ELECTRONIC EIGENVALUES AND EIGENFUNCTIONS IN CRYSTALS BY A PSEUDOPOTENTIAL METHOD

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by

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CONTENTS

CHAPTER I

CHAPTER II

CHAPTER III

ABSTRACT

The electronic band structure of a face-centred monatomic crystal is calculated by a plane wave method. A model pseudopotential is used depending on two adjustable parameters.

The object of this work is mainly to investigate how the change of the potential affects the band structure, for the case of a potential similar in some respect to pseudopotentials which have been used for real metals.

A detailed calculation is made for the points of symmetry and along the axis of symmetry within the Brillouin Zone. Five different sets of parameters for the pseudopotential are considered and the corresponding Energy v. Wave vector graphs are plotted.

Also the coefficients of the Fourier expansion of the wave function, the so-called momentum eigenfunctions, are plotted against the wave vector $\underline{k}$ in an extended zone scheme.

The features of the band structure which are independent of the potential and those which are sensitive to any change of it are found.

Finally the results given by this model are compared with the band structure of actual elements having a face-centred cubic lattice.

CHAPTER I

1. The Symmetry Operations of Crystals

The diffraction of X-rays by solids applied to the study of crystal structure, showed a regularity of the atomic arrangement. Thus a crystal can be divided into unit cells each one containing one or more atoms.

If we consider a point in a unit cell we may obtain any other equivalent point (called lattice point) in another unit cell, by a linear combination of three non-coplanar vectors $\underline{a}_1$, $\underline{a}_2$, $\underline{a}_3$ that is by the following translation operation,

$$\underline{R}_n = n_1\underline{a}_1 + n_2\underline{a}_2 + n_3\underline{a}_3 \qquad (1.1)$$

where n_1, n_2, n_3 are integers. The vectors $\underline{a}_1$, $\underline{a}_2$, $\underline{a}_3$ are called primitive vectors and the infinite three dimensional array of points derived by using the operation $\underline{R}_n$ is called Bravais lattice. There are 14 such lattices.

In addition to the translational operations, crystals possess the symmetry operations of the point group, which consist of rotations and reflections that leave the crystal invariant.

Combining the rotation and reflection operations of a point group with translations we form a space group. There are 230 possible space groups, which are made by combining 14 different sets of vectors $\underline{a}_1$, $\underline{a}_2$, $\underline{a}_3$ (leading to the Bravais lattices), with 32 possible point groups. Each of these 32 point groups is said to form a crystal class.

In this work we are concerned with the face-centred cubic lattice, for which the space group is denoted by O_h^5 and the corresponding point group by O_h.

The requirements which must be satisfied when operations are to form a group are the following:

a) The successive application of two operations of the group must give an operation of the group. Thus a multiplication table exists for each group.

b) The identity and the inverse operation to each operation must be included in the set of operations.

c) The associative law holds. That is three operations R_1, R_2, R_3 satisfy the equation:

$$R_1(R_2 R_3) = (R_1 R_2) R_3$$

2. The Unit Cells

A unit cell is the smallest volume of a crystal lattice which will generate this lattice through the use of the primitive translation.

The fourteen Bravais lattices are classified into the following seven systems : the cubic, triclinic, monoclinic, orthorhombic, tetragonal, trigonal and hexagonal. In the cubic system there are three Bravais lattices called the simple cubic, the face-centred cubic and the body centred cubic lattices.

We consider the face centred cubic lattice and construct the unit cell for it. We take a cube of side a (fig.1)

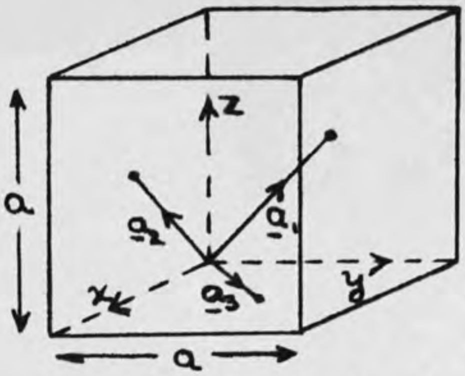

Fig. 1

This cube can not be a unit cell since it contains four lattice points. So we choose the three vectors

$$\underline{a}_1 = a/2\,(\underline{j}+\underline{k}) \qquad \underline{a}_2 = a/2\,(\underline{k}+\underline{i}) \qquad \underline{a}_3 = a/2\,(\underline{i}+j) \qquad (2.1)$$

as the primitive vectors for the face-centred cubic lattice. The unit cell is then the parallelopiped bounded by these vectors. Its volume is :

$$\Omega = \underline{a}_1\,(\underline{a}_2 \times \underline{a}_3) = a^3/4 \qquad (2.2)$$

But thisunit cell does not show the symmetry of the point group. To make use of this symmetry an alternative construction for the unit cell of a monatomic substance, has been made by Wigner and Seitz in the following way:

We draw lines connecting an atom to its nearest and next nearest neighbour and consider the planes bisecting these lines perpendicularly. Now the smallest polyhedron surrounding the central atom and bounded by these planes is the Wigner - Seitz cell. In the case of the face-centred cubic lattice the W-S cell is a rhombododecahedron which remains unchanged under the operations of the cubic point groups (Fig. 2)

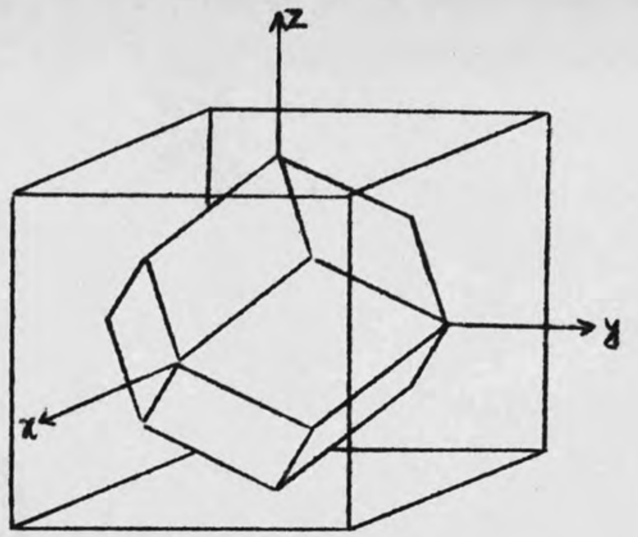

Fig. 2

3. Bloch's Theorem

Considering the periodic electrostatic field in which an electron moves within a crystal and neglecting any surface effects, the potential energy of the electron is periodic with the periodicity of the lattice, that is

$$V(\underline{r}) = V(\underline{r}+\underline{R}_n) \qquad (3.1)$$

where $\underline{R}_n$ is defined by equation (1.1)

This potential includes the nuclear attraction and the averaged repulsions of the other electrons. So for consistency the electron distribution must have the same periodicity as the potential, i.e.

$$\left|\psi(\underline{r}+R_n)\right|^2 = \left|\psi(\underline{r})\right|^2 \qquad (3.2)$$

or $$\psi(\underline{r}+\underline{R}_n) = e^{i\theta}\psi(\underline{r}) \qquad (3.3)$$

where θ is a phase shift which is fixed for a given displacement $\underline{R}_n$ So from equation (1.1) we conclude that θ is proportional to $\underline{R}_n$ i.e.

$$\theta = \underline{k}\cdot\underline{R}_n \qquad (3.4)$$

where $\underline{k}$ is a real vector, called the wave vector, which characterizes the wave function of an electron in a periodic potential.

Using equations (3.3) and (3.4) one finds:

$$\psi_{\underline{k}}(\underline{r}+R_n) = e^{i\underline{k}\underline{R}_n}\psi_{\underline{k}}(r) \qquad (3.5)$$

This is known as Bloch's theorem and is taken as boundary condition to solve Schrodinger's equation in the periodic potential.

The following equivalent form of this theorem can be found by introducing a function $u_k(\underline{r})$, which satisfies the relation:

$$\psi_{\underline{k}}(\underline{r}) = e^{i\underline{k}\cdot\underline{r}}u_{\underline{k}}(\underline{r}) \qquad (3.6)$$

Using (3.5) and (3.6),

$$\psi_{\underline{k}}(\underline{r}+\underline{R}_n) = e^{i\underline{k}(\underline{r}+\underline{R}_n)}u_{\underline{k}}(\underline{r}+\underline{R}_n) = e^{i\underline{k}\cdot\underline{R}_n}e^{i\underline{k}\cdot\underline{r}}u_{\underline{k}}(\underline{r}) \qquad (3.7)$$

which gives $$u_{\underline{k}}(\underline{r}+\underline{R}_n) = u_{\underline{k}}(\underline{r}) \qquad (3.8)$$

that is $u_{\underline{k}}$ has the periodicity of the lattice.

If $u_{\underline{k}}$ is a constant the wave function becomes

$$\psi(\underline{r}) = e^{i\underline{k}\cdot\underline{r}} \qquad (3.9)$$

which is the solution of Schrodinger's equation for a constant potential.

Consider the translation operators $T(\underline{R}_n)$ which satisfy the condition:

$$T(\underline{R}_n)f(\underline{r}) = f(\underline{r}+R_n) \qquad (3.10)$$

where $f(\underline{r})$ is any function of position.

As a result of (3.1) the operators $T(\underline{R}_w)$ commute with the Hamiltonian operator,

$$H = -\hbar^2/2m\ \nabla^2 + V(\underline{r}) \qquad (3.11)$$

Therefore the wave function of the electron may be chosen to be simultaneously an eigenfunction of the energy and of all translations $T(\underline{R}_w)$. Hence the wave vector $\underline{k}$ is a constant of the motion and also may be considered as a set of three quantum numbers which label the various crystal states.

It can also be proved, by applying the correspondence principle and Hamilton's equations, that $\underline{k}$ satisfies the following relations:

$$\underline{F} = \hbar\, d\underline{k}/dt \qquad \underline{v}(\underline{k}) = 1/\hbar\ \mathrm{grad}_{\underline{k}} E(\underline{k}) \qquad (3.12)$$

where $\underline{F}$ is an external force acting on the electron and $\underline{v}(\underline{k})$ is the average velocity of the electron in a stationary state.

From equation (3.12), which expresses a Newtonian law, one notices that the quantity $\hbar\underline{k}$ - called crystal momentum- plays the role of the classical momentum.

4. The Reciprocal Lattice and the Brillouin Zones

The study of the wave vector $\underline{k}$ led to the idea of the reciprocal lattice. This lattice is defined as follows:

A set of vectors $\underline{b}_1$, $\underline{b}_2$, $\underline{b}_3$ and the primitive vectors $\underline{a}_1$, $\underline{a}_2$, $\underline{a}_3$ of the Bravais lattice are required to satisfy the following condition:

$$\underline{a}_i \underline{b}_j = 2\pi\delta_{ij} \qquad (i,j = 1,2,3) \qquad (4.1)$$

where δ_{ij} is the Kronecker's delta.

The meaning of this relation is that the vectors $\underline{b}_1$, $\underline{b}_2$, $\underline{b}_3$ are perpendicular to the planes of the axes $\underline{a}_1$, $\underline{a}_2$, $\underline{a}_3$. The vectors $\underline{b}_1$, $\underline{b}_2$, $\underline{b}_3$ are called reciprocal vectors and the linear combinations of them:

$$\underline{K}_m = m_1\underline{b}_1 + m_2\underline{b}_2 + m_3\underline{b}_3 \qquad (4.2)$$

defines a set of points which forms what is called reciprocal lattice, with $\underline{K}_m$ the fundamental vector of this lattice.

In order to consider the reciprocal lattice for the face-centred cubic lattice equation (4.1) is written in the equivalent forms:

$$\underline{b}_1 = 2\pi/D\ \underline{a}_2 \times \underline{a}_3 \quad \underline{b}_2 = 2\pi/D\ \underline{a}_3 \times \underline{a}_1 \quad \underline{b}_3 = 2\pi/D\ \underline{a}_1 \times \underline{a}_2 \qquad (4.3)$$

where $D = \underline{a}_1 (\underline{a}_2 \times \underline{a}_3)$

Then substituting $\underline{a}_1$, $\underline{a}_2$, $\underline{a}_3$ from equations (2.1) we find:

$$\underline{b}_1 = 2\pi/a(-\underline{i} + \underline{j} + \underline{k}) \quad \underline{b}_2 = 2\pi/a(\underline{i} - \underline{j} + \underline{k}) \quad \underline{b}_3 = 2\pi/a(\underline{i} + \underline{j} - \underline{k}) \qquad (4.4)$$

Now we may take as unit cell in the reciprocal space the parallelopiped whose sides are parallel to the vectors $\underline{b}_1$, $\underline{b}_2$, $\underline{b}_3$ (Fig.3)

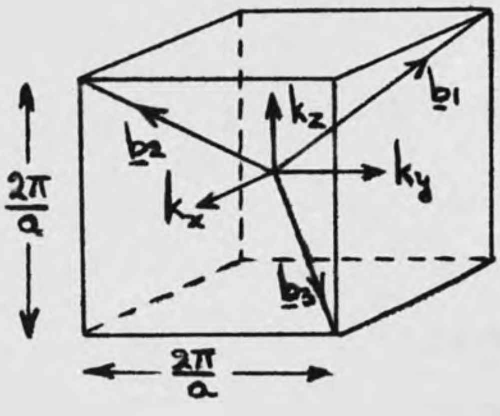

Fig. 3

The volume of this unit cell will be:

$$\Omega_B = \underline{b}_1 \, (\underline{b}_2 \times \underline{b}_3) = 32\pi^3/a^3 \qquad (4.5)$$

But again, as in the ordinary space, this parallelopiped does not possess the characteristic symmetry of the point group of the crystal. So a cell analogous to the Wigner - Seitz cell is constructed, which is called first Brillouin Zone and which remains invariant under the symmetry operations of the crystal. The B.Z. for the face-centred cubic lattice is a truncated octahedron (Fig.4)

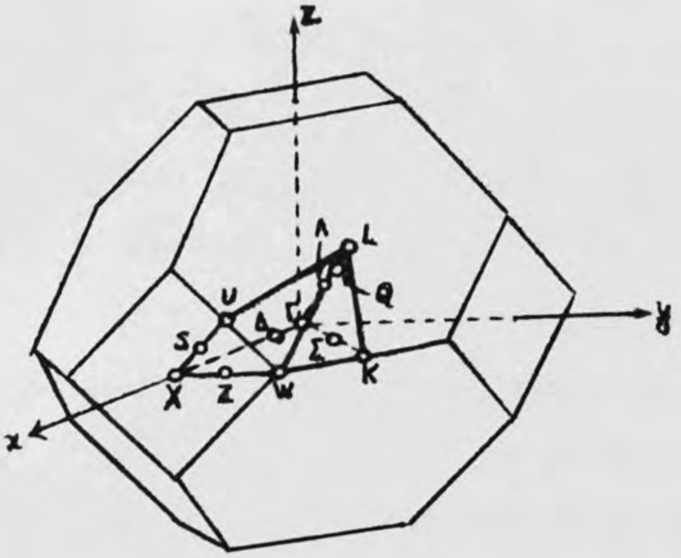

Fig. 4

Regions of the first Brillouin Zone may be translated through reciprocal lattice vectors to form polyhedra symmetrically surrounding the first zone. The region between the first zone and the second smallest polyhedra is then called the second Brillouin Zone. In the same way one may construct 3rd 4th etc. Brillouin Zones.

Since any point of the reciprocal space may be obtained by a lattice translation from a point in the first B.Z. all Brillouin Zones have the same volume Ω_B which, due to the definition of reciprocal lattice (equation 4.1) satisfies the following condition:

$$\Omega\Omega_B = (2\pi)^3 \qquad (4.6)$$

where Ω is the volume of the unit cell in ordinary space.

Since the wave function $\psi_k(r)$ is, according to Bloch's theorem, a periodic function of k such will also be the energy. So we solve Schrodinger equation by restricting the k vectors to the 1st Brillouin Zone. The energy is then a multivalued function of k (Reduced Zone Scheme).

An alternative way of finding the relation between the energy and the wave vector, is to let k be extended throughout the higher Zones. Now the energy is a singlevalued function of k and has a discontinuity on the boundaries of each Brillouin Zone. This procedure is called " Extended Zone Scheme ".

Both the reduced and extended zone schemes are equally valid and which one is used is a matter of convenience.

6

5. Classification of Crystal States

Since the electronic states of the crystals are identified by k vectors, we shall investigate the symmetry operations which leave the given k invariant. These operations form the point group of the given k and their number varies for the different k - points.

For the cubic structures at $k = 0$, there are 48 operations which leave a cube invariant. These operations form the full cubic group O_h and are divided into the following ten classes (Two operations R_1 , R_2 belong to the same class if there is some element X in the group such that $X^{-1}R_1X = R_2$):

1) The identity E which leaves the cube in its original position.
2) Class C_4. Six rotations by ±90° about an axis of fourfold symmetry.
3) Class C_4^2. Three rotations by 180° about the same axis.
4) Class C_2. Six rotations by 180° about an axis of twofold symmetry.
5) Class C_3. Eight rotations by ±120° about an axis of threefold symmetry.
6) The inversion J with respect to the origin.
7) Class JC_4, Combination of C_4 with the inversion.
8) Class JC_4^2. Combination of C_4^2 with the inversion.
9) Class JC_2. Combination of C_2 with the inversion.
10) Class JC_3. Combination of C_3 with the inversion.

We may describe the operations of the cubic group by considering a position vector R with components x, y, z. Then the possible rearrangements or permutations of x, y, z, including changes of sign, give the operations of the cubic group. (Table 1). We also reproduce from Slater (1965) the multiplication table (Table 2) of the point group T_d which contains the 24 operations of the first five classes of the full cubic group. To form the multiplication table of the point group O_h, we find the subscript of the product operation from Table 2; and if both factors are unprimed or both primed, the product operation is unprimed; if one is primed and the other unprimed, the product is primed.

It must be mentioned here that the Hamiltonian operator commutes with each operation of the point group, though these operators do not all commute with each other. This leads to the conclusion that the energy must have full cubic symmetry in k-space.

As a consequence of this we solve Schrodinger's equation for k vectors lying in the interior or on the surface of the first Brillouin zone. Only 1/48 of the zone need be considered since the zone has the full cubic symmetry. The symmetry points of the zone are labelled according to the notation suggested by Bouckaert, Smoluchowski and Wigner (1936). Thus referring to the figure 4, we list the symmetry points or the points along symmetry axes for the Brillouin Zone of a face-centred cubic lattice.

