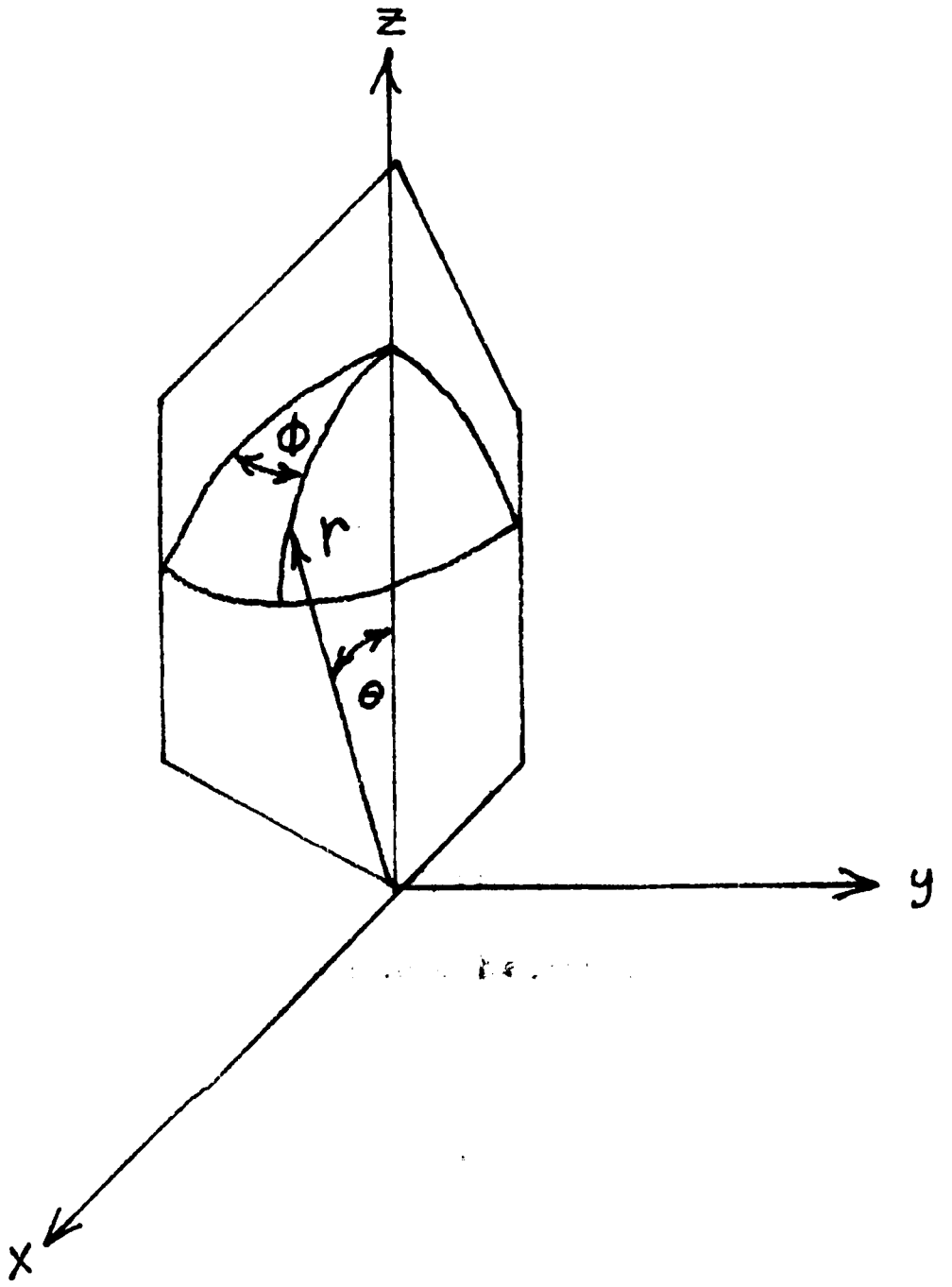

Fig. 5. Surface of Constant Frequency with One Penetration, r .