Γ : $2\pi/a$ (ooo) Δ : $2\pi/a$ (xoo)   where $o<x<1$

$X : 2\pi/a\ (100)$ $\qquad Z : 2\pi/a\ (1y0)$ where $0<y<\frac{1}{2}$

$W : 2\pi/a\ (1\frac{1}{2}0)$ $\qquad Q : 2\pi/a\ (x\frac{1}{2}z)$ where $\frac{1}{2}<x<1\ ,\ 0<z<\frac{1}{2}$

$L : 2\pi/a\ (\frac{1}{2}\frac{1}{2}\frac{1}{2})$ $\qquad \Lambda : 2\pi/a\ (xxx)$ where $0<x<\frac{1}{2}$

$\Sigma : 2\pi/a\ (xx0)$ where $0<x<\frac{3}{4}$ $\qquad K : 2\pi/a\ (\frac{3}{4}\frac{3}{4}0)$

6. The Irreducible Representations. Characters. Basis Functions.

If the elements of a group are substituted by square matrices B_n which follow the same multiplication table, the matrices are called a regular representation of the group. The order of the matrices, which is the same for all elements, is called the dimension of the representation.

To construct the regular representation of the full cubic group for instance, we consider a solution of Schrodinger equation for the wave vector $\underline{0} + \underline{K}_n$. Applying the operations of the full cubic group we obtain, in general, 48 different vectors corresponding to 48 different solutions of Shrodinger equation. So any operation of the group changes any solution ψ_i into one of the other 47 solutions or into itself. The operation which makes this transformation is a regular representation and it is represented by a 48 x 48 matrix, with only one element different from 0 in each row and column.

A matrix M is said to be the direct sum of matrices m_1, m_2... if all its elements are zero except for square blocks of terms (the sub-matrices m_1, m_2....) along the diagonal. Now if each matrix of a representation can be expressed as a direct sum, and the dimensions of the corresponding sub-matrices are the same in every case, then the sub-matrices are a representation of the group, and the original representation has been reduced. To carry out this reduction a unitary transformation U is applied, which brings the matrices B_n to the required form $M_n = U^{-1} B_n U$.

In the present wave mechanical problem the above reduction means that linear combinations of the eigenfunctions have been found, which have the symmetry of the point group.

If having applied unitary transformations, it is impossible to find any more of them which express a representation as a direct sum, then the sub-matrices themselves form irreducible representations of the group. For example in the case of the cubic group O_h the original 48 x 48 matrices can be expressed as the direct sum of four 3 x 3 matrices each repeated three times, two 2 x 2 matrices each repeated twice and four 1 x 1 matrices. That is the original representation is reduced to ten irreducible representations.

The traces of the matrices of an irreducible representation are called characters, usually denoted by χ. All operations of one class have the same character. The calculation of the characters depends on two theorems which we state without proof.

A) The number of irreducible representations is equal to the number of classes.

B) The sum of the squares of the dimensions of the representations equals the number of elements of the group.

In a band structure calculation one needs to know functions which transform according to a row of a particular irreducible representation. These functions are called basis functions and can be found by considering elements of the form $x^n y^m z^\ell$ and their linear combinations.

In the following pages we reproduce from Slater (1965) and Callaway (1964) tables with the matrix elements, the characters and the basis functions for the irreducible representations to be used in our calculations.

In writing Chapter I we had in mind a series of postgraduate lectures on Energy Band Theory given by Dr. L. Pincherle and the text books by Jones (1960), Callaway (1964), Ziman (1964) and Slater (1965).

TABLE I

THE CUBIC GROUP

Class	Operation				Class	Operation			
E	R_1:	x	y	z	J	R'_1:	-x	-y	-z
C_4^2	R_2:	x	-y	-z	JC_4^2	R'_2:	-x	y	z
	R_3:	-x	y	-z		R'_3:	x	-y	z
	R_4:	-x	-y	z		R'_4:	x	y	-z
C_3	R_5:	y	z	x	JC_3	R'_5:	-y	-z	-x
	R_6:	-y	z	-x		R'_6:	y	-z	x
	R_7:	-y	-z	x		R'_7:	y	z	-x
	R_8:	y	-z	-x		R'_8:	-y	z	x
	R_9:	z	x	y		R'_9:	-z	-x	-y
	R_{10}:	-z	-x	y		R'_{10}:	z	x	-y
	R_{11}:	z	-x	-y		R'_{11}:	-z	x	y
	R_{12}:	-z	x	-y		R'_{12}:	z	-x	y
C_4	R_{13}:	-x	z	-y	JC_4	R'_{13}:	x	-z	y
	R_{14}:	-x	-z	y		R'_{14}:	x	z	-y
	R_{15}:	-z	-y	x		R'_{15}:	z	y	-x
	R_{16}:	z	-y	-x		R'_{16}:	-z	y	x
	R_{17}:	y	-x	-z		R'_{17}:	-y	x	z
	R_{18}:	-y	x	-z		R'_{18}:	y	-x	z
C_2	R_{19}:	x	z	y	JC_2	R'_{19}:	-x	-z	-y
	R_{20}:	x	-z	-y		R'_{20}:	-x	z	y
	R_{21}:	z	y	x		R'_{21}:	-z	-y	-x
	R_{22}:	-z	y	-x		R'_{22}:	z	-y	x
	R_{23}:	y	x	z		R'_{23}:	-y	-x	-z
	R_{24}:	-y	-x	z		R'_{24}:	y	x	-z

Table 2

Multiplication table for Group T_d. Table gives k, where $R_iR_j = R_k$

$i \backslash j$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
1	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
2	2	1	4	3	7	8	5	6	12	11	10	9	14	13	21	22	24	23	20	19	15	16	18	17
3	3	4	1	2	8	7	6	5	10	9	12	11	20	19	16	15	23	24	14	13	22	21	17	18
4	4	3	2	1	6	5	8	7	11	12	9	10	19	20	22	21	18	17	13	14	16	15	24	23
5	5	8	6	7	9	12	10	11	1	4	2	3	18	24	14	20	16	22	23	17	19	13	21	15
6	6	7	5	8	11	10	12	9	4	1	3	2	17	23	20	14	21	15	24	18	13	19	16	22
7	7	6	8	5	12	9	11	10	2	3	1	4	23	17	13	19	22	16	18	24	20	14	15	21
8	8	5	7	6	10	11	9	12	3	2	4	1	24	18	19	13	15	21	17	23	14	20	22	16
9	9	11	12	10	1	3	4	2	5	7	8	6	22	15	24	17	20	13	21	16	23	18	19	14
10	10	12	11	9	3	1	2	4	8	6	5	7	21	16	18	23	13	20	22	15	17	24	14	19
11	11	9	10	12	4	2	1	3	6	8	7	5	15	22	23	18	14	19	16	21	24	17	13	20
12	12	10	9	11	2	4	3	1	7	5	6	8	16	21	17	24	19	14	15	22	18	23	20	13
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22	22	15	21	16	17	24	18	23	14	19	13	20	11	9	2	4	5	7	10	12	3	1	8	6
23	23	17	18	24	19	13	14	20	21	15	16	22	6	7	10	11	2	3	5	8	9	12	1	4
24	24	18	17	23	13	19	20	14	16	22	21	15	5	8	12	9	3	2	6	7	11	10	4	1

Table 3

Matrix elements and characters at point Γ, cubic groups (explanation follows table)

	R_1	R_2	R_3	R_4	R_5	R_6	R_7	R_8	R_9	R_{10}	R_{11}	R_{12}	R_{13}	R_{14}	R_{15}	R_{16}	R_{17}	R_{18}	R_{19}	R_{20}	R_{21}	R_{22}	R_{23}	R_{24}	**Basis functions**
Γ_1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
Γ_2	1	1	1	1	1	1	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	Γ_2' xyz
$(\Gamma_{12})_{11}$	1	1	1	1	−½	−½	−½	−½	−½	−½	−½	−½	1	1	−½	−½	−½	−½	1	1	−½	−½	−½	−½	
$(\Gamma_{12})_{21}$	0	0	0	0	$\frac{\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	$-\frac{\sqrt{3}}{2}$	$-\frac{\sqrt{3}}{2}$	$-\frac{\sqrt{3}}{2}$	$-\frac{\sqrt{3}}{2}$	0	0	$-\frac{\sqrt{3}}{2}$	$-\frac{\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	0	0	$-\frac{\sqrt{3}}{2}$	$-\frac{\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	$x^2 - y^2$,
$(\Gamma_{12})_{12}$	0	0	0	0	$-\frac{\sqrt{3}}{2}$	$-\frac{\sqrt{3}}{2}$	$-\frac{\sqrt{3}}{2}$	$-\frac{\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	0	0	$-\frac{\sqrt{3}}{2}$	$-\frac{\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	0	0	$-\frac{\sqrt{3}}{2}$	$-\frac{\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	$2z^2 - x^2 - y^2$
$(\Gamma_{12})_{22}$	1	1	1	1	−½	−½	−½	−½	−½	−½	−½	−½	−1	−1	½	½	½	½	−1	−1	½	½	½	½	
$\chi(\Gamma_{12})$	2	2	2	2	−1	−1	−1	−1	−1	−1	−1	−1	0	0	0	0	0	0	0	0	0	0	0	0	
$(\Gamma'_{25})_{11}$	1	1	−1	−1	0	0	0	0	0	0	0	0	−1	−1	0	0	0	0	1	1	0	0	0	0	
$(\Gamma'_{25})_{21}$	0	0	0	0	1	−1	−1	1	0	0	0	0	0	0	0	0	1	−1	0	0	0	0	1	−1	
$(\Gamma'_{25})_{31}$	0	0	0	0	0	0	0	0	1	−1	1	−1	0	0	−1	1	0	0	0	0	1	−1	0	0	
$(\Gamma'_{25})_{12}$	0	0	0	0	0	0	0	0	1	−1	−1	1	0	0	0	0	−1	1	0	0	0	0	1	−1	
$(\Gamma'_{25})_{22}$	1	−1	1	−1	0	0	0	0	0	0	0	0	0	0	−1	−1	0	0	0	0	1	1	0	0	xy, yz, zx
$(\Gamma'_{25})_{32}$	0	0	0	0	1	1	−1	−1	0	0	0	0	1	−1	0	0	0	0	1	−1	0	0	0	0	
$(\Gamma'_{25})_{13}$	0	0	0	0	1	−1	1	−1	0	0	0	0	0	0	1	−1	0	0	0	0	1	−1	0	0	
$(\Gamma'_{25})_{23}$	0	0	0	0	0	0	0	0	1	1	−1	−1	−1	1	0	0	0	0	1	−1	0	0	0	0	
$(\Gamma'_{25})_{33}$	1	−1	−1	1	0	0	0	0	0	0	0	0	0	0	0	0	−1	−1	0	0	0	0	1	1	
$\chi(\Gamma'_{25})$	3	−1	−1	−1	0	0	0	0	0	0	0	0	−1	−1	−1	−1	−1	−1	1	1	1	1	1	1	
$(\Gamma'_{15})_{11}$	1	1	−1	−1	0	0	0	0	0	0	0	0	1	1	0	0	0	0	−1	−1	0	0	0	0	
$(\Gamma'_{15})_{21}$	0	0	0	0	1	−1	−1	1	0	0	0	0	0	0	0	0	−1	1	0	0	0	0	−1	1	
$(\Gamma'_{15})_{31}$	0	0	0	0	0	0	0	0	1	−1	1	−1	0	0	1	−1	0	0	0	0	−1	1	0	0	
$(\Gamma'_{15})_{12}$	0	0	0	0	0	0	0	0	1	−1	−1	1	0	0	0	0	1	−1	0	0	0	0	−1	1	
$(\Gamma'_{15})_{22}$	1	−1	1	−1	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	−1	−1	0	0	
$(\Gamma'_{15})_{32}$	0	0	0	0	1	1	−1	−1	0	0	0	0	−1	1	0	0	0	0	−1	1	0	0	0	0	Γ_{15} x, y, z
$(\Gamma'_{15})_{13}$	0	0	0	0	1	−1	1	−1	0	0	0	0	0	0	−1	1	0	0	0	0	−1	1	0	0	
$(\Gamma'_{15})_{23}$	0	0	0	0	0	0	0	0	1	1	−1	−1	1	−1	0	0	0	0	−1	1	0	0	0	0	
$(\Gamma'_{15})_{33}$	1	−1	−1	1	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	−1	−1	
$\chi(\Gamma'_{15})$	3	−1	−1	−1	0	0	0	0	0	0	0	0	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1	

The matrix elements and characters are given for the unprimed operations. For the irreducible representations Γ_1, Γ_2, Γ_{12}, Γ'_{25}, and Γ'_{15} listed (in the notation of Bouckaert, Smoluchowski, and Wigner), the matrix elements for the primed operations are identical with those for the unprimed operations. For the operations Γ'_1, Γ'_2, Γ'_{12}, Γ_{15}, and Γ_{25}, the matrix elements and characters for the unprimed operations are identical with those for Γ_1, Γ_2, Γ_{12}, Γ'_{25}, and Γ'_{15}, respectively, but those for the primed operations are the negatives of those for the unprimed operations. These same notations for the irreducible representations are used by Herring [*J. Franklin Inst.*, **233**:525 (1942)] for the group O_h^7 (*Fd3m*). For the group T_d^2 (*F*$\bar{4}$3*m*), where we have only the operators of the point group T_d, the complete table of matrix elements is given in the table. In this case, following the convention of Parmenter [*Phys. Rev.*, 100:573 (1955)], the five irreducible representations of the table are denoted in succession as Γ_1, Γ_2, Γ_{12}, Γ_{15}, Γ_{25}.

Table 4 Group Δ

	R_1	R_2	R_{19}	R_{20}	R'_3	R'_4	R'_{13}	R'_{14}	Basis functions
Δ_1	1	1	1	1	1	1	1	1	1
Δ'_2	1	1	1	1	-1	-1	-1	-1	yz
Δ_2	1	1	-1	-1	1	1	-1	-1	$y^2 - z^2$
Δ'_1	1	1	-1	-1	-1	-1	1	1	$yz(y^2 - z^2)$
$(\Delta_5)_{11}$	1	-1	0	0	-1	1	0	0	y, z
$(\Delta_5)_{21}$	0	0	1	-1	0	0	-1	1	
$(\Delta_5)_{12}$	0	0	1	-1	0	0	1	-1	
$(\Delta_5)_{22}$	1	-1	0	0	1	-1	0	0	
$\chi(\Delta_5)$	2	-2	0	0	0	0	0	0	

Table 5 Group X

	R_1	R_2	R_3	R_4	R_{13}	R_{14}	R_{19}	R_{20}	R'_1	R'_2	R'_3	R'_4	R'_{13}	R'_{14}	R'_{19}	R'_{20}	Basis functions
X_1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
X_2	1	1	1	1	−1	−1	−1	−1	1	1	1	1	−1	−1	−1	−1	$y^2 - z^2$
X_3	1	1	−1	−1	−1	−1	1	1	1	1	−1	−1	−1	−1	1	1	yz
X_4	1	1	−1	−1	1	1	−1	−1	1	1	−1	−1	1	1	−1	−1	$yz(y^2 - z2)$
X'_1	1	1	1	1	−1	−1	−1	−1	−1	−1	−1	−1	1	1	1	1	$xyz(y^2 - z^2)$
X'_2	1	1	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1	−1	−1	xyz
X'_3	1	1	−1	−1	1	1	−1	−1	−1	−1	1	1	−1	−1	1	1	$x(y^2 - z^2)$
X'_4	1	1	−1	−1	−1	−1	1	1	−1	−1	1	1	1	1	−1	−1	x
$(X_6)_{11}$	1	−1	−1	1	0	0	0	0	1	−1	−1	1	0	0	0	0	xy, xz
$(X_6)_{21}$	0	0	0	0	−1	1	1	−1	0	0	0	0	−1	1	1	−1	
$(X_6)_{12}$	0	0	0	0	1	−1	1	−1	0	0	0	0	1	−1	1	−1	
$(X_6)_{22}$	1	−1	1	−1	0	0	0	0	1	−1	1	−1	0	0	0	0	
$\chi(X_6)$	2	−2	0	0	0	0	0	0	2	−2	0	0	0	0	0	0	
$(X'_6)_{11}$	1	−1	1	−1	0	0	0	0	−1	1	−1	1	0	0	0	0	y, z
$(X'_6)_{21}$	0	0	0	0	1	−1	1	−1	0	0	0	0	−1	1	−1	1	
$(X'_6)_{12}$	0	0	0	0	−1	1	1	−1	0	0	0	0	1	−1	−1	1	
$(X'_6)_{22}$	1	−1	−1	1	0	0	0	0	−1	1	1	−1	0	0	0	0	
$\chi(X'_6)$	2	−2	0	0	0	0	0	0	−2	2	0	0	0	0	0	0	

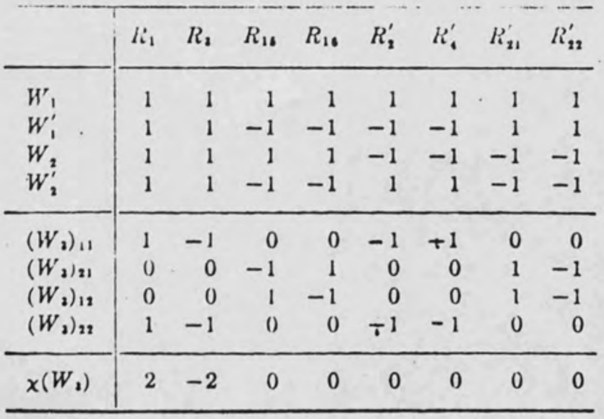
Table 6 Group Z

	R_1	R_3	R_2'	R_4'	Basis functions
Z_1	1	1	1	1	1
Z_2	1	1	-1	-1	$z(x - y)$
Z_3	1	-1	-1	1	z
Z_4	1	-1	1	-1	$x - y$

Table 7 Group Q

	R_1	R_{21}'	Basis functions
Q_1	1	1	1
Q_2	1	-1	$x(y^2 - z^2) + y(z^2 - x^2) + z(x^2 - y^2)$

Table 8 Group W



	R_1	R_3	R_{15}	R_{16}	R_2'	R_4'	R_{21}'	R_{22}'
W_1	1	1	1	1	1	1	1	1
W_1'	1	1	−1	−1	−1	−1	1	1
W_2	1	1	1	1	−1	−1	−1	−1
W_2'	1	1	−1	−1	1	1	−1	−1
$(W_3)_{11}$	1	−1	0	0	−1	+1	0	0
$(W_3)_{21}$	0	0	−1	1	0	0	1	−1
$(W_3)_{12}$	0	0	1	−1	0	0	1	−1
$(W_3)_{22}$	1	−1	0	0	+1	−1	0	0
$\chi(W_3)$	2	−2	0	0	0	0	0	0