CHAPTER VI

DEVICES AND METHODS USED IN THE CODE

Because the secular determinant is transcendental it is necessary to build into the program certain numerical techniques for finding the values of r belonging to a definite angular position. This is done by providing a trial value for r and then using the Newton-Raphson method[7] to converge on a solution point. This iterative convergence routine was programed so as to give results to six place accuracy. In the actual code several of these convergence routines were used, each one making use of either the factored expressions of the secular determinant for the various branches, or the secular determinant itself. Use of the factored expressions provided a definite separation of the three branches belonging to a given λ in the symmetry planes. This is an aid in arriving at a trial value of r and in separating the three branches wherever the factored expressions are not available.

The method of arriving at a trial value of r is that of a parabolic extrapolation. This is permitted in any plane of ϕ with one exception. Whenever $\phi=\Delta\phi$ a linear

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[7] J. B. Scarborough, Numerical Mathematical Analysis (The Johns Hopkins Press, Baltimore, 1958) p. 192.

approximation is used to obtain a trial value of r . This is justified by remembering that the surfaces intercept the Z axis perpendicularly, and because we have been able to establish the value of the z intercept. By making use of the symmetry properties wherever necessary the trial value for the general $r(\theta > \Delta\theta)$ is found by fitting a parabola[8] to the three preceding values of r belonging to the current ϕ plane. The trial value of r was taken to be that which would be the next point on the parabola. In this manner a large number of points on the surfaces are obtained. The number of points depends entirely on the size of the increments $\Delta\theta$ and $\Delta\phi$. The r's for a particular value of λ for each branch are stored in the computer memory in an array.

The volume under any particular surface of constant frequency is found by summing up small volume elements. Each element of volume belongs to one r array point on the surface.

$$\Delta V = \frac{1}{3}\ \Delta\theta\Delta\phi r^3 \sin\theta$$

With $\frac{n}{\alpha}$ set, the volumes beneath a number of constant frequency surfaces for each branch are determined.

Actually, the memory of the computer has stored an

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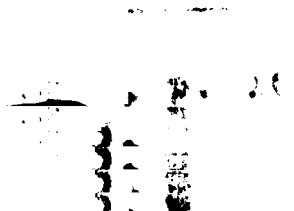
8 F. B. Hildebrand, Introduction to Numerical Analysis, McGraw-Hill Book Company, Inc. (1956) p. 61

array of volumes for each branch. There is a volume corresponding to every value of λ used by the program. The points in this volume array can be thought of as the curve V vs. λ . The program then allows the computer to take any three consecutive points on this curve and fit a parabola to them. Then it evaluates the derivative of the parabola at the value of the second of the three points. This procedure is repeated until $\frac{dV}{d\lambda}$ is evaluated at every point of the curve. Another array of values is thus obtained, that is, G (λ) the distribution function.

A graph of G (λ) is found for each of the three branches [G (λ) vs. λ]. The sum of the curves G (λ) for each branch constitutes the lattice spectrum.



CHAPTER VII

RESULTS

Fig. (6) is a plot of volume vs. λ for the three branches with $\frac{\gamma}{\alpha}$ set equal to zero. The upper limit is the volume maximum set by the boundary conditions. Branches I and II are remarkably smooth considering the nature of the function generating them. The sudden increase in the Branch III volume at the higher values of λ is surprising but not totally unexpected.

Fig. (7) is a plot of the unnormalized distribution function G (λ) vs. λ , for each of the three branches with $\frac{\gamma}{\alpha}$ set equal to zero, that is, ignoring the next nearest neighbor interaction. Branch III requires some extrapolation at values greater than N=22 due to the method used to evaluate volumes exceeding the limits set by the boundary conditions. This extrapolation is substantiated in the data generated by the array which produce the points on the surfaces of constant frequency.

The results plotted in Fig. (7) are to be compared with those obtained by Leighton,[9] Fig. (8). In this cited work the volumes of constant frequency were obtained using plaster-of-paris models. Of particular note in Fig. (7) is the complementary nature of the three branches yielding a comparatively smooth total spectrum.

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[9] Reference 5, p. 165

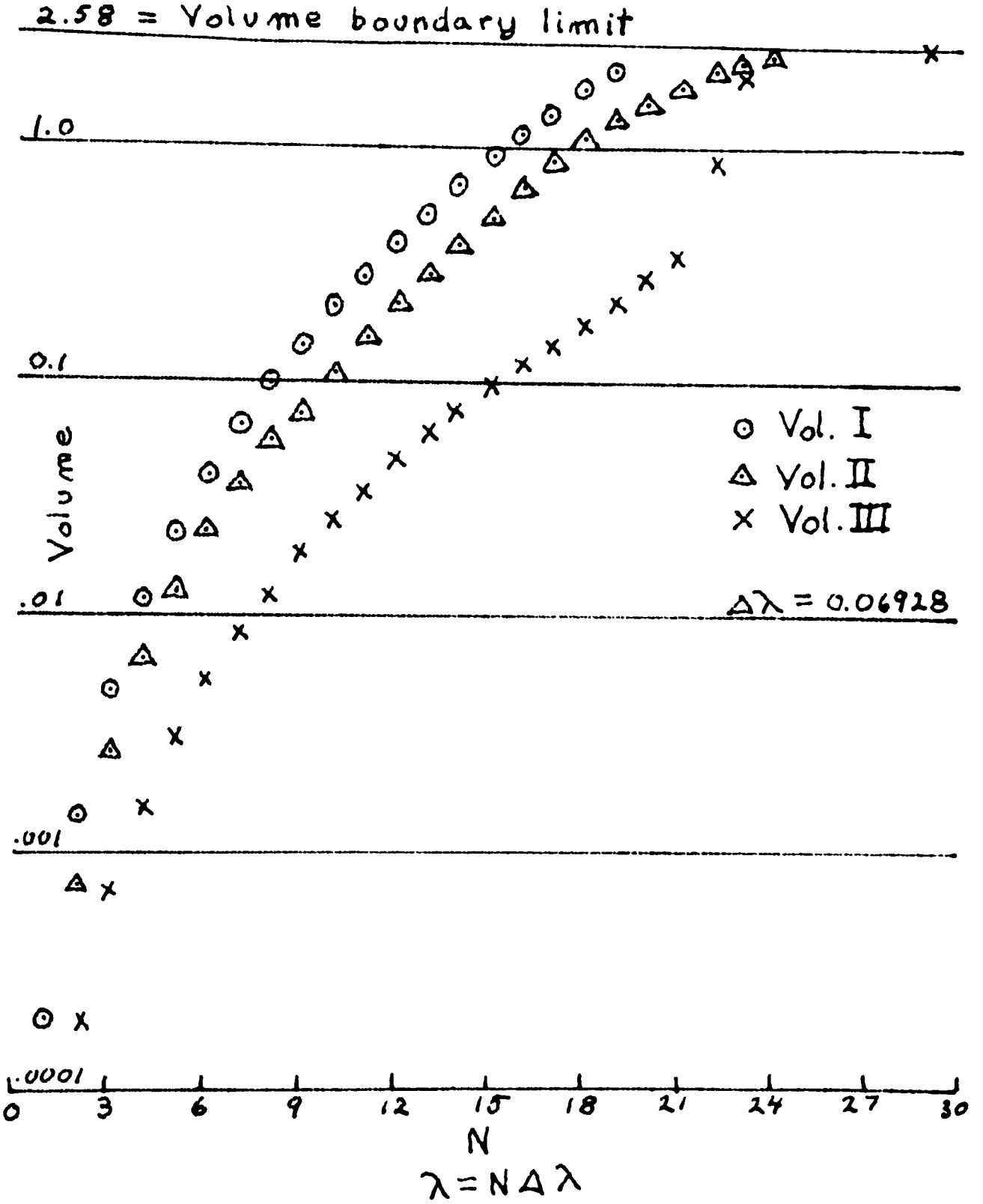
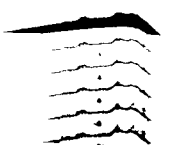