Basis functions

1
xz
xyz
y

xy, yz

Table 9 **Group Σ, K**

	R_1	R_{23}	R'_4	R'_{24}	Basis functions
Σ_1	1	1	1	1	1
Σ_2	1	-1	-1	1	$z(x - y)$
Σ_3	1	1	-1	-1	z
Σ_4	1	-1	1	-1	$x - y$

Table 10 **Group Λ**

	R_1	R_5	R_9	R_{19}	R_{21}	R_{23}	**Basis functions**
Λ_1	1	1	1	1	1	1	1
Λ_2	1	1	1	−1	−1	−1	$x(y^2 - z^2) + y(z^2 - x^2) + z(x^2 - y^2)$
$(\Lambda_3)_{11}$	1	$-\frac{1}{2}$	$-\frac{1}{2}$	1	$-\frac{1}{2}$	$-\frac{1}{2}$	
$(\Lambda_3)_{21}$	0	$\frac{\sqrt{3}}{2}$	$\frac{-\sqrt{3}}{2}$	0	$\frac{-\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	$2x - y - z$, $y - z$
$(\Lambda_3)_{12}$	0	$\frac{-\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	0	$\frac{-\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	
$(\Lambda_3)_{22}$	1	$-\frac{1}{2}$	$-\frac{1}{2}$	−1	$\frac{1}{2}$	$\frac{1}{2}$	
$\chi(\Lambda_3)$	2	−1	−1	0	0	0	

Table 11 **Group L**

	R_1	R_5	R_9	R_{19}	R_{21}	R_{23}	R'_1	R'_5	R'_9	R'_{19}	R'_{21}	R'_{23}	**Basis functions**
L_1	1	1	1	1	1	1	1	1	1	1	1	1	1
L_2	1	1	1	−1	−1	−1	1	1	1	−1	−1	−1	$yz(y^2 - z^2)$ + etc.
L'_1	1	1	1	−1	−1	−1	−1	−1	−1	1	1	1	$x(y^2 - z^2)$ + etc.
L'_2	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1	$x + y + z$
$(L_3)_{11}$	1	$-\frac{1}{2}$	$-\frac{1}{2}$	1	$-\frac{1}{2}$	$-\frac{1}{2}$	1	$-\frac{1}{2}$	$-\frac{1}{2}$	1	$-\frac{1}{2}$	$-\frac{1}{2}$	
$(L_3)_{21}$	0	$\frac{\sqrt{3}}{2}$	$\frac{-\sqrt{3}}{2}$	0	$\frac{-\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	0	$\frac{\sqrt{3}}{2}$	$\frac{-\sqrt{3}}{2}$	0	$\frac{-\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	$2x^2 - y^2 - z^2$,
$(L_3)_{12}$	0	$\frac{-\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	0	$\frac{-\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	0	$\frac{-\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	0	$\frac{-\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	$y^2 - z^2$
$(L_3)_{22}$	1	$-\frac{1}{2}$	$-\frac{1}{2}$	−1	$\frac{1}{2}$	$\frac{1}{2}$	1	$-\frac{1}{2}$	$-\frac{1}{2}$	−1	$\frac{1}{2}$	$\frac{1}{2}$	
$\chi(L_3)$	2	−1	−1	0	0	0	2	−1	−1	0	0	0	
$(L_4)_{11}$	1	$-\frac{1}{2}$	$-\frac{1}{2}$	1	$-\frac{1}{2}$	$-\frac{1}{2}$	−1	$\frac{1}{2}$	$\frac{1}{2}$	−1	$\frac{1}{2}$	$\frac{1}{2}$	
$(L_4)_{21}$	0	$\frac{\sqrt{3}}{2}$	$\frac{-\sqrt{3}}{2}$	0	$\frac{-\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	0	$\frac{-\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	0	$\frac{\sqrt{3}}{2}$	$\frac{-\sqrt{3}}{2}$	$y - z$,
$(L_4)_{12}$	0	$\frac{-\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	0	$\frac{-\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	0	$\frac{\sqrt{3}}{2}$	$\frac{-\sqrt{3}}{2}$	0	$\frac{\sqrt{3}}{2}$	$\frac{-\sqrt{3}}{2}$	$2x - y - z$
$(L_4)_{22}$	1	$-\frac{1}{2}$	$-\frac{1}{2}$	−1	$\frac{1}{2}$	$\frac{1}{2}$	−1	$\frac{1}{2}$	$\frac{1}{2}$	1	$-\frac{1}{2}$	$-\frac{1}{2}$	
$\chi(L_4)$	2	−1	−1	0	0	0	−2	1	1	0	0	0	

CHAPTER II

1. The Approximations Used in the Band Theory

In the problems of Energy Band Theory one assumes that the nuclei are kept fixed and deals with the electronic motions in the field of the stationary nuclei (Born-Oppenheimer approximation).

A second approximation (one-electron approximation) is based on the assumption that the Schrodinger equation of a system of N electrons can be separated into N Schrodinger equations with a periodic potential.

To find this potential one considers the many-electron system where the electrons interact with nuclei and with each other. The Hamiltonian is then :

$$H = \sum_{i=1}^{N} \left[- \hbar^2/2m \; V_i^2 + V(\underline{r}_i) + \tfrac{1}{2} \sum_{j}^{N} e^2/r_{ij} \right] \qquad (1.1)$$

where the first term represents the kinetic energy of the electrons; the second their potential energy due to the nuclear attractions and the third the electrostatic interaction of the electrons with each other. Note that $\underline{r}_i$ is the position of electron i and r_{ij} is the distance between electrons i and j.

The Schrodinger equation with such Hamiltonian is not separable because of the interaction term. So an approximation has to be made and this is known as Hartree-Fork method. In this method the wave function of the system is approximated by a determinant of orthonormal one-electron functions, i.e.

$$\Psi(\underline{r}_1, \ldots \underline{r}_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_1(\underline{r}_1) & \ldots & \psi_N(\underline{r}_1) \\ \cdots & & \cdots \\ \psi_1(\underline{r}_N) & \ldots & \psi_N(\underline{r}_N) \end{vmatrix} \qquad (1.2)$$

$\underline{r}_i$ includes generally the spin coordinate though spin will not be considered in this work.

Application of the variational principle using this determinantal wave function leads in the following equations for the one-electron functions ψ_i

$$\left[-\hbar^2/2m\ \nabla_1^2 + V(\underline{r}_1) + e^2 \sum_j^N \int \left|\psi_j(\underline{r}_2)\right|^2 / r_{12}\, d\underline{r}_2\right] \psi_i(\underline{r}_1) - e^2 \sum_j^N \left[\int \psi_j^*(\underline{r}_2)\psi_i(\underline{r}_2)/r_{12}\, d\underline{r}_2\right] \psi_j(\underline{r}_1) = \mathcal{E}_i \psi_i(\underline{r}_1) \qquad (1.3)$$

which are called Hartree-Fock equations.

In equation (1.3) the third term, known as Hartree's potential, represents the average electrostatic potential energy of an electron in the field of the other electrons and the fourth term, (exchange interaction), takes into account the Pauli principle according to which electrons of the same spin keep away one from the other.

Slater (1951) suggested an exchange potential of the following form :

$$V_{ex} = 1/\psi_i(\underline{r}_1) \sum_j^N \psi_j(\underline{r}_1) \int \psi_j^*(\underline{r}_2)\, e^2/r_{12}\, \psi_i(\underline{r}_2)\, d\underline{r}_2 \qquad (1.4)$$

which leads to the usual approximation to the Hartree-Fock equation, i.e.

$$\nabla^2\psi + 2m/\hbar^2 \left[W - V(\underline{r}) - V_o(\underline{r}) - V_{ex}(\underline{r})\right]\psi = 0 \qquad (1.5)$$

where V(r) is the potential energy of one electron due to the nuclear attraction and $V_o(r)$ is the Hartree potential.

Slater approximated V_{ex} by a potential which is the same for all states. He proposed that the exchange potential may be taken the same as in a free electron gas.

Since there is a mutual dependence between the potential and the states which are occupied by electrons a self-consistent potential is required in order to solve equation (1.5). But such a potential is very difficult to obtain, because it involves extreemely laborious computation.

However the pseudopotential method whose ideas form the basis of the present work, has made considerable progress towards the solution of the problem of a self-consistent field. The whole philosophy of the pseudopotential method, which is discussed in detail in section 5 of this Chapter is based on the Hartree-Fock approach as it is the case in most band structure calculations.

2. The Many-Body Problem

The correlation effect, which accounts for the repulsion between electrons of opposite spins because of their electric charge, is neglected by the Hartree-Fock approach and this is justified by modern many-body theory.

This problem of the electron-electron interaction is treated by the method of quasi particles. This is the study of the possible types of spectra of quantized systems by introducing quasi-particles having these spectra.

We outline here one of the many-body theories, i.e. the theory of plasma oscillations of Bohn and Pines (1951-55) who discussed the problem by using the concept of plasma. A plasma is an ionized gas consisting of positive ions and free electrons, with zero total charge. Bohn and Pines regarded a metal as a plasma where due to fluctuation in the thermal motion the electron gas is set to vibration. These oscillations are called plasma oscillations and can be represented by a finite set of harmonic oscillators (plasmons) with angular frequency ω_p.

The Coulomb interaction of the electrons may be divided into two parts : a long-range part, whose effect is described by the plasma oscillations and a short-range part, which is a screened Coulomb interaction with screening distance of the order of 1A, for the electron densities ordinarily found in metals.

It is found that the excitation energy $\hbar\omega_p$ of a plasma oscillation is much greater than the thermal energy which any electron possesses at normal temperatures. This means that plasmons can not be excited at ordinary temperatures and therefore have no active part in many electronic processes. Hence, since the long-range part of the Coulomb interaction is responsible for the plasmons, it follows that this interaction can be ignored when no plasma oscillations occur.

The short-range interaction has a very small effective range and may be neglected too.

Therefore the theory of plasma oscillations gives a justification to the one-electron approximation, answering to the question how the simple one-electron model leads to at least qualitatively correct solutions.

3. The Method of Momentum Eigenfunctions

There are two main approaches to the problem of solving the one-electron Schrodinger equation in a rigid, infinite, periodic lattice. The first is the atomic orbitals approximation which considers the electrons as tightly bound to a nucleus and their wave functions only slightly overlapping. The second is the nearly free-electron approximation which assumes that the electrons move through the whole crystal and their wave functions can be represented by only slightly modified plane waves.

The method to be used in this work is based on the nearly free-electron approximation and is known as "method of momentum eigenfunctions" or "method of linear combinations of plane waves". In the following the whole theory of the method is developed.

According to Bloch's theorem, the solution of Schrodinger's equation must satisfy the relation :

$$\psi_{\underline{k}}(\underline{r}) = e^{i\underline{k}\cdot\underline{r}}u_{\underline{k}}(\underline{r}) \qquad (3.1)$$

where $u_{\underline{k}}(\underline{r})$ is a periodic function having the periodicity of the lattice, that is

$$u_{\underline{k}}(\underline{r}) = u_{\underline{k}}(\underline{r} + \underline{R}_n) \qquad (3.2)$$

Therefore $u_{\underline{k}}(\underline{r})$ may be expanded in a Fourier series in ordinary space and in terms of the reciprocal lattice vectors $\underline{K}_n$, i.e.

$$u_{\underline{k}}(\underline{r}) = \sum_{\underline{K}_n} A_{\underline{k}}(\underline{K}_n)e^{i\underline{K}_n\cdot\underline{r}} \qquad (3.3)$$

with $$A_{\underline{k}}(\underline{K}_n) = 1/\Omega \int_{u.c.} u_{\underline{k}}(\underline{r}) e^{-i\underline{K}_n\cdot\underline{r}} d\underline{r} \qquad (3.4)$$

This integration is over the unit cell of volume Ω in ordinary space.

Using equations (3.1) and (3.3) a Fourier expansion for the wave function $\psi_{\underline{k}}(\underline{r})$ is obtained :

$$\psi_{\underline{k}}(r) = \sum_{\underline{K}_n} A(\underline{k}+\underline{K}_n) e^{i(\underline{k}+\underline{K}_n)\cdot\underline{r}} \qquad (3.5)$$

with $$A(\underline{k}+\underline{K}_n) = 1/\Omega \int_{u.c.} \psi_{\underline{k}}(\underline{r}) e^{-i(\underline{k}+\underline{K}_n)\cdot\underline{r}} d\underline{r} \qquad (3.6)$$

where $\underline{k}$ is a particular point in reciprocal space.

The coefficients $A(\underline{k}+\underline{K}_n)$ are called momentum eigenfunctions and they represent the probability of finding the electron with a given crystal momentum, in the same way as the ordinary eigenfunction is the probability of finding the electron with a given coordinate.

The periodic potential $V(\underline{r})$ can also be expanded in a Fourier series in ordinary space and in terms of the reciprocal lattice vectors $\underline{K}_n$, i.e.

$$V(\underline{r}) = \sum_{\underline{K}_n} V(\underline{K}_n) e^{i\underline{K}_n\cdot\underline{r}} \qquad (3.7)$$

with $$V(\underline{K}_n) = 1/\Omega \int_{u.c.} V(\underline{r}) e^{-i\underline{K}_n\cdot\underline{r}} dr \qquad (3.8)$$

Now substituting equations (3.5) and (3.7) into Schrodinger equation (1.5) multiplying by $e^{-i(\underline{k}+\underline{K}_l)\cdot\underline{r}}$ integrating over the unit cell and taking into account the orthogonality of the waves $e^{i\underline{K}_n\cdot\underline{r}}$, one finds :

$$\left[\hbar^2/2m\left|\underline{k}+\underline{K}_i\right|^2 - W\right] A(\underline{k}+\underline{K}_i) + \sum_{\underline{K}_m} V(\underline{K}_m)\ A\ (\underline{k}+\underline{K}_i-\underline{K}_m) = 0 \qquad (3.9\ )$$

Equations (3.9) form a system of honogeneous algebraic equations for the momentum eigenfunctions $A(\underline{k}+\underline{K}_i)$. Therefore this system has non-zero solutions only if the determinant of the coefficients $A(\underline{k}+\underline{K}_i)$ vanishes. This determinant provides a secular equation of infinite degree, determining the energies $W_n(k)$ for a given $\underline{k}$. For any $W_n(\underline{k})$ the system (3.9) gives the ratios of the $A_n(\underline{k}+\underline{K}_i)$. In order to find the actual values of the momentum eigenfunctions a normalization condition must be added to equations (3.9).

In practice the W_n and A_n are found by successive approximations, solving (3.9) with more and more terms included in the summation. The convergence depends on how many of the coefficients of the potential have an appreciable value.

The justification for this "plane wave" approach is found in the method of pseudopotentials where, as we shall see in the following, the effective potential is weak and expanded in Fourier series gives small components suitable for this type of calculation.

4. The Symmetrized Combinations of Plane Waves

We saw in the previous section that the expansion of the wave function in plane waves provides a method for solving Schrodinger's equation for the periodic problem. In addition the use of symmetrized functions reduces the order of the secular equations which must be solved at the symmetry points and along symmetry axes in the Brillouin zone. Hence we form symmetrized linear combinations of plane waves, which transform according to the irreducible representations of the group of the wave vector k.

Such combinations are found by using the projection operator :

$$\Psi^{(j)}_{sym} = \sum_R \left[D^{(j)} R\right]_{ii} R\,\psi \qquad (4.1)$$

where $\Psi^{(j)}_{sym}$ is the symmetrized function, $\left[D^{(j)} R\right]_{ii}$ is the iith element of the matrix for the representation in question, R are the symmetry operations of that particular group, and ψ a plane wave.

We shall now give a proof for equation (4.1). A function ψ_i^j which transforms according to the ith row of the jth irreducible representation satisfies the following equation :

$$R\,\psi_i^j = \sum_m \left[D^{(j)}R\right]_{mi} \psi_m^j \qquad (4.2)$$

where $\left[D^{(j)}R\right]_{mi}$ is the mith matrix element of the matrix representation of the operator R, m takes the values from 1 to d where d is the dimension of the irreducible representation j. If we multiply equation (4.2) by $\left[D^{(j')}R\right]_{m'i'}$ and sum over R we have :

$$\sum_R \left[D^{(j')}R\right]_{m'i'} R\psi_i^j = \sum_R \sum_m \left[D^{(j')}R\right]_{m'i'} \left[D^{(j)}R\right]_{mi} \psi_m^j \qquad (4.3)$$

The following theorem is now used (see Wigner 1959 p.79)

$$\sum_R \left[D^{(j')}R\right]_{m'i'} \left[D^{(j)}R\right]_{mi} = h/d\ \delta_{ii'}\delta_{jj'}\delta_{mm'} \qquad (4.4)$$

where h is the order of the group.

So using equation (4.4), equation (4.3) gives :

$$\sum_R \left[D^{(j')}R\right]_{m'i'} R\psi_i^j = h/d\ \delta_{ii'}\delta_{jj'}\psi_{m'}^j \qquad (4.5)$$

and for $m' = i' = i$ and $j = j'$ we obtain :

$$\psi_i^j = d/h \sum \left[D^{(j)}R\right]_{ii} R\psi_i^j \qquad (4.6)$$

which is the required formula. The constant d/h is generally included in the normalization factor.

The matrix elements of the irreducible representations are found by applying the operators R to the basis functions, and those concerning the face-centred cubic lattice are listed in the tables of the first chapter.

To illustrate the procedure which is followed to find the symmetrized combinations of plane waves, the following examples are given :

1) One-dimensional representation Δ_2 Basis function $y^2 - z^2$.
Operations : R_1, R_2, R_{19}, R_{20}, R'_3, R'_4, R'_{13}, R'_{14} (see Table 1)

The basis function remains unchanged for the operations R_1, R_2, R'_3, R'_4 which we represent by +1, and changes sign for the rest of the operations which we represent by -1. So we have the combinations for a vector of, say, the type (020).

(020)+(0-20)-(002)-(00-2)

2) Two-dimensional representation X_5'. Basis function y, z.