Fig. 6

Volume vs. λ , for $\frac{\tau}{\alpha} = 0$



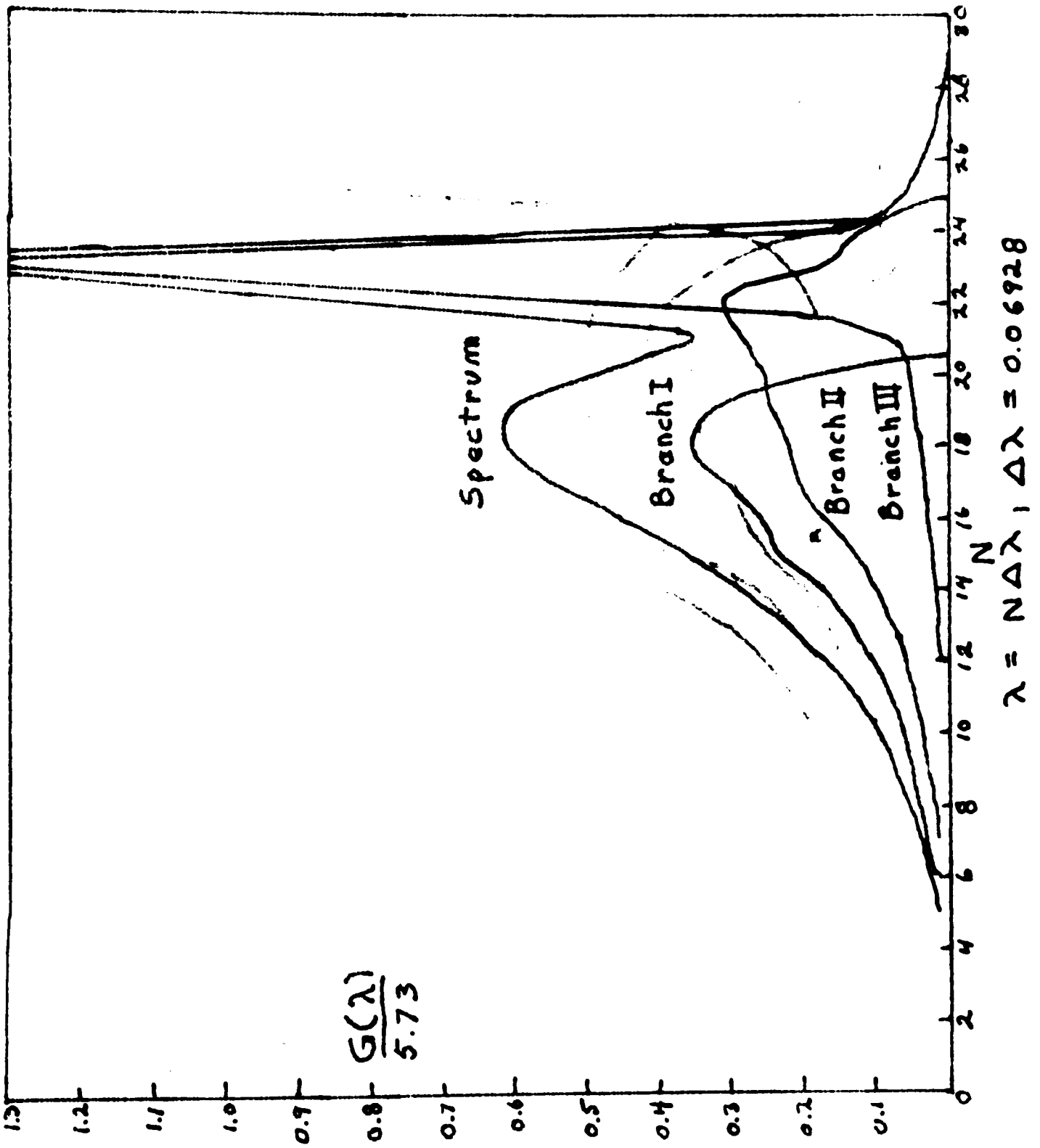


Fig. 7

The un-normalized distribution function for $\frac{\alpha}{\gamma} = 0$

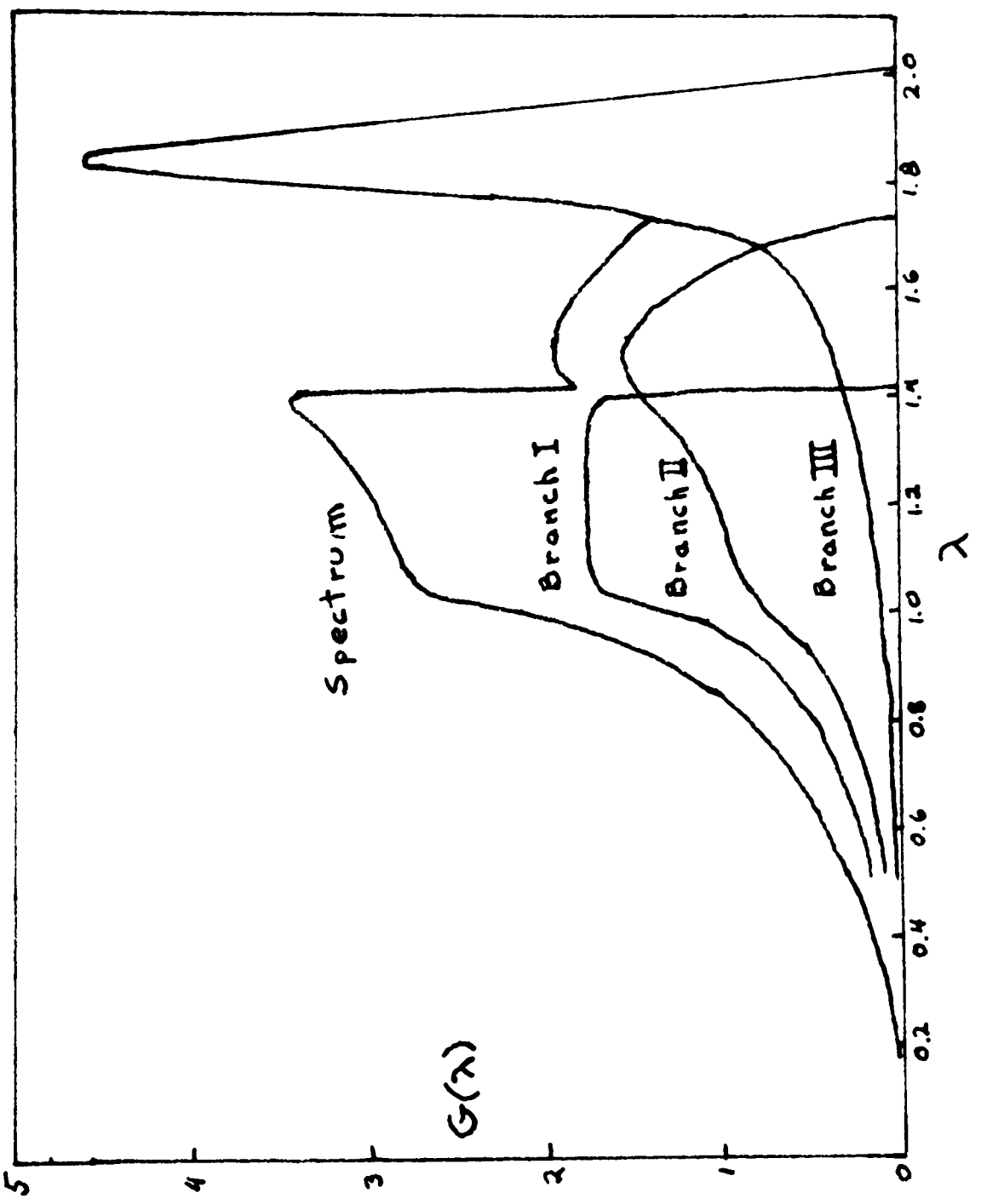


Fig. 8

The frequency spectrum of a face-centered cubic lattice according to Leighton ($\frac{\gamma}{\alpha}=0$)

CHAPTER VIII

CONCLUSIONS

The method of programing the problem of determining the frequency spectrum has left as parameters the following: $\Delta\theta$, $\Delta\phi$, $\Delta\lambda$, $\frac{\tau}{\alpha}$. It should be pointed out that the incremental terms are to be chosen sufficiently small so that this approximation is consistent with the overall dimensions of the program.

It is readily seen that the overall program can be adapted to other lattice structures by using the appropriate secular equation wherever called for in the program.

The program as described should be particularly valuable in the analysis of the inert gas solids, with the possible exception of helium. The central force interaction is physically realizable in these nearly perfect (theoretically perfect) crystals. Empirical evidence along with some previous work along this same line have indicated that letting the interaction reach no further than that of the next nearest neighbor is quite sufficient.

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