Operations: R_1, R_2, R_3 R_4, R_{13}, R_{14}, R_{19}, R_{20},

R_1', R_2', R_3', R_4', R_{13}', R_{14}', R_{19}', R_{20}',

The following assignment of matrices to operations is made:

$$R_1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad R_2 = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} \quad R_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad R_4 = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$R_{13} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \quad R_{14} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad R_{19} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad R_{20} = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$$

and similarly for the primed operations.

Considering the iith element of the above matrices, it is found that the basis functions remain unchanged for the operations R_1, R_3, R_2', R_4' and change sign for the operations R_2, R_4, R_1', R_3'. The rest of the operations give no contribution to the combinations.

For example for a vector of the type (111) we have :

(111)+(11-1)-(1-1-1)-(1-11)

3) Three-dimensional representation Γ_{15}. Basis function x,y,z

Operations: The 48 operations of the cubic group. (Table 1)

The following assignment of matrices to operations is made :

$$R_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad R_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad R_3 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

and similarly for the rest of the operations (Table 3).

Considering again the iith elements of those matrices, it is found that the basis functions remain unchanged for the operations R_1, R_2, R_{19}, R_{20}, R'_3, R'_4, R'_{13}, R'_{14} and change sign for the operations R_3, R_4, R_{13}, R_{14}, R'_1, R'_2, R'_{19}, R'_{20}. The rest of the operations having 0 iith element, give no contribution to the combinations. For example for a vector of the type (220) we have :

$$(220)+(2-20)+(202)+(20-2)-(-220)-(-2-20)-(-20-2)-(-202)$$

It must be noted here that in constructing these combinations one must consider the vector $\underline{k}+\underline{K}_n$ and not just $\underline{K}_n$, though is some cases this is immaterial.

Our combinations found as explained above, have been checked by a method of "generators" suggested by Schlosser (1962). Schlosser tabulated in a systematic way the symmetrized combinations of plane waves for the cubic lattices.

Here we give an example of how to use these tables. Consider the point L, $k = 2\pi/a(\frac{1}{2}\frac{1}{2}\frac{1}{2})$ in the face-centred cubic lattice. We are going to construct symmetrized combinations transforming according to the representation L'_2. Schlosser, designating a particular plane wave by $[ijk]$, gives for L'_2 the following generator:

$$A'[ijk] \qquad (4.7)$$

where $A' = (I-J)A$ and $A = \sum_{n}(I+R_{23})P_{1n}$ with $n = 1,2,3$

and where $P_{11} = I = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ $J = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$

$$R_{12} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad R_{13} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \qquad R_{23} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

$$P_{12} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \qquad P_{13} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

Now if $[ijk]$ is considered as a column vector, equation (4.7) gives :

$$\left\{(I-J)\ (I + R_{23} + P_{12} + R_{12} + P_{13} + R_{13})\right\}[ijk] =$$

$$= [ijk]+[ikj]+[kij]+[jik]+[jki]+[kji]-[-i-j-k]-[-i-k-j]-[-k-i-j]-$$
$$-[-j-i-k]-[-j-k-i]-[-k-j-i]$$

From this, one finds for a vector of the type, say $(\frac{3}{2}\,-\frac{1}{2}\,-\frac{1}{2})$

$$(\tfrac{3}{2}\,-\tfrac{1}{2}\,-\tfrac{1}{2})+(-\tfrac{1}{2}\,\tfrac{3}{2}\,-\tfrac{1}{2})+(-\tfrac{1}{2}\,-\tfrac{1}{2}\,\tfrac{3}{2})-(-\tfrac{3}{2}\,\tfrac{1}{2}\,\tfrac{1}{2})-(\tfrac{1}{2}\,-\tfrac{3}{2}\,\tfrac{1}{2})-(\tfrac{1}{2}\,\tfrac{1}{2}\,-\tfrac{3}{2})$$

or subtracting $\underline{k} = (\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2})$

$$(1-1-1)+(-11-1)+(-1-11)-(-200)-(0-20)-(00-2)$$

In the following pages we tabulate the symmetrized combinations of plane waves for a face-centred cubic lattice.

SYMMETRIZED COMBINATIONS OF PLANE WAVES

Γ_1

K_0; (000)
K_1: (111)+(1-11)+(11-1)+(1-1-1)+(-1-1-1)+(-1-11)+(-11-1)+(-111)
K_2 (200)+(020)+(002)+(-200)+(0-20)+(00-2)
K_3: (220)+(-220)+(2-20)+(-2-20)+(202)+(20-2)+(-20-2)+(-202)+(022)+(02-2)
+(0-22)+(0-2-2)
K_4: (311)+(3-1-1)+(-31-1)+(-3-11)+(113)+(-11-3)+(-1-13)+(1-1-3)+(131)+(-1-31)
+(1-3-1)+(-13-1)+(-3-1-1)+(-311)+(3-11)+(31-1)+(-1-1-3)+(1-13)+(11-3)
+(-113)+(-1-3-1)+(13-1)+(-131)+(1-31)
K_5: (222) as K_1
K_6: (400) as K_2

Γ_{15}

K_1: (111)+(1-11)+(11-1)+(1-1-1)-(-1-1-1)-(-1-11)-(-11-1)-(-111)
K_2: (200)-(-200)
K_3: (220)-(-220)+(2-20)-(-2-20)+(202)+(20-2)-(-20-2)-(-202)
K_4: (311)-(-311)+(3-11)+(31-1)-(-3-11)-(-31-1)+(3-1-1)-(-3-1-1)
K_5: (222) as K_1
K_6: (400) as K_2

Γ'_{25}

K_1 : (111)-(1-11)+(11-1)-(1-1-1)+(-1-1-1)+(-1-11)-(-11-1)-(-111)
K_3: (220)+(-2-20)-(2-20)-(-220)
K_4: (113)+(11-3)-(-11-3)-(-113)-(1-13)-(1-1-3)+(-1-13)+(-1-1-3)
K_5: (222) as K_1

Γ_{12}

K_2: (200)+(-200)-(020)-(0-20)
K_3: (202)-(022)+(-202)-(0-22)+(20-2)-(02-2)+(-20-2)-(0-2-2)
K_4: (311)-(131)+(-311)-(1-31)+(3-11)+(-31-1)-(-131)+(31-1)-(13-1)+(-3-11)
-(-1-31)-(1-3-1)+(3-1-1)-(-13-1)+(-3-1-1)-(-1-3-1)
K_6: (400) as K_2

Γ'_2

K_1: (111)-(1-11)-(11-1)+(1-1-1)-(-1-1-1)+(-1-11)+(-11-1)-(-111)
K_4: (311)+(3-1-1)+(-31-1)+(-3-11)+(113)+(-11-3)+(-1-13)+(1-1-3)+(131)+(-1-31)
+(1-3-1)+(-13-1)-(-3-1-1)-(-311)-(3-11)-(31-1)-(-1-1-3)-(1-13)-(11-3)
-(-113)-(-1-3-1)-(13-1)-(-131)-(1-31)
K_5: (222) as K_1

SYMMETRIZED COMBINATIONS OF PLANE WAVES

Δ_1

K_0: (000)
K_1: (-1-1-1)+(-1-11)+(-11-1)+(-111)

K_2: (-200)

K_3: (111)+(1-11)+(11-1)+(1-1-1)

K_4: (020)+(002)+(0-20)+(00-2)

K_5: (200)

K_6: (-220)+(-2-20)+(-202)+(-20-2)

K_7: (022)+(02-2)+(0-22)+(0-2-2)

K_8: (220)+(2-20)+(202)+(20-2)

K_9: (-311)+(-3-11)+(-31-1)+(-3-1-1)

K_{10} (-131)+(-113)+(-1-31)+(-11-3)+(-13-1)+(-1-13)+(-1-3-1)+(-1-1-3)

K_{11}: (131)+(113)+(1-31)+(11-3)+(13-1)+(1-13)+(1-3-1)+(1-1-3)

K_{12} (311)+(3-11)+(31-1)+(3-1-1)

K_{13} (-2-2-2)+(-2-22)+(-22-2)+(-222)

K_{14} (222)+(2-22)+(22-2)+(2-2-2)

K_{15} (-400)

Δ_2

K_4: (020)+(0-20)-(002)-(00-2)

K_6: (-220)+(-2-20)-(-202)-(-20-2)

K_8: (220)+(2-20)-(202)-(20-2)

K_{10} (-131)+(-1-3-1)+(-1-31)+(-13-1)-(-113)-(-1-1-3)-(-11-3)-(-1-13)

K_{11} (131)+(1-3-1)+(1-31)+(13-1)-(113)-(1-1-3)-(11-3)-(1-13)

SYMMETRIZED COMBINATIONS OF PLANE WAVES

Δ_2'

K_1 : (-1-1-1)+(-111)-(-1-11)-(-11-1)

K_3 : (111)+(1-1-1)-(1-11)-(11-1)

K_7 : (022)+(0-2-2)-(0-22)-(02-2)

K_9 : (-311)+(-3-1-1)-(-3-11)-(-31-1)

K_{10}: (-131)+(-1-3-1)+(-1-1-3)+(-113)-(-1-13)-(-11-3)-(-1-31)-(-13-1)

K_{11}: (131)+(1-3-1)+(1-1-3)+(113)-(1-13)-(11-3)-(1-31)-(13-1)

K_{12}: (311)+(3-1-1)-(3-11)-(31-1)

K_{13}: (-2-2-2)+(-222)-(-2-22)-(-22-2)

K_{14}: (222)+(2-2-2)-(2-22)-(22-2)

Δ_5

K_1 : (-111)+(-11-1)-(-1-11)-(-1-1-1)

K_3: (111)+(11-1)-(1-11)-(1-1-1)

K_4: (020)-(0-20)

K_6: (-220)-(-2-20)

K_7: (022)+(02-2)-(0-2-2)-(0-22)

K_8: (220)-(2-20)

K_9: (-311)+(-31-1)-(-3-1-1)-(-3-11)

K_{10}: (-131)+(-13-1)-(-1-3-1)-(-1-31)

K_{11}: (131)+(13-1)-(1-3-1)-(1-31)

K_{12}: (311)+(31-1)-(3-1-1)-(3-11)

K_{13}: (-222)+(-22-2)-(-2-22)-(-2-2-2)

K_{14}: (222)+(22-2)-(2-22)-(2-2-2)

SYMMETRIZED COMBINATIONS OF PLANE WAVES

X_1

K_0 : (000)+(-200)

K_1 : (-111)+(-1-11)+(-11-1)+(-1-1-1)

K_2 : (020)+(002)+(0-20)+(00-2)+(-220)+(-202)+(-2-20)+(-20-2)

K_3 : (111)+(1-11)+(11-1)+(1-1-1)+(-311)+(-3-11)+(-31-1)+(-3-1-1)

K_4 : (200)+(-400)+(022)+(0-22)+(02-2)+(0-2-2)+(-222)+(-2-22)+(-22-2)+ (-2-2-2)

K_5 (-131)+(-113)+(-1-31)+(-13-1)+(-1-13)+(-11-3)+(-1-3-1)+(-1-1-3)

K_6 (220)+(2-20)+(202)+(20-2)+(-4-20)+(-420)+(-402)+(-40-2)

K_7 (131)+(113)+(1-31)+(11-3)+(13-1)+(1-13)+(1-3-1)+(1-1-3)+(-331)+ (-313)+(-3-31)+(-31-3)+(-33-1)+(-3-13)+(-3-3-1)+(-3-1-3)

X_4'

K_0 : (000)-(-200)

K_1 : (020)+(0-20)+(002)+(00-2)-(-220)-(-2-20)-(-202)-(-20-2)

K_2 : (111)+(1-1-1)+(1-11)+(11-1)-(-311)-(-3-1-1)-(-3-11)-(-31-1)

K_3 : (022)+(0-2-2)+(0-22)+(02-2)-(-222)-(-2-2-2)-(-2-22)-(-22-2)+ (200)-(-400)

K_4 : (220)+(2-20)+(202)+(20-2)-(-420)-(-4-20)-(-402)-(-40-2)

K_5 : (131)+(1-3-1)+(113)+(1-1-3)+(1-31)+(1-13)+(13-1)+(11-3)- (-331)-(-3-3-1)-(-313)-(-3-1-3)-(-3-31)-(-3-13)-(-33-1)-(-31-3)

X_3

K_0 : (-111)+(-1-1-1)-(-1-11)-(-11-1)

K_1 : (111)+(1-1-1)-(1-11)-(11-1)+(-311)+(-3-1-1)-(-3-11)-(-31-1)

K_2 : (022)+(0-2-2)-(0-22)-(02-2)+(-222)+(-2-2-2)-(-2-22)-(-22-2)

K_3 : (-131)+(-113)+(-1-1-3)+(-1-3-1)-(-1-31)-(-13-1)-(-11-3)-(-1-13)

K_4 : (131)+(113)+(1-1-3)+(1-3-1)-(1-31)-(13-1)-(11-3)-(1-13)+(-331)+ (-313)+(-3-1-3)-(-3-3-1)-(-3-31)-(-33-1)-(-31-3)-(-3-13)

SYMMETRIZED COMBINATIONS OF PLANE WAVES

X_5'

K_0 : (-111)+(-11-1)-(-1-1-1)-(-1-11)

K_1 : (020)-(0-20)+(-220)-(-2-20)

K_2 : (111)+(11-1)-(-1-1-1)-(1-11)+(-311)+(-31-1)-(-3-1-1)-(-3-11)

K_3 : (022)+(02-2)-(0-2-2)-(0-22)+(-222)+(-22-2)-(-2-2-2)-(-2-22)

K_4 : (-131)+(-13-1)-(-1-3-1)-(-1-31)

K_5 : (220)-(2-20)+(-420)-(-4-20)

K_6 : (131)+(13-1)-(-13-1)-(1-31)+(-331)+(-33-1)-(-3-3-1)-(-3-31)

X_2

K_0 : (020)+(0-20)-(002)-(00-2)+(-220)+(-2-20)-(-202)-(-20-2)

K_1 : (-131)+(-13-1)+(-1-31)+(-1-3-1)-(-113)-(-11-3)-(-1-13)-(-1-1-3)

K_2 : (220)+(2-20)-(202)-(20-2)+(-420)+(-4-20)-(-402)-(-40-2)

K_3 : (131)+(13-1)+(1-31)+(1-3-1)-(113)-(11-3)-(1-13)-(1-1-3)-(-331) -
(-33-1)-(-3-31)-(-3-3-1)+(-313)+(-31-3)+(-3-13)+(-3-1-3)

X_5

K_0 : (020)+(-2-20)-(0-20)-(-220)

K_1 : (111)+(11-1)+(-3-11)+(-3-1-1)-(1-1-1)-(-31-1)-(-311)-(1-11)

K_2 : (022)+(02-2)+(-2-22)+(-2-2-2)-(0-2-2)-(-22-2)-(-222)-(0-22)

K_3 : (220)+(-4-20)-(2-20)-(-420)

K_4 : (131)+(13-1)+(-3-31)+(-3-3-1)-(1-3-1)-(-33-1)-(-331)-(1-31)

X_3'

K_0 : (020)+(0-20)-(002)-(00-2)+(-202)+(-20-2)-(-220)-(-2-20)

K_1 : (220)+(2-20)-(202)-(20-2)+(-402)+(-40-2)-(-420)-(-4-20)

K_2 : (131)+(1-3-1)+(1-31)+(13-1)-(113)-(1-1-3)-(1-13)-(11-3)+
(-31-3)+(-3-13)+(-3-1-3)+(-313)-(-33-1)-(-3-31)-(-3-3-1)-(-331)

SYMMETRIZED COMBINATIONS OF PLANE WAVES

Z_1

K_0: (000)+(-200)
K_1: (-1-11)+(-1-1-1)
K_2: (-111)+(-11-1)
K_3: (0-20)+(-2-20)
K_4: (002)+(00-2)+(-202)+(-20-2)
K_5: (1-11)+(1-1-1)+(-3-11)+(-3-1-1)
K_6: (020)+(-220)
K_7: (111)+(11-1)+(-311)+(-31-1)
K_8: (0-22)+(0-2-2)+(-2-22)+(-2-2-2)
K_9: (-1-31)+(-1-3-1)
K_{10}: (200)+(-400)
K_{11}: (-1-13)+(-1-1-3)
K_{12}: (022)+(02-2)+(-222)+(-22-2)
K_{13}: (-113)+(-11-3)
K_{14}: (-131)+(-13-1)
K_{15}: (2-20)+(-4-20)
K_{16}: (1-31)+(1-3-1)+(-3-31)+(-3-3-1)

Z_3

K_0: (000)-(-200)
K_3: (0-20)-(-2-20)
K_4: (002)+(00-2)-(-202)-(-20-2)
K_5: (1-11)+(1-1-1)-(-3-11)-(-3-1-1)
K_6: (020)-(-220)
K_7: (111)+(11-1)-(-311)-(-3+1-1)
K_8: (0-22)+(0-2-2)-(-2-22)-(-2-2-2)
K_{10}: (200)-(-400)
K_{12}: (022)+(02-2)-(-222)-(-22-2)
K_{15}: (2-20)-(-4-20)
K_{16}: (1-31)+(1-3-1)-(-3-31)-(-3-3-1)

SYMMETRIZED COMBINATIONS OF PLANE WAVES

Z_4

K_1 : (-1-11)-(-1-1-1)
K_2 : (-111)-(-11-1)
K_4 : (002)-(00-2)+(-202)-(-20-2)
K_5 : (1-11)-(1-1-1)+(-3-11)-(-3-1-1)
K_7 : (111)-(11-1)+(-311)-(-31-1)
K_8 : (0-22)-(0-2-2)+(-2-22)-(-2-2-2)
K_9 : (-1-31)-(-1-3-1)
K_{11}: (-1-13)-(-1-1-3)
K_{12}: (022)-(02-2)+(-222)-(-22-2)
K_{13}: (-113)-(-11-3)
K_{14}: (-131)-(-13-1)
K_{16}: (1-31)-(1-3-1)+(-3-31)-(-3-3-1)

W_1

K_0 : (000)+(-200)+(-1-11)+(-1-1-1)
K_1 : (-111)+(-11-1)+(0-20)+(-2-20)
K_2 : (002)+(00-2)+(-202)+(-20-2)+(1-11)+(1-1-1)+(-3-11)+(-3-1-1)
K_3 : (020)+(-220)+(111)+(11-1)+(-311)+(-31-1)+(0-22)+(0-2-2)+(-2-22)
+(-2-2-2)+(-1-31)+(-1-3-1)
K_4 : (200)+(-400)+(-1-13)+(-1-1-3)
K_5 : (022)+(02-2)+(-222)+(-22-2)+(-113)+(-11-3)+(2-20)+(-4-20)+(1-31)
+(1-3-1)+(-3-31)+(-3-3-1)
K_6 : (-131)+(-13-1)+(1-13)+(1-1-3)+(-3-13)+(-3-1-3)+(202)+(20-2)+(-402)
+(-40-2)+(0-40)+(-2-40)

W_1'

K_0 : (000)+(-200)-(-1-11)-(-1-1-1)
K_1 : (0-20)+(-2-20)-(-111)-(-11-1)
K_2 : (002)+(00-2)+(-202)+(-20-2)-(1-11)-(1-1-1)-(-3-11)-(-3-1-1)
K_3 : (020)+(-220)+(111)+(11-1)+(-311)+(-31-1)-(0-22)-(0-2-2)-(-2-22)
(-2-2-2)-(-1-31)-(-1-3-1)
K_4 : (200)+(-400)-(-1-13)-(-1-1-3)
K_5 : (022)+(02-2)+(-222)+(-22-2)+(-113)+(-11-3)-(2-20)-(-4-20)-(1-31)
-(1-3-1)-(-3-31)-(-3-3-1)
K_6 : (202)+(20-2)+(-402)+(-40-2)+(0-40)+(-2-40)-(-131)-(-13-1)-(1-13)
-(1-1-3)-(-3-13)-(-3-1-3)

SYMMETRIZED COMBINATIONS OF PLANE WAVES

W_3

K_0: (000)-(-200)
K_1: (0-20)-(-2-20)
K_2: (002)+(00-2)-(202)-(20-2)
K_3: (020)-(-220)+(111)+(11-1)-(-311)-(-31-1)
K_4: (200)-(-400)
K_5: (022)+(02-2)-(-222)-(-22-2)+(-113)-(-11-3)
K_6: (202)+(20-2)-(-402)-(-40-2)+(0-40)-(-2-40)

Q_1

K_0: (000)+(-1-1-1)
K_1: (1-1-1)+(00-2)
K_2: (-11-1)+(0-20)
K_3: (-1-11)+(11-1)+(-200)+(0-2-2)
K_4: (1-11)+(-20-2)
K_5: (-111)+(200)+(-2-20)+(-1-1-3)
K_6: (111)+(020)+(20-2)+(-1-3-1)+(1-1-3)+(-2-2-2)
K_7: (002)+(2-20)+(02-2)+(-11-3)+(1-3-1)+(-3-1-1)
K_8: (11-3)+(2-2-2)
K_9: (-220)+(-1-31)+(0-22)+(-31-1)
K_{10}: (-202)+(-3-11)+(3-1-1)+(00-4)+(1-31)+(-22-2)

Q_2

K_0: (000)-(-1-1-1)
K_1: (00-2)-(1-1-1)
K_2: (0-20)-(-11-1)
K_3: (-200)+(0-2-2)-(-1-11)-(11-1)
K_4: (-20-2)-(1-11)
K_5: (200)+(-2-20)-(-111)-(-1-1-3)
K_6: (020)+(20-2)+(-2-2-2)-(111)-(-1-3-1)-(1-1-3)
K_7: (002)+(2-20)+(02-2)-(-11-3)-(1-3-1)-(-3-1-1)
K_8: (2-2-2)-(11-3)
K_9: (-220)+(0-22)-(-1-31 -(-31-1)
K_{10}: (-202)+(00-4)+(-22-2)-(-3-11)-(3-1-1)-(1-31)

L_1

K_0: (000)+(-1-1-1)
K_1: (1-1-1)+(-1-11)+(-11-1)+(-200)+(00-2)+(0-20)
K_2: (-111)+(11-1)+(1-11)+(0-2-2)+(-2-20)+(-20-2)
K_3: (111)+(-2-2-2)+(200)+(002)+(020)+(-3-1-1)+(-1-1-3)+(-1-3-1)
K_4: (2-20)+(-202)+(02-2)+(20-2)+(0-22)+(-220)+(-31-1)+(1-1-3)
+(-1-31)+(-3-11)+(-11-3)+(1-3-1)
K_5: (-311)+(11-3)+(1-31)+(2-2-2)+(-2-22)+(-22-2)
K_6: (022)+(220)+(202)+(-1-3-3)+(-3-3-1)+(-3-1-3)+(3-1-1)+(-1-13)
+(-13-1)+(-400)+(00-4)+(0-40)

SYMMETRIZED COMBINATIONS OF PLANE WAVES

L_2'

K_0: (000)-(-1-1-1)

K_1: (1-1-1)+(-1-11)+(-11-1)-(-200)-(00-2)-(0-20)

K_2: (-111)+(11-1)+(1-11)-(0-2-2)-(-2-20)-(-20-2)

K_3: (111)-(-2-2-2)+(200)+(002)+(020)-(-3-1-1)-(-1-1-3)-(-1-3-1)

K_4: (2-20)+(-202)+(02-2)+(20-2)+(0-22)+(-220)-(-31-1)-(1-1-3)
-(-1-31)-(-3-11)-(-11-3)-(1-3-1)

K_5: (-311)+(11-3)+(1-31)-(2-2-2)-(-2-22)-(-22-2)

K_6: (022)+(220)+(202)-(-1-3-3)-(-3-3-1)-(-3-1-3)+(3-1-1)+(-1-13)
+(-13-1)-(-400)-(00-4)-(0-40)

L_3

K_1: 2(1-1-1)-(-1-11)-(-11-1)+2(-200)-(00-2)-(0-20)

K_2: 2(-111)-(11-1)-(1-11)+2(0-2-2)-(-2-20)-(-20-2)

K_3: 2(200)-(002)-(020)+2(-3-1-1)-(-1-1-3)-(-1-3-1)

K_4: 2(2-20)-(-202)-(02-2)+2(20-2)-(0-22)-(-220)+2(-31-1)-(1-1-3)
-(-1-31)+2(-3-11)-(-11-3)-(1-3-1)

K_5: 2(-311)-(11-3)-(1-31)+2(2-2-2)-(-2-22)-(-22-2)

K_6: 2(022)-(220)-(202)+2(-1-3-3)-(-3-3-1)-(-3-1-3)+2(3-1-1)-(-1-13)
-(-13-1)+2(-400)-(00-4)-(0-40)

L_3'

K_1: 2(1-1-1)-(-1-11)-(-11-1)-2(-200)+(00-2)+(0-20)

K_2: 2(-111)-(11-1)-(1-11)-2(0-2-2)+(-2-20)+(-20-2)

K_3: 2(200)-(002)-(020)-2(-3-1-1)+(-1-1-3)+(-1-3-1)

K_4: 2(2-20)-(-202)-(02-2)+2(20-2)-(0-22)-(-220)-2(-31-1)+(1-1-3)
+(-1-31)-2(-3-11)+(-11-3)+(1-3-1)

K_5: 2(-311)-(11-3)-(1-31)-2(2-2-2)+(-2-22)+(-22-2)

K_6: 2(022)-(220)-(202)-2(-1-3-3)+(-3-3-1)+(-3-1-3)+2(3-1-1)-(-1-13)
-(-13-1)-2(-400)+(00-4)+(0-40)

Λ_3

K_2: 2(1-1-1)-(-1-11)-(-11-1)

K_3: 2(-200)-(00-2)-(0-20)

K_4: 2(-111)-(11-1)-(1-11)

K_6: 2(200)-(002)-(020)

K_7: 2(0-2-2)-(-2-20)-(-20-2)

K_8: 2(2-20)-(-202)-(02-2)-(0-22)+2(20-2)-(-220)

K_9: 2(-3-1-1)-(-1-1-3)-(-1-3-1)

K_{11}: 2(-31-1)-(1-1-3)-(-1-31)+2(-3-11)-(-11-3)-(1-3-1)

K_{12}: 2(022)-(220)-(202)

K_{13}: 2(-311)-(11-3)-(1-31)

K_{14}: 2(2-2-2)-(-2-22)-(-22-2)

K_{15}: 2(3-1-1)-(-1-13)-(-13-1)

SYMMETRIZED COMBINATIONS OF PLANE WAVES

Λ_1

K_0: (000)
K_1: (-1-1-1)
K_2: (1-1-1)+(-1-11)+(-11-1)
K_3: (-200)+(00-2)+(0-20)
K_4: (-111)+(11-1)+(1-11)
K_5: (111)
K_6: (200)+(002)+(020)
K_7: (0-2-2)+(-2-20)+(-20-2)
K_8: (2-20)+(-202)+(o2-2)+(20-2)+(0-22)+(-220)
K_9: (-3-1-1)+(-1-1-3)+(-1-3-1)
K_{10}: (-2-2-2)
K_{11}: (-31-1)+(1-1-3)+(-1-31)+(-3-11)+(-11-3)+(1-3-1)
K_{12}: (022)+(220)+(202)
K_{13}: (-311)+(11-3)+(1-31)
K_{14}: (2-2-2)+(-2-22)+(-22-2)
K_{15}: (3-1-1)+(-1-13)+(-13-1)

Σ_1

K_0: (000)
K_1: (-1-11)+(-1-1-1)
K_2: (-200)+(0-20)
K_3: (1-11)+(1-1-1)+(-11-1)+(-111)
K_4: (002)+(00-2)
K_5: (111)+(11-1)
K_6: (-2-20)
K_7: (200)+(020)
K_8: (-202)+(-20-2)+(0-22)+(0-2-2)
K_9: (2-20)+(-220)
K_{10}: (-3-11)+(-3-1-1)+(-1-31)+(-1-3-1)
K_{11}: (-2-22)+(-2-2-2)
K_{12}: (202)+(20-2)+(022)+(02-2)
K_{13}: (-1-13)+(-1-1-3)
K_{14}: (-311)+(-31-1)+(1-31)+(1-3-1)
K_{15}: (220)

Σ_3

K_1: (-1-11)-(-1-1-1)
K_3: (1-11)-(1-1-1)-(-11-1)+(-111)
K_4: (002)-(00-2)
K_5: (111)-(11-1)
K_8: (-202)-(-20-2)+(0-22)-(0-2-2)
K_{10}: (-3-11)-(-3-1-1)+(-1-31)-(-1-3-1)
K_{11}: (-2-22)-(-2-2-2)
K_{12}: (202)-(20-2)+(022)-(02-2)
K_{13}: (-1-13)-(-1-1-3)
K_{14}: (-311)-(-31-1)+(1-31)-(1-3-1)

SYMMETRIZED COMBINATIONS OF PLANE WAVES

Σ_4

K_2 : (-200)-(0-20)

K_3 : (1-11)+(1-1-1)-(-11-1)-(-111)

K_7 : (200)-(020)

K_8 : (-202)+(-20-2)-(0-22)-(0-2-2)

K_9 : (2-20)-(-220)

K_{10}: (-3-11)+(-3-1-1)-(-1-31)-(-1-3-1)

K_{12}: (202)+(20-2)-(022)-(02-2)

K_{14}: (-311)+(-31-1)-(1-31)-(1-3-1)

Σ_2

K_3 : (1-11)-(1-1-1)+(-11-1)-(-111)

K_8 : (-202)-(-20-2)+(0-22)-(0-2-2)

K_{10}: (-3-11)-(-3-1-1)-(-1-31)+(-1-3-1)

K_{12}: (202)-(20-2)-(022)+(02-2)

K_{14}: (-311)-(-31-1)-(1-31)+(1-3-1)

5. The pseudopotential method.

The basic idea of pseudopotential comes from the orthogonalized plane wave method (Herring 1940, Phillips and Kleinman 1959). In the OPW method plane waves are used as basic functions which have been made orthogonal to the core states, so that the lowest eigenvalue corresponds to levels in the valence band.

In the pseudopotential method one writes the wave function for a valence electron in the form :

$$\psi = v - \sum \langle \phi_n , v \rangle \phi_n \qquad (5.1)$$

where ϕ_n are the eigenfunctions of the core states and ψ is orthogonal to all ϕ_n.

v is a smooth function which is expressed as a sum of symmetrized combinations of plane waves.

Schrodinger equation gives for the core function,

$$H\phi_n = E_n \phi_n \qquad (5.2)$$

and for the valence function,

$$H\psi = E\psi \qquad (5.3)$$

Using equations (5.1), (5.2), (5.3) one obtains,

$$Hv - \sum_n \langle \phi_n , v \rangle (E_n - E) \phi_n = Ev \qquad (5.4)$$

Introducing a repulsive potential, the so-called pseudopotential,

$$V_p = \sum_n \langle \phi_n , v \rangle (E_n - E) \frac{\phi_n}{v} \qquad (5.5)$$

equation (5.4) becomes,

$$(H + V_p)v = Ev \qquad (5.6)$$

where the function v may be called a pseudo-wave-function.

Equation (5.6) may be written as,

$$(-\nabla^2 + V' + V_p)v = Ev \qquad (5.7)$$

where V' is the true lattice potential.

The symbol V_p stands for a non-localized potential operator :

$$V_p v(\underline{r}) = \int V_p(\underline{r},\underline{r}')v(\underline{r}')d\underline{r}'$$

where $$V_p(\underline{r},\underline{r}') = \sum_n (E-E_n)\phi_n^*(\underline{r}')\phi_n(\underline{r})$$

However in practice V_p is treated as a localized operator.

It turns out that the positive psudopotential V_p cancels to a large extent within the core region the negative crystal potential V'. Therefore the effective potential is weak and is also a smooth function which expanded in a Fourier series gives quite small components very convenient for a plane wave computation. This cancellation can be improved by suitable choice of the core functions. Cohen and Heine(1961) observed that the pseudopotential V_p is not uniquely defined. They showed that any linear combination of the core wave functions ϕ_n can be added to the pseudo-wave-function v without altering the valence function ψ. This can be seen by noticing that the pseudopotential operator V_p

projects v on the core states; and since ψ is orthogonal to all ϕ_n the addition of V_p to the Hamiltonian operator makes no difference to the eigenvalue problem for the valence states. So in equation (5.5) we replace $\langle\phi_n, v\rangle(E_n - E)$ with $\langle F, v\rangle$ where F can be conveniently chosen to give good cencellation. We put $F = -V'\phi_n$ and then the effective potential $V' + V_p$ operating on v gives :

$$(V'+V_p)v = V'v - \sum_n \langle V'\phi_n, v\rangle \phi_n \qquad (5.8)$$

This shows that we can subtract from V' a sum of core functions and this explains why the effective potential can be very small. If the occupied core states formed a complete system the cancellation would be total.

Bassani and Celli (1961) showed that the effective potential, due to its weakness, may be treated by second order perturbation theory. Austin, Heine and Sham (1962) proved that there exists a wider class of pseudopotentials which all give the same valence energy levels.

Ziman (1965) showed that the "Green's function" method for the calculation of electronic band structure is closely related with the pseudopotential method.

Crystal band structure calculations have been carried out with assumed crystal potentials, that is the term $V' + V_p$ in equation (5.7) has been substituted by the particular form of potential which has been chosen. Such a calculation was performed by Pincherle and Lee (1961) and it is discussed in the next section.

It must be noted at this stage that the term pseudopotential is often used to describe an assumed potential. This is the case in the present work where the pseudopotential which has been chosen is of the form :

$$V(r) = A/r + Br + C$$

where A, B, C are constants to be considered in the following chapter.

The term model pseudopotential suggested by Heine and his co-workers is more appropriate in our case.

6. Review of Calculations Using Pseudopotentials.

The idea of pseudopotential was first introduced by Hellmann and Kassatotschkin (1936). In their work on the cohesive energies of the alkali metals they introduced a potential energy for the valence electron of the form $-2/r$ for large r, but containing a repulsive part at small r.

In 1958 Callaway calculated the energy bands of sodium by using for the valence electron a pseudopotential of the form :

$$V(r) = -2/r + Ae^{-\beta r}/r$$

where the constants A and B have been determined from spectroscopic data. He applied the method of plane wave expansion (note that the effect of the core states is contained in the pseudopotential so that the orthogonalization procedure is unnecessary), and calculated the energy levels of s and p symmetry at four points of the Brillouin zone. His results are in good agreement with calculations by Ham (1962) using the quantum defect method, and by Howarth and Jones (1952) and Von der Lage and Bethe (1947) using the cellular method and the Prokofjew potential.

Phillips and Kleinman (1959) estimated their pseudopotential by using Slater's (1930-32) simplified analytic expressions for the wave functions in the core region. They assumed that the radial part of the "pseudowave-function" v (see previous section) is given by

$$v \sim r^{n} e^{-\lambda r}$$

where n and λ are variational parameters. They also assumed the "Coulomb" potential V' to have the form,

$$V'(r) = - 2Z/r - 2(A-Z)/r\ e^{-\lambda r}$$

where A is the atomic number of the atom considered and Z, λ are varied to give the correct core and valence levels as determined from Hartree calculations. They carried out calculations for Si with two choices of Z and λ, concluding that within the core region the repulsive potential (which it may be said that represents the positive kinetic energy of the electron) very nearly cancels the attractive potential (which represents the negative potential energy inside the core). This explains the rapid convergence of orthogonalized plane wave calculation for s-states. For the p-states they did not find such a cancellation in agreement with the slow convergence of O.P.W calculations.

This cancellation between kinetic and potential energy was demonstrated more clearly by Cohen and Heine (1961). Phillips and Kleinman in their second paper of 1959 applied their method to diamond. They constructed approximate self-consistent potentials and found that the charge densities and the energy gaps were in good agreement with experiment. In 1960 they used the pseudopotential method for cubic boron nitride and found an energy gap about twice that of diamond, a result which is consistent with the results for other zincblende crystals. They also observed that the maximum of valence band and the minimum in the conduction band are at the centre and (100) face of the Brillouin zone, respectively. The most important feature of their work is the ease with which it leads to a self-consistent crystal potential.

Antoncik (1959) working independently from Phillips and Kleinman developed a pseudopotential which is an extension to metals of the following potential derived for atoms by Gombás (1956):

$$G_\ell = -\pi^2 D_\ell^2/4(2\ell+1) - \ell^2/4a_0 r^2$$

where D_ℓ is the radial density of all states with angular momentum quantum number l energetically lower than the state of the valence electron characterized by the same quantum number l, and a_0 is the Bohr radius. Antoncik wrote Schrodinger's equation in he form

$$(H + V_{rep})\psi = E\psi$$

where V_{rep} is an operator defined in terms of the above potential. He tested his method on diamond and found his results in agreement with Herman's (1952) O.P.W. calculation.

Antoncik's "l-dependent" pseudopotential was used by Cornwell and Wohlfarth (1960) to calculate the band structure of the alkali metals and metallic beryllium. Also Cornwell (1961) performed calculations, using Phillips type pseudopotential, for the noble metals. He concluded that the optical data are inconsistent with the low temperatures specific heats and the (111) neck areas given by the de-Haas Van Alphen effect, but the cyclotron resonance effective masses are correct.

Harrison (1960a) employed the pseudopotential method to find the band structure of aluminium. He determined the necessary parameters from Heine's (1957) results for the point W, and he constructed the Fermi surface. Comparing his results with experimental measurements which determine the characteristics of the Fermi surface, he found that the geometry of it is given quite well, but that there is a discrepancy of a factor of order two between the derived and measured effective masses.

Harrison (1960b) extended his calculations and constructed the Fermi surfaces for face-centered-cubic and body-centered-cubic polyvalent metals. He found his results in semiquantitative agreement with experiment in all cases. He also observed agreement with experiment within a few hundredths of a rydberg in his band structure calculation of zinc (1962, 1963) when the potential used was based on the Hartree-Fock field for neutral zinc.

Pincherle and Lee (1961) studied the electronic band structure of a simple cubic and a face-centred-cubic monatomic substance by a plane-wave method using an assumed potential which was taken to be constant within the sphere inscribed in the Wigner-Seitz cell and zero outside. They calculated the bands at the points Γ, X, W and L for two different depths of the potential wells, and sketched their graphs, without any calculation for the intermediate points, using the compatibility relations. They found that the lowest band has its minimum at $\underline{k}=0$ and maxima at W and X. The second (p) band was found to have its maximum at $\underline{k}=0$ and minima at L and X. The third (d) band showed a minimum at X. It was concluded that changes in the potential leave the main pattern of the band structure unchanged.

The same type of potential was used by Zaher Hassan (1965) to determine by a plane-wave method the electronic band structure of a model of a sodium chloride crystal.. Her conclusions do not agree with Howland's (1958) "tight binding" calculation, but they do agree with some experimental results.

The present work is aiming to investigate the effect of a more complicated model pseudopotential on the band structure. It will be necessary to perform calculations for the intermediate points Δ, Z, Q and Λ in order to plot more reliable graphs.

Heine and Abarenkov (1964) introduced a model pseudopotential method which is not based on the orthogonalized plane wave method but is an extension of the quantum-defect approach.

Their pseudopotential for the free ion is

$$V_M = -\sum A_\ell(E) P_\ell \qquad \text{for } r < R_M$$

$$V_M = -Z/r \qquad \text{for } r > R_M$$

in atomic units ($e = \hbar = m = 1$)

where A_ℓ is a constant independent of r, depending on the energy E of the incident conduction electron and the radius R_M of a sphere constructed around the ion. P_ℓ is a projection operator which picks out the lth spherical harmonic of the incident wave function.

A_ℓ (E) is fitted to spectroscopic data for the energy levels of the free ions.

Heine and Abarenkov considered the potential of all ions in the metal as a sum of potentials of the above type and a potential due to the conduction electrons which is obtained from the dielectric screening calculation of Cohen and Phillips (1961).

To obtain the matrix elements they used a plane wave expansion, and their results for the band structure of the alkali metals gave better agreement with experiment than previous results (Ham 1962).

The same method has been used by Animalu and Heine (1966) to obtain matrix elements between states on the Fermi surface for a number of metals.

We wish to mention here in addition to the references given in the text, the references given at the end of Chapter I and the books by Kittel (1963) and Harrison (1966).

CHAPTER III

1. The pseudopotential used.

A face-centred cubic structure is considered whose Wigner-Seitz cell is a rhombododecahedron. (Fig. 2 1st Chapter). In each W-S cell a model pseudopotential is assumed to be a spherically symmetrical one of the form:

$$V(r) = A/r + Br + C \qquad (1.1)$$

for $\lambda R < r < R$ and zero otherwise (Fig. 1), where λ will be taking the values 0,25 , 0.50 , 0.75.

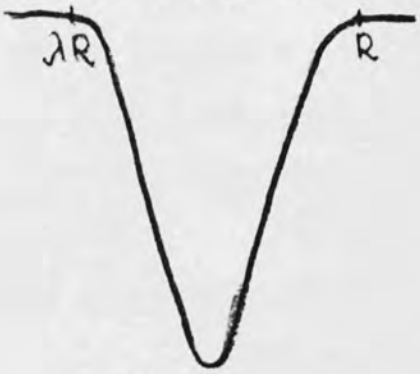


Fig 1

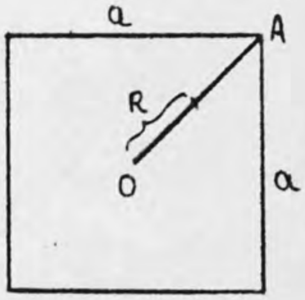


Fig 2

R is the radius of the sphere inscribed into the Wigner-Seitz cell and it is chosen as follows : (Fig. 2)

$$R = OA/2 = a\sqrt{2}/4 \qquad \text{and} \qquad R/a = \sqrt{2}/4 = b$$

where a is the length of the side of the fundamental cube.

By imposing the boundary conditions, $V(r) = 0$ at $r = R$ and $r = \lambda R$ the constants A and B in (1.1) may be expressed in terms of C, that is :

$$\begin{aligned} A/R + BR + C &= 0 \\ A/\lambda R + B\lambda R + C &= 0 \end{aligned} \qquad (1.2)$$

The system (1.2) gives the solution :

$$A = -R\lambda C/1+\lambda \qquad B = -C/R(1+\lambda) \qquad (1.3)$$

Therefore the pseudopotential will have the form :

$$V(r) = C\left[-\lambda R/(1+\lambda)r - r/(1+\lambda)R + 1\right] \qquad (1.4)$$

where C must be a negative constant.

In order to find the "depth" of the well, equation (1.4) is differentiated with respect to r ,

$$dV/dr = -C\left[-\lambda R/(1+\lambda)r^2 + 1/(1+\lambda)R\right] = 0$$

which gives $r = R\sqrt{\lambda}$

So the minimum value of the potential is

$$V_{min} = C\left(1 - 2\sqrt{\lambda}/1+\lambda\right) \qquad (1.5)$$

2. Calculation of the Fourier coefficients of the pseudopotential.

In this work in order to find the energy bands the method of plane wave expansion will be followed. The Fourier coefficients of the cr stal potential may be found as follows:

$$V(\underline{K}_n) = 1/\Omega \int_{u.c} V(\underline{r})e^{-i\underline{K}_n\cdot\underline{r}}d\underline{r}$$

where Ω is the volume of the Wigner-Seitz cell.

Having considered a face-centred cubic structure in which there are four atoms per unit cell, the volume of the unit cell is :

$$\Omega = a^3/4$$

a being the lenght of the side of the fundamental cube.

Using spherical polar coordinates with the polar axis along the direction of $\underline{K}_n$ one obtains,

$$V(K'_n) = 1/\Omega\int_{\lambda R}^{R} V(r)r^2dr\int_0^{\pi} e^{-iK'_n r\cos\theta}\sin\theta d\theta\int_0^{2\pi} d\Phi$$

$$= -\,2\pi/\Omega\int_{\lambda R}^{R} V(r)r^2dr\int_0^{\pi} e^{-iK'_n r\cos\theta}d(\cos\theta)$$

$$= -\,2\pi/\Omega\int_{\lambda R}^{R} V(r)r^2dr\int_0^{\pi} 1/-iK'_n r\cdot e^{-iK'_n r\cos\theta}d(-iK'_n r\cos\theta)$$

$$-= 2\pi/\Omega\int_{\lambda R}^{R} V(r)r^2dr\left[1/iK'_n r\cdot e^{-iK'_n r\cos\theta}\right]_0^{\pi}$$

$$= 2\pi/\Omega\int_{\lambda R}^{R} V(r)r^2dr\left(e^{iK'_n r} - e^{-iK'_n r}\right)/iK'_n r$$

$$= 4\pi/\Omega\int_{\lambda R}^{R} V(r)r^2dr\ \sin(K'_n r)/K'_n r$$

$$= 4\pi/\Omega K'^2_n\int_{\lambda R}^{R} V(r)r\sin(K'_n r)d(K'_n r)$$

Now the expression (1.4) for the potential V(r) is used, i.e.

$$V(K'_n) = 4\pi C/\Omega K'^2_n\Bigg[-\lambda R/1+\lambda\int_{\lambda R}^{R}\sin(K'_n r)d(K'_n r) -$$

$$-\,1/(1+\lambda)RK'^2_n\int_{\lambda R}^{R}(K'_n r)^2\sin(K'_n r)d(K'_n r) +$$

$$+\,1/K'_n\int_{\lambda R}^{R}(K'_n r)\sin(K'_n r)d(K'_n r)\Bigg]$$

$$= 4\pi C/\Omega K_n'^2 \Big\{ \lambda R/1+\lambda \left[\cos(K_n'R) - \cos(\lambda K_n'R) \right]$$

$$- 1/(1+\lambda) RK_n'^2 \Big[2K_n'R\sin(K_n'R) - (K_n'^2R^2-2)\cos(K_n'R) -$$

$$-2\lambda K_n'R\sin(\lambda K_n'R) + (\lambda^2K_n'^2R^2-2)\cos(\lambda K_n'R) \Big]$$

$$+ 1/K_n' \left[\sin(K_n'R) - K_n'R\cos(K_n'R) - \sin(\lambda K_n'R) + \lambda K_n'R\cos(\lambda K_n'R) \right] \Big\}$$

The reciprocal vectors K_n' for the face-centered cubic structure are:

$$2\pi/a\ (000)\ ,\ 2\pi/a\ (111)\ ,\ 2\pi/a\ (200)\ ,\ 2\pi/a\ (220)\ \text{ etc.}$$

Substituting $K_n = 2\pi(xyz)$ and using the relations $R = ba$ and $\Omega = a^3/4$, it is found that:

$$K_n'R = K_nb\ ,\ \ \Omega K_n'^2 = a^3/4\ .K_n^2/a^2 = aK\ /4$$

and $RK_n'^2 = ba\ K_n^2/a^2 = bK_n^2/a$

Therefore the following expression for $V(K')$ is found, which is independent of a.

$$V(K_n') = 16\pi C/K_n^2 \left[\lambda b/1+\lambda \cdot X(K_n) - 1/(1+\lambda) bK_n^2 \cdot Y(K_n) + 1/K_n Z(K_n) \right] \qquad (1.3)$$

where $X(K_n) = \cos K_nb - \cos\lambda K_nb$

$$Y(K_n) = 2K_nb\sin K_nb - (K_n^2b^2-2)\cos K_nb - 2\lambda K_nb\sin\lambda K_nb + (\lambda^2K_n^2b^2-2)\cos\lambda K_nb$$

$$Z(K_n) = \sin K_nb - K_nb\cos K_nb - \sin\lambda K_nb + \lambda K_nb\cos\lambda K_nb$$

Using the formula (1.3) the Fourier coefficients of table I have been found.

The coefficient $V(K_0')$ is found as follows:

$$
\begin{aligned}
V(K_0') &= 1/\Omega \int_{u.c} V(r)\,d\underline{r} = 1/\Omega \int_{\lambda R}^{R} V(r) r^2 dr \int_0^{\pi} \sin\theta\, d\theta \int_0^{2\pi} d\phi \\
&= 2\pi/\Omega \int_{\lambda R}^{R} V(r) r^2 dr \int_0^{\pi} \sin\theta\, d\theta = 4\pi/\Omega \int_{\lambda R}^{R} V(r) r^2 dr \\
&= 4\pi C/\Omega \int_{\lambda R}^{R} \left[-\lambda R r/(1+\lambda) \;-\; r^3/(1+\lambda)R \;+\; r^2\right] dr \\
&= 4\pi C/\Omega \left[-\lambda R(R^2-\lambda^2 R^2)/2(1+\lambda) - (R^4-\lambda^4 R^4)/4R(1+\lambda) + \frac{(R^3-\lambda^3 R^3)}{3}\right. \\
&= 4\pi C R^3/\Omega \left[-\lambda(1-\lambda)/2 - (1+\lambda^2)(1-\lambda)/4 + (1-\lambda)(\lambda^2+\lambda+1)/3\right.
\end{aligned}
$$

and $V(K_0') = 16\pi C b^3 (\lambda-1)\left[\lambda/2 + (\lambda^2+1)/4 - (\lambda^2+\lambda+1)/3\right]$

Using the above formula we found the V_0 of Table 1.

Table 1

THE FOURIER COEFFICIENTS OF THE PSEUDOPOTENTIAL USED

			$V'_0 = -100$	
K_n		$V(K_n) \cdot V'_0$ $\lambda = 0.25$	$V(K_n) \cdot V'_0$ $\lambda = 0.50$	$V(K_n) \cdot V'_0$ $\lambda = 0.75$
$2\pi(000)$	V_0	-7.80954	-2.31390	-0.28922
$2\pi(111)$	V_1	-1.76047	-0.18504	0.01867
$2\pi(200)$	V_2	-0.75058	0.11586	0.04902
$2\pi(220)$	V_3	0.76553	0.37990	0.03501
$2\pi(311)$	V_4	0.70446	0.20129	-0.00671
$2\pi(222)$	V_5	0.61444	0.13263	-0.01708
$2\pi(400)$	V_6	0.23428	-0.07576	-0.03279
$2\pi(331)$	V_7	0.05066	-0.13865	-0.02399
$2\pi(420)$	V_8	0.01381	-0.12694	-0.01897
$2\pi(422)$	V_9	-0.04026	-0.11639	0.00249
$2\pi(333)$ $2\pi(511)$	V_{10}	-0.02230	-0.07054	0.01443
$2\pi(440)$	V_{11}	0.02849	0	0.02037
$2\pi(531)$	V_{12}	0.04533	0.02579	0.01662
$2\pi(442)$ $2\pi(600)$	V_{13}	0.04743	0.03130	0.01457
$2\pi(620)$	V_{14}	0.03979	0.03972	0.00462
$2\pi(533)$	V_{15}	0.02215	0.03562	-0.00287
$2\pi(622)$	V_{16}	0.01516	0.03313	0.00501
$2\pi(444)$	V_{17}	-0.01348	0.02056	-0.01138
$2\pi(551)$ $2\pi(711)$	V_{18}	-0.03143	0.01136	-0.01326
$2\pi(640)$	V_{19}	-0.03619	0.00869	-0.01337
$2\pi(642)$	V_{20}	-0.04802	0.00102	-0.01150
$2\pi(800)$	V_{21}	-0.04118	-0.00090	-0.00171

$$V(K'_n) = C \cdot V(K_n)$$

3. Formation of the secular equations

We saw in the section 3 of the second chapter that using the method of momentum eigenfunctions the problem of solving Schrodinger equation reduces to the system of algebraic equations (3.9). Putting $\underline{K}'_m = \underline{K}'_l - \underline{K}'_n$ and using primed K's, for reason which becomes apparent below, we rewrite equation (3.9) in the form,

$$\left[\hbar^2/2m \left| \underline{k}' + \underline{K}'_l \right|^2 - W \right] A(\underline{k}' + \underline{K}'_l) + \sum_{\underline{K}'_l - \underline{K}'_n} V(\underline{K}'_l - \underline{K}'_n) A(\underline{k}' + \underline{K}'_n) = 0 \qquad (3.1)$$

Then the following substitutions are introduced :

$\underline{K}' = \underline{K}/a$ where $\underline{K} = 2\pi(xyz)$

$2ma^2 C/\hbar^2 = V'_0$ where C is the negative constant in terms of which the Fourier coefficients of the pseudopotential have been found.

$2ma^2 W/\hbar^2 = E$ where E expresses the energy in dimensionless units. For example for aluminium a = 4.04 A , hence E = 1 in this substance corresponds to W = 0.23 eV. The quantity V'_0 is also dimensionless and in our calculation it will be taking the values -100 , -500 and -2000.

We tabulate below the values for V_{min} expressed in dimensionless units as found from equation (1.5) :

λ / V'_0	-100	-500	-2000
0.25	-20	-100	-400
0.50	-5.72	-28.6	-114.4
0.75	-1.03	-5.15	-20.6

Having made the above substitutions equations (3.1) become :

$$\left[\left|\underline{k}+\underline{K}_1\right|^2 - E\right] A(\underline{k}+\underline{K}_1) + \sum_{\underline{K}_1-\underline{K}_n} V_0' V(\underline{K}_1-\underline{K}_n) A(\underline{k}+\underline{K}_n) = 0 \qquad (3.2)$$

Equations (3.2) provide the secular equations for our band structure calculation in the different points within the Brillouin zone. These equations are of the form:

$$\begin{aligned} \left[a_{11} - E\right] A(\underline{k}+K_0) + a_{12} A(\underline{k}+\underline{K}_1) + a_{13} A(\underline{k}+\underline{K}_2) + \ldots &= 0 \\ a_{21} A(\underline{k}+\underline{K}_0) + \left[a_{22} - E\right] A(\underline{k}+\underline{K}_1) + a_{23} A(\underline{k}+\underline{K}_2) + \ldots &= 0 \qquad (3.3) \\ a_{31} A(\underline{k}+\underline{K}_0) + a_{32} A(\underline{k}+\underline{K}_1) + \left[a_{33} - E\right] A(\underline{k}+\underline{K}_2) + \ldots &= 0 \\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots & \end{aligned}$$

In these equations we have $a_{12} = a_{21}$, $a_{13} = a_{31}$, $a_{23} = a_{32}$ etc. The small a's have been calculated using the Fourier coefficients of the pseudopotential and the symmetrized combinations of plane waves.

As we have explained in the second chapter (section 3) the vanishing determinant of the coefficients A givesthe values for the energy E. For finding the momentum eigenfunctions A we normalized them to unity.

The whole calculation was performed on the Atlas computer of the University of London using a library program, which calculates the eigenvalues and eigenvectors of a symmetric matrix.

In the following pages we tabulate the matrix elements of our secular equation. These tables are followed by tables containing our results showing the convergence achieved.

MATRIX ELEMENTS OF THE SECULAR EQUATION

Rep.	a_{11}	$a_{12}=a_{21}$	$a_{13}=a_{31}$	$a_{14}=a_{41}$	$a_{15}=a_{51}$
Γ_1	K_0^2	$8^{\frac{1}{2}}V_1$	$6^{\frac{1}{2}}V_2$	$12^{\frac{1}{2}}V_3$	$24^{\frac{1}{2}}V_4$
Γ_{15}	$K_1^2+V_2-V_3-V_5$	$2(V_1-V_4)$	$2(V_1-V_7)$	$V_2+2V_3+V_5-V_6$ $-2V_8-V_9$	$V_1+V_4-V_7-V_{10}$
Γ_{12}	$K_2^2-2V_3+V_6$	$2^{\frac{1}{2}}(V_2-2V_5+V_8)$	$2(V_1-V_4-V_7+V_{10})$	$V_2-2V_8+V_{13}$	
Γ_{25}'	$K_1^2-V_2-V_3+V_5$	$2^{\frac{1}{2}}(V_1-2V_4+V_7)$	$V_2-2V_3+V_5+V_6$ $-2V_8+V_9$	$V_1-V_4-V_7+V_{10}$	
Γ_2'	$K_1^2-3V_2+3V_3+V_5$	$(\frac{1}{3})^{\frac{1}{2}}(3V_2-6V_3+$ $3V_5-3V_6+6V_8-3V_9)$	$V_1-3V_4+3V_7-V_{10}$		
Δ_1	$(k+K_0)^2$	$2V_1$	$2V_1$	V_2	$2V_2$
Δ_2	$(k+K_4)^2-2V_3+V_6$	$V_2-2V_5+V_8$	$V_2-2V_5+V_8$	$2^{\frac{1}{2}}(V_1-V_4-V_7+V_{10})$	$2^{\frac{1}{2}}(V_1-V_4-V_7+V_{10})$
Δ_2'	$(k+K_1)^2-2V_2+V_3$	$V_2-2V_3+V_5$	$V_1-2V_4+V_7$	$V_2-2V_3+V_5$	$2^{\frac{1}{2}}(V_2-V_3-V_6+V_8)$
Δ_5	$(k+K_1)^2-V_3$	V_2-V_5	$2^{\frac{1}{2}}(V_1-V_4)$	$2^{\frac{1}{2}}(V_1-V_4)$	V_1-V_7
X_1	$(k+K_0)^2+V_2$	$8^{\frac{1}{2}}V_1$	$2(V_2+V_3)$	$2(V_1+V_4)$	$(\frac{1}{5})^{\frac{1}{2}}(V_2+4V_3+$ $+4V_5+V_6)$
X_4'	$(k+K_0)^2-V_2$	$2(V_2-V_3)$	$2(V_1-V_4)$	$(\frac{1}{5})^{\frac{1}{2}}(V_2+4V_3-4V_5-V_6)$	$2(V_3-V_8)$
X_3	$(k+K_1)^2-2V_2+V_3$	$2^{\frac{1}{2}}(V_2-2V_3+V_5)$	$2^{\frac{1}{2}}(V_1-2V_4+V_7)$	$2^{\frac{1}{2}}(V_2-V_3-V_6+V_8)$	$2(V_3-V_5-V_8+V_9)$
X_5'	$(k+K_1)^2-V_3$	$2(V_1-V_4)$	$2^{\frac{1}{2}}(V_2-V_5)$	$2^{\frac{1}{2}}(V_1-V_7)$	$V_2+V_3-V_6-V_8$
X_5	$(k+K_2)^2-V_2-V_6+V_8$	$2^{\frac{1}{2}}(V_1-2V_4+V_7)$	$2^{\frac{1}{2}}(V_2-V_3-V_8+V_9)$	$V_2-V_6-V_8+V_{11}$	$2^{\frac{1}{2}}(V_1-V_4-V_{10}+V_{12})$
X_2	$(k+K_2)^2+V_2-2V_3$ $-2V_5+V_6+V_8$	$2(V_1-V_4-V_7+V_{10})$	$V_2-2V_5+V_6+V_8-2V_9+V$	$2^{\frac{1}{2}}(V_1-2V_7+V_{12})$	

MATRIX ELEMENTS OF THE SECULAR EQUATION

Rep.	a_{22}	$a_{23}=a_{32}$	$a_{24}=a_{42}$	$a_{25}=a_{52}$	$a_{26}=a_{62}$
Γ_1	$K_1^2+3V_2+3V_3+V_5$	$12^{\frac{1}{2}}(V_1+V_4)$	$6^{\frac{1}{2}}(V_1+2V_4+V_7)$	$(\frac{1}{3})^{\frac{1}{2}}(3V_2+6V_3+3V_5$ $+3V_6+6V_8+3V_9)$	$V_1+3V_4+3V_7+V_{10}$
Γ_{15}	$K_2^2+V_6$	$2(V_2-V_8)$	$2(V_1-V_{10})$	$2(V_3-V_9)$	V_2-V_{13}
Γ_{12}	$K_3^2-2V_3+2V_6-$ $-2V_9+V_{11}$	$2^{\frac{1}{2}}(V_1-2V_7+V_{12})$	$2^{\frac{1}{2}}(V_3-2V_9-V_{14})$		
Γ_{25}'	$K_3^2-2V_6+V_{11}$	$2^{\frac{1}{2}}(V_4-2V_7+V_{10})$	$2^{\frac{1}{2}}(V_2-2V_8+V_{13})$		
Γ_2'	$K_4^2-2V_2+3V_3-2V_5-4V_8$ $+4V_9+2V_{11}-3V_{13}+2V_{14}-V_{16}$	$(\frac{1}{3})^{\frac{1}{2}}(V_1-2V_4+V_7-V_{10}+2V_{12}-V_{15})$			
Δ_1	$(k+K_1)^2+2V_2+V_3$	$V_2+2V_3+V_5$	$2V_1$	$2(V_1+V_4)$	$2V_4$
Δ_2	$(k+K_6)^2-2V_3+V_6$	$V_6-2V_9+V_{11}$	$2^{\frac{1}{2}}(V_1-V_4-V_7+V_{10})$	$2^{\frac{1}{2}}(V_4-V_7-V_{10}+V_{12})$	
Δ_2'	$(k+K_3^2)^2-2V_2+V_3$	$V_1-2V_4+V_7$	$V_6-2V_8+V_9$	$2^{\frac{1}{2}}(V_3-V_5-V_8+V_9)$	$V_4-2V_7+V_{10}$
Δ_5	$(k+K_3)^2-V_3$	$2^{\frac{1}{2}}(V_1-V_4)$	$2^{\frac{1}{2}}(V_4-V_7)$	V_1-V_7	V_6-V_9
X_1	$(k+K_1)^2+2V_2+V_3$	$8^{\frac{1}{2}}(V_1+V_4)$	$2^{\frac{1}{2}}(V_2+2V_3+V_5)$	$\frac{4}{\sqrt{10}}(V_1+3V_4+V_7)$	$2^{\frac{1}{2}}(V_2+V_3+V_6+V_8)$
X_4'	$(k+K_2)^2-V_2+2V_3$ $-2V_5+V_6-V_8$	$2(V_1-V_7)$	$\frac{2}{\sqrt{5}}(2V_2-V_3+V_8-2V_9)$	$V_2+2V_5-V_6+V_8$ $-2V_9-V_{11}$	$2^{\frac{1}{2}}(V_1-V_{12})$
X_3	$(k+K_3)^2-2V_2+V_3$ $+V_6-2V_8+V_9$	$V_1-V_4-V_7+V_{10}$	$2(V_3-V_5-V_8+V_9)$	$2^{\frac{1}{2}}(V_2-V_3-V_6+2V_8$ $-V_9-V_{11}+V_{13})$	
X_5'	$(k+K_2)^2+V_2-V_6-V_8$	$2^{\frac{1}{2}}(V_1-V_7)$	$2^{\frac{1}{2}}(V_2+V_3-V_8-V_9)$	$2(V_1-V_{10})$	$V_2+V_6-V_8-V_{11}$
X_5	$(k+K_3)^2-V_3-V_6+V_9$	$V_1-V_4-V_7+V_{10}$	$2^{\frac{1}{2}}(V_1-V_4-V_{10}+V_{12})$	$V_2+V_3-V_6-2V_8+V_{11}-V_9+V_{13}$	
X_2	$(k+K_5)^2+V_2-V_3-2V_8$ $-V_{11}+V_{13}+V_{14}$	$2(V_4-V_7-V_{10}+V_{12})$	$2^{\frac{1}{2}}(V_2+V_3-V_5-2V_9-V_{13}+V_{14}+V_{16})$		

MATRIX ELEMENTS OF THE SECULAR EQUATION

Rep.	a_{33}	$a_{34}=a_{43}$	$a_{35}=a_{53}$	$a_{36}=a_{63}$
Γ_1	$K_2^2+4V_3+V_6$	$8^{\frac{1}{2}}(V_2+V_5+V_8)$	$2(V_1+2V_4+2V_7+V_{10})$	$12^{\frac{1}{2}}(V_3+V_9)$
Γ_{15}	$K_3^2+2V_3-2V_9-V_{11}$	$2(V_1+V_4-V_{10}-V_{12})$	$2(V_2-V_{13})$	$2(V_3-V_{14})$
Γ_{12}	$K_4^2+2V_2-V_5-2V_8-$ $-2V_9-V_{11}+2V_{14}+V_{16}$	$2(V_1-V_7-V_{12}-V_{18})$		
Γ_{25}'	$K_4^2-2V_2+V_3+V_{13}-2V_{14}$ $+V_{16}$	$V_1-2V_4+V_7+V_{10}$ $-2V_{12}+V_{15}$		
Γ_2'	$K_5^2-3V_6+3V_{11}-V_{17}$			
Δ_1	$(k+K_3)^2+2V_2+V_3$	$2V_4$	$2(V_1+V_4)$	$2V_1$
Δ_2	$(k+K_8)^2-2V_3+V_6$	$2^{\frac{1}{2}}(V_4-V_7-V_{10}+V_{12})$	$2^{\frac{1}{2}}(V_1-V_4-V_7+V_{10})$	
Δ_2'	$(k+K_7)^2-2V_6+V_{11}$	$V_4-2V_7+V_{10}$	$2^{\frac{1}{2}}(V_1-V_4-V_{10}+V_{12})$	$V_2-2V_8+V_{13}$
Δ_5	$(k+K_4)^2-V_6$	V_2-V_8	$2^{\frac{1}{2}}(V_2-V_8)$	$2^{\frac{1}{2}}(V_4-V_7)$
X_1	$(k+K_2)^2+V_2+2V_3+2V_5$ $+V_6+V_8$	$2(V_1+2V_4+V_7)$	$(\frac{4}{5})^{\frac{1}{2}}(2V_2+3V_3+3V_8+2V_9)$	$2(V_1+V_4+V_7+V_{10})$
X_4'	$(k+K_3)^2+2V_2+V_3-V_6$ $-2V_8-V_9$	$(\frac{4}{5})^{\frac{1}{2}}(2V_1+V_4-V_7-2V_{10})$	$2(V_1+V_4-V_{10}-V_{12})$	$2^{\frac{1}{2}}(V_2+V_3+V_6-V_9-V_{11}-V_1$
X_3	$(k+K_4)^2-2V_6+V_2-2V_8$ $+V_{11}+V_{13}$	$2(V_1-V_4-V_{10}+V_{12})$	$2^{\frac{1}{2}}(V_1-V_7-V_{10}+V_{15})$	
X_5'	$(k+K_3)^2-V_3+V_6-V_9$	$V_1+V_4-V_7-V_{10}$	$2^{\frac{1}{2}}(V_3+V_5-V_8-V_9)$	$2^{\frac{1}{2}}(V_1-V_4+V_{10}-V_{12})$
X_5	$(k+K_4)^2-V_2-V_{11}+V_{13}$	$2^{\frac{1}{2}}(V_3-V_8-V_9+V_{13})$	$V_1-V_7-V_{10}+V_{15}$	
X_2	$(k+K_6)^2-2V_3+V_6+V_{13}$ $-2V_{16}+V_{19}$	$2^{\frac{1}{2}}(V_1-V_4-V_7+2V_{10}$ $-V_{12}-V_{15}+V_{18})$		

MATRIX ELEMENTS OF THE SECULAR EQUATIONS

Rep.	a_{44}	$a_{45}=a_{54}$	$a_{46}=a_{64}$	$a_{47}=a_{74}$
Γ_1	$K_3^2+4V_3+2V_6+4V_9+V_{11}$	$2^{\frac{1}{2}}(2V_1+3V_4+2V_7+3V_{10}+2V_{12})$	$6^{\frac{1}{2}}(V_2+2V_8+V_{13})$	$8^{\frac{1}{2}}(V_3+V_9+V_{14})$
Γ_{15}	$K_4^2+2V_2+V_3-V_{13}-2V_{14}-V_{16}$	$V_1+2V_4+V_7-V_{10}-2V_{12}-V_{15}$	$2(V_1-V_{18})$	
Γ_{12}	$K_6^2-2V_{11}+V_{21}$			
Γ_{25}'	$K_5^2-V_6-V_{11}+V_{17}$			
Δ_1	$(k+K_2)^2$	$2V_3$	V_6	$2V_2$
Δ_2	$(k+K_{10})^2+V_2-V_3-2V_8-V_{11}+V_{13}+V_{14}$	$V_2+V_3-V_5-2V_9-V_{13}+V_{14}+V_{16}$		
Δ_2'	$(k+K_9)^2-2V_2+V_3$	$2^{\frac{1}{2}}(V_3-V_5-V_8+V_9)$	$V_1-2V_4+V_7$	$2^{\frac{1}{2}}(V_8-V_9-V_{11}+V_{13})$
Δ_5	$(k+K_6)^2-V_6$	$2^{\frac{1}{2}}(V_3-V_9)$	$2^{\frac{1}{2}}(V_1-V_4)$	V_6-V_{11}
X_1	$(k+K_3)^2+2V_2+V_3+V_6+2V_8+V_9$	$(\frac{4}{5})^{\frac{1}{2}}(2V_1+3V_4+3V_7+2V_{10})$	$2(V_3+V_5+V_8+V_9)$	$2(V_1+V_4+V_{10}+V_{12})$
X_4'	$(k+K_4)^2-\frac{4}{5}(V_2-V_{11})+\frac{8}{5}(V_5+V_6-V_8-V_9)-V_{13}$	$(\frac{4}{5})^{\frac{1}{2}}(V_2+2V_3-2V_8+2V_9-2V_{13}-V_{14})$	$(\frac{16}{10})^{\frac{1}{2}}(V_1+V_4-V_7+V_{10}-V_{12}-V_{15})$	
X_3	$(k+K_5)^2-V_2+V_3-2V_8+V_{11}-V_{13}+V_{14}$	$2^{\frac{1}{2}}(V_2-V_3+V_5-2V_9+V_{13}-V_{14}+V_{16})$		
X_5'	$(k+K_4)^2+V_2-V_{11}-V_{13}$	$2^{\frac{1}{2}}(V_1+V_4-V_{10}-V_{12})$	$2^{\frac{1}{2}}(V_3+V_8-V_9-V_{13})$	$V_1+2V_4+V_7-V_{10}-2V_{12}-V_{15}$
X_5	$(k+K_6)^2-V_6-V_{13}+V_{19}$	$2^{\frac{1}{2}}(V_1-2V_{10}+V_{18})$		
X_2	$(k+K_7)^2+V_2-V_3+V_6-V_8-V_9-V_{11}-V_{13}+V_{14}-V_{17}+V_{14}+V_{20}$			

MATRIX ELEMENTS OF THE SECULAR EQUATIONS

Rep	a_{55}	$a_{56}=a_{65}$	$a_{57}=a_{75}$	$a_{58}=a_{85}$
Γ_1	$K_4^2+2V_2+3V_3+2V_5+4V_8$ $+4V_9+2V_{11}+3V_{13}+2V_{14}+V_{16}$	$(\frac{1}{5})^{\frac{1}{2}}(V_1+2V_4+V_7$ $+V_{10}+2V_{12}+V_{15})$	$2(V_1+2V_7+2V_{12}+V_{18})$	
Γ_{15}	$K_5^2+V_6-V_{11}-V_{17}$	$2(V_5-V_{16})$		
Δ_1	$(k+K_4)^2+2V_3+V_6$	$2V_3$	$-V_2+2V_5+V_8$	$2(V_2+V_8)$
Δ_2	$(k+K_{11})^2+V_2-V_3-2V_8$ $-V_{11}+V_{13}+V_{14}$			
Δ_2'	$(k+K_{10})^2-V_2+V_3-2V_8$ $+V_{11}-V_{13}+V_{14}$	$2^{\frac{1}{2}}(V_1-V_4-V_{10}+V_{12})$	$V_2-V_3+V_5-2V_9$ $+V_{13}-V_{14}+V_{16}$	$2^{\frac{1}{2}}(V_8-V_9-V_{11}+V_{13})$
Δ_5	$(k+K_7)^2-V_{11}$	V_4-V_{10}	$2^{\frac{1}{2}}(V_3-V_9)$	$V_1+V_4-V_{10}-V_{12}$
X_1	$(k+K_4)^2+\frac{4}{5}(V_2+2V_5+$ $+2V_6+2V_8+2V_9+V_{11})+V_{13}$	$(\frac{16}{5})^{\frac{1}{2}}(V_1+V_4+V_7+V_{10}+V_{12})$	$(\frac{4}{5})^{\frac{1}{2}}(V_2+2V_3+2V_8$ $+2V_9+2V_{13}+V_{14})$	$(\frac{8}{5})^{\frac{1}{2}}(V_1+3V_4+V_7+3V_{12}$ $+V_{10}+V_{15})$
X_4'	$(k+K_6)^2+2V_3+V_6-V_{13}$ $-2V_{16}-V_{19}$	$2^{\frac{1}{2}}(V_1+V_4+V_7-V_{12}$ $-V_{15}-V_{18})$		
X_3	$(k+K_7)^2-V_2+V_3+V_6-3V_8$ $+V_9+V_{11}-3V_{13}+V_{14}+V_{17}-V_{19}+V_{20}$			
X_5'	$(k+K_5)^2+V_2-V_{13}-V_{14}$	$2(V_4-V_{12})$	$2^{\frac{1}{2}}(V_2+V_3-V_{14}-V_{16})$	
X_5	$(k+K_7)^2+V_2-V_6-V_8-V_{13}$ $-V_{14}+V_{19}+V_{20}$			

MATRIX ELEMENTS OF THE SECULAR EQUATION

Rep.	a_{66}	$a_{67}=a_{76}$	$a_{68}=a_{86}$	$a_{69}=a_{96}$
Γ_1	$K_5^2+3V_6+3V_{11}+V_{17}$	$12^{\frac{1}{2}}(V_5+V_{16})$		
Γ_{15}	$K_6^2-V_{21}$			
Δ_1	$(k+K_5)^2$	$2V_8$	$2V_5$	$2V_2$
Δ_2'	$(k+K_{13})^2-2V_6+V_{11}$	$2^{\frac{1}{2}}(V_4-V_7-V_{12}+V_{15})$	$V_{10}-2V_{12}+V_{15}$	$V_6-2V_{11}+V_{17}$
Δ_5	$(k+K_9)^2-V_3$	$2^{\frac{1}{2}}(V_{10}-V_{12})$	$V_3+V_5-V_8-V_9$	V_1-V_7
X_1	$(k+K_5)^2+V_2+V_3+2V_8$ $+V_{11}+V_{13}+V_{14}$	$2(V_4+V_7+V_{10}+V_{12})$	$2^{\frac{1}{2}}(V_2+V_3+V_5+2V_9$ $+V_{13}+V_{14}+V_{16})$	
X_4'	$(k+K_7)^2+V_2+V_3-V_6$ $+V_8-V_9+V_{11}-V_{13}+V_{14}$ $-V_{17}-V_{19}-V_{20}$			
X_5'	$(k+K_6)^2-V_6+V_{13}-V_{19}$	$2^{\frac{1}{2}}(V_1-V_{18})$		

	a_{77}	$a_{78}=a_{87}$	$a_{79}=a_{97}$	$a_{710}=a_{10.7}$
Γ_1	$K_6^2+4V_{11}+V_{21}$			
Δ_1	$(k+K_6)^2+2V_3+V_6$	$2(V_3+V_9)$	$V_6+2V_9+V_{11}$	$2(V_1+V_4)$
Δ_2'	$(k+K_{11})^2-V_2+V_3$ $-2V_8+V_{11}-V_{13}+V_{14}$	$2^{1/2}(V_3-V_5-V_8+V_9)$	$2^{1/2}(V_1-V_4-V_{10}+V_{12})$	
Δ_5	$(k+K_8)^2-V_6$	$2^{1/2}(V_4-V_{12})$	$2^{1/2}(V_8-V_{13})$	$2^{1/2}(V_1-V_{10})$
X_1	$(k+K_6)^2+2V_3+V_6+V_{13}$ $+2V_{16}+V_{19}$	$2^{1/2}(V_1+V_4+V_7+2V_{10}$ $+V_{12}+V_{15}+V_{18})$		
X_5'	$(k+K_7)^2+V_2+V_6+V_8$ $-V_{13}-V_{14}-V_{19}-V_{20}$			

MATRIX ELEMENTS OF THE SECULAR EQUATION

Rep.	$a_{16}=a_{61}$	$a_{17}=a_{71}$	$a_{18}=a_{81}$	$a_{19}=a_{91}$	$a_{1,10}=a_{10,1}$
Γ_1	$8^{\frac{1}{2}}V_5$	$6^{\frac{1}{2}}V_6$			
Γ_{15}	$2(V_4-V_{10})$				
Δ_1	V_2	$2V_3$	$2V_3$	$2V_3$	$2V_4$
Δ_2'	$V_1-2V_4+V_7$	$2^{\frac{1}{2}}(V_3-V_5-V_8+V_9)$	$V_6-2V_8+V_9$	$V_4-2V_7+V_{10}$	
Δ_5	V_2-V_5	$2^{\frac{1}{2}}(V_4-V_7)$	$V_2+V_3-V_6-V_8$	V_1-V_7	$V_3+V_5-V_8-V_9$
X_1	$4V_4$	$2(V_3+V_8)$	$8^{\frac{1}{2}}(V_4+V_7)$		
X_4'	$8^{\frac{1}{2}}(V_4-V_7)$				
X_5'	$2(V_4-V_7)$	$2^{\frac{1}{2}}(V_3+V_5-V_8-V_9)$			

	$a_{37}=a_{73}$	$a_{38}=a_{83}$	$a_{39}=a_{93}$	$a_{3,10}=a_{10,3}$	$a_{3,11}=a_{11,3}$
Γ_1	$V_2+4V_8+V_{13}$				
Δ_1	$2(V_4+V_7)$	$V_1+2V_4+V_7$	$2(V_1+V_4)$	$V_6+2V_8+V_9$	$2^{\frac{1}{2}}(V_3+V_5+V_8+V_9$
Δ_2'	$2^{\frac{1}{2}}(V_1-V_4-V_{10}+V_{12})$	$V_4-2V_7+V_{10}$	$V_2-2V_8+V_{13}$		
Δ_5	V_2-V_8	$2^{\frac{1}{2}}(V_1-V_{10})$	$2^{\frac{1}{2}}(V_3-V_9)$	$2^{\frac{1}{2}}(V_1-V_{10})$	$2^{\frac{1}{2}}(V_4-V_7)$
X_1	$V_2+2V_5+V_6$ $+V_8+2V_9+V_{11}$	$2^{\frac{1}{2}}(V_1+2V_4+2V_7$ $+2V_{10}+V_{12})$			
X_5'	$V_2+V_3-V_6$ $+V_9-V_{11}-V_{13}$				

MATRIX ELEMENTS OF THE SECULAR EQUATION

Rep.	$a_{27}=a_{72}$	$a_{28}=a_{82}$	$a_{29}=a_{92}$	$a_{2,10}=a_{10,2}$
Γ_1	$12^{\frac{1}{2}}(V_4+V_{10})$			
Δ_1	$2(V_1+V_4)$	$V_1+2V_4+V_7$	$2(V_4+V_7)$	$V_2+2V_3+V_5$
Δ_2'	$2^{1/2}(V_2-V_3-V_6+V_8)$	$V_2-2V_3+V_5$	$V_1-2V_4+V_7$	
Δ_5	$2^{1/2}(V_1-V_4)$	$V_3+V_5-V_8-V_9$	V_4-V_{10}	$V_2+V_3-V_6-V_8$
X_1	$8^{1/2}(V_4+V_7)$	$2(V_3+V_5+V_8+V_9)$		
X_5'	$2^{1/2}(V_1+V_4-V_{10}-V_{12})$			

	$a_{48}=a_{84}$	$a_{49}=a_{94}$	$a_{4,10}=a_{10,4}$	$a_{4,11}=a_{11,4}$
Δ_1	$2V_5$	$2V_8$	$2V_1$	$8^{\frac{1}{2}}V_4$
Δ_2'	$V_{13}-2V_{14}+V_{16}$	$V_{10}-2V_{12}+V_{15}$		
Δ_5	$2^{\frac{1}{2}}(V_1-V_{10})$	$2^{\frac{1}{2}}(V_2-V_8)$	$2^{\frac{1}{2}}(V_4-V_{12})$	$2^{\frac{1}{2}}(V_{10}-V_{12})$
X_1	$2^{1/2}(V_2+V_3+V_6+2V_8$ $+V_9+V_{11}+V_{13})$			

	$a_{59}=a_{95}$	$a_{5,10}=a_{10,5}$	$a_{5,11}=a_{11,5}$	$a_{5,12}=a_{12,5}$
Δ_1	$V_2+2V_5+V_8$	$2(V_4+V_7)$	$2^{\frac{1}{2}}(V_1+V_4+V_7+V_{10})$	$2^{\frac{1}{2}}(V_1+V_4+V_7+V_{10})$
Δ_2'	$2^{\frac{1}{2}}(V_4-V_7-V_{12}+V_{15})$			
Δ_5	V_2-V_{13}	$V_1+V_4-V_{10}-V_{12}$	V_4-V_{10}	V_2-V_{13}

MATRIX ELEMENTS OF THE SECULAR EQUATION

Rep.	a_{11}	$a_{12}=a_{21}$	$a_{13}=a_{31}$	$a_{14}=a_{41}$
Z_1	$(k+K_0)^2+V_2$	$2V_1$	$2V_1$	V_2+V_3
Z_3	$(k+K_0)^2-V_2$	V_2-V_3	$2^{\frac{1}{2}}(V_2-V_3)$	$2^{\frac{1}{2}}(V_1-V_4)$
Z_4	$(k+K_1)^2-V_2$	V_2-V_3	$2^{\frac{1}{2}}(V_1-V_4)$	$2^{\frac{1}{2}}(V_2-V_3)$
W_1	$(k+K_0)^2+2V_1+V_2$	$2V_1+V_2+V_3$	$2^{\frac{1}{2}}(V_1+V_2+V_3+V_4)$	$(\frac{1}{3})^{\frac{1}{2}}(2V_1+V_2+3V_3+4V_4+2V_5)$
W'_2	$(k+K_0)^2-2V_1+V_2$	$-2V_1+V_2+V_3$	$2^{\frac{1}{2}}(-V_1+V_2+V_3-V_4)$	$(\frac{1}{3})^{\frac{1}{2}}(2V_1+V_2-V_3-2V_5)$
W_3	$(k+K_0)^2-V_2$	V_2-V_3	$2^{\frac{1}{2}}(V_2-V_3)$	$(\frac{1}{3})^{\frac{1}{2}}(2V_1+V_2-V_3-2V_4)$
Q_1	$(k+K_0)^2+V_1$	V_1+V_2	V_1+V_2	$(\frac{1}{2})^{\frac{1}{2}}(2V_1+V_2+V_3)$
Q_2	$(k+K_0)^2-V_1$	$-V_1+V_2$	$-V_1+V_2$	$(\frac{1}{2})^{\frac{1}{2}}(-2V_1+V_2+V_3)$
L_1	$(k+K_0)^2+V_1$	$3^{\frac{1}{2}}(V_1+V_2)$	$3^{\frac{1}{2}}(V_1+V_3)$	$\frac{1}{2}(V_1+3V_2+3V_4+V_5)$
L'_2	$(k+K_0)^2-V_1$	$3^{\frac{1}{2}}(V_1-V_2)$	$3^{\frac{1}{2}}(V_1-V_3)$	$\frac{1}{2}(V_1+3V_2-3V_4-V_5)$
L_3	$(k+K_1)^2-V_1-V_3+V_4$	$V_1-V_2-V_4+V_5$	$V_1-V_3-V_4+V_6$	$(\frac{1}{2})^{\frac{1}{2}}(2V_1-V_2-V_4-V_5-V_7+2V_8)$
L'_3	$(k+K_1)^2+V_1-V_3-V_4$	$-V_1-V_2+V_4+V_5$	$V_1+V_3-V_4-V_6$	$(\frac{1}{2})^{\frac{1}{2}}(2V_1+V_2-V_4+V_5-V_7-2V_8)$
Λ_1	$(k+K_0)^2$	V_1	$3^{\frac{1}{2}}V_1$	$3^{\frac{1}{2}}V_2$
Λ_3	$(k+K_2)^2-V_3$	$-V_1+V_4$	$-V_2+V_5$	V_1-V_4
Σ_1	$(k+K_0)^2$	$2^{1/2}V_1$	$2^{1/2}V_2$	$2V_1$
Σ_2	$(k+K_3)^2-V_2-V_3+V_5$	$-V_1+2V_4-V_7$	$-V_3+V_5+V_6-V_8$	$V_1-2V_4+V_7$
Σ_3	$(k+K_1)^2-V_2$	$2^{1/2}(V_2-V_3)$	V_1-V_4	V_3-V_5
Σ_4	$(k+K_2)^2-V_3$	$2^{1/2}(-V_1+V_4)$	$-V_3+V_6$	$2^{1/2}(V_2-V_5)$
X'_3	$(k+K_2)^2-V_2-2V_3$ $+2V_5+V_6-V_8$	$V_2-2V_5-V_6+V_8$ $+2V_9-V_{11}$	$2^{1/2}(V_1-2V_4+2V_{10}-V_{12})$	

MATRIX ELEMENTS OF THE SECULAR EQUATION

Rep.	$a_{15}=a_{51}$	$a_{16}=a_{61}$	$a_{17}=a_{71}$	$a_{18}=a_{81}$
Z_1	$\sqrt{2}\ (V_2+V_3)$	$\sqrt{2}\ (V_1+V_4)$	V_2+V_3	$\sqrt{2}\ (V_1+V_4)$
Z_3	V_2-V_3	$\sqrt{2}\ (V_1-V_4)$	$\sqrt{2}\ (V_3-V_5)$	V_2-V_6
Z_4	$\sqrt{2}\ (V_3-V_5)$	$\sqrt{2}\ (V_1-V_4)$	V_2-V_3	V_2-V_6
W_1	$V_2+2V_4+V_6$	$1/\sqrt{3}\ (3V_3+4V_4$ $+2V_5+2V_7+V_8)$	$1/\sqrt{3}(2V_3+4V_4$ $+V_6+2V_7+3V_8)$	
W_2'	$V_2-2V_4+V_6$	$1/\sqrt{3}(V_3+2V_5$ $-2V_7-V_8)$	$1/\sqrt{3}(2V_3-4V_4$ $+V_6-2V_7+3V_8)$	
W_3	V_2-V_6	$2/\sqrt{3}(V_3-V_5)$	$1/\sqrt{3}(2V_3+V_6-3V_8)$	
Q_1	V_1+V_3	$1/\sqrt{2}(V_1+V_2+V_3+V_4)$	$1/\sqrt{3}(V_1+V_2+V_3$ $+2V_4+V_5)$	$1/\sqrt{3}(V_2+2V_3+3V_4)$
Q_2	$-V_1+V_3$	$1/\sqrt{2}(-V_1+V_2+V_3-V_4)$	$1/\sqrt{3}(-V_1+V_2+V_3$ $-2V_4+V_5)$	$1/\sqrt{3}(V_2+2V_3-3V_4)$
L_1	$\sqrt{6}\ (V_3+V_4)$	$\sqrt{3}\ (V_4+V_5)$	$\sqrt{3/2}(V_3+V_4+V_6+V_7)$	
L_2'	$\sqrt{6}(V_3-V_4)$	$\sqrt{3}(V_4-V_5)$	$\sqrt{3/2}(V_3+V_4-V_6-V_7)$	
L_3	$V_1-V_3-V_7+V_9$	$1/\sqrt{2}(V_2-2V_4+V_5$ $+V_7-2V_8+V_{10})$		
L_3'	$-V_1-V_3+V_7+V_9$	$1/\sqrt{2}(V_2-V_5+V_7-V_{10})$		
Λ_1	$\sqrt{3}V_1$	V_1	$\sqrt{3}V_2$	$\sqrt{3}V_3$
Λ_3	V_1-V_4	$1/\sqrt{2}(2V_1-V_4-V_7)$	$-V_3+V_6$	$1/\sqrt{2}(-V_2-V_5+2V_8)$
Σ_1	$\sqrt{2}V_2$	$\sqrt{2}V_1$	V_3	$\sqrt{2}V_2$
Σ_2	$-V_2+V_3+V_8-V_9$			
Σ_3	$\sqrt{2}(V_1-V_4)$	$\sqrt{2}(V_2-V_3)$	V_1-V_4	$\sqrt{2}(V_4-V_7)$
Σ_4	$-V_2+V_8$	$\sqrt{2}(V_1-V_4)$	$\sqrt{2}(-V_5+V_8)$	$\sqrt{2}(V_1-V_7)$

MATRIX ELEMENTS OF THE SECULAR EQUATION

Rep.	a_{22}	$a_{23}=a_{32}$	$a_{24}=a_{42}$	$a_{25}=a_{52}$
Z_1	$(k+K_1)^2+V_2$	V_2+V_3	$2V_1$	$2^{\frac{1}{2}}(V_1+V_4)$
Z_3	$(k+K_4)^2-V_2$	$2^{\frac{1}{2}}(V_3-V_5)$	$2^{\frac{1}{2}}(V_1-V_4)$	V_6-V_8
Z_4	$(k+K_3)^2-V_2$	$2^{\frac{1}{2}}(V_1-V_4)$	$2^{\frac{1}{2}}(V_3-V_5)$	$2^{\frac{1}{2}}(V_2-V_3)$
W_1	$(k+K_2)^2+V_2+2V_4$	$2^{\frac{1}{2}}(V_1+V_3+V_4+V_5)$	$(\frac{1}{3})^{\frac{1}{2}}(2V_1+2V_2+2V_3+$ $+2V_4+V_6+2V_7+V_8)$	$V_3+2V_4+V_8$
W_2'	$(k+K_2)^2+V_2-2V_4$	$2^{\frac{1}{2}}(-V_1+V_3-V_4+V_5)$	$(\frac{1}{3})^{\frac{1}{2}}(-2V_1-2V_2-2V_3+$ $+2V_4+V_6+2V_7+V_8)$	$V_3-2V_4+V_8$
W_3	$(k+K_2)^2-V_2$	$2^{\frac{1}{2}}(V_3-V_5)$	$(\frac{1}{3})^{\frac{1}{2}}(2V_4+V_6-2V_7-V_8)$	V_3-V_8
Q_1	$(k+K_2)^2+V_1$	V_1+V_3	$(\frac{1}{2})^{\frac{1}{2}}(V_1+V_2+V_3+V_4)$	V_2+V_4
Q_2	$(k+K_2)^2-V_1$	$-V_1+V_3$	$(\frac{1}{2})^{\frac{1}{2}}(-V_1+V_2+V_3-V_4)$	V_2-V_4
L_1	$(k+K_1)^2+2V_1+2V_3+V_4$	$V_1+2V_2+2V_4+V_5$	$(\frac{3}{4})^{\frac{1}{2}}(V_1+3V_3+3V_4+V_6)$	$2^{\frac{1}{2}}(V_1+V_2+V_4+V_5+V_7+V_8)$
L_2'	$(k+K_1)^2-2V_1+2V_3-V_4$	$-V_1+2V_2-2V_4+V_5$	$(\frac{3}{4})^{\frac{1}{2}}(V_1-V_3+V_4-V_6)$	$2^{\frac{1}{2}}(V_1-V_2+V_4-V_5+V_7-V_8)$
L_3	$(k+K_2)^2-V_3-V_4+V_7$	$-V_1+V_4+V_5-V_8$	$(\frac{1}{2})^{\frac{1}{2}}(-V_1+2V_3-V_4-V_6$ $+2V_7-V_9)$	$V_2-V_4-V_8+V_{10}$
L_3'	$(k+K_2)^2-V_3+V_4-V_7$	$-V_1+V_4-V_5+V_8$	$(\frac{1}{2})^{\frac{1}{2}}(-V_1-2V_3-V_4+V_6$ $+2V_7+V_9)$	$V_2+V_4-V_8-V_{10}$
Λ_1	$(k+K_1)^2$	$3^{\frac{1}{2}}V_2$	$3^{\frac{1}{2}}V_1$	$3^{\frac{1}{2}}V_3$
Λ_3	$(k+K_3)^2-V_3$	V_1-V_4	$-V_3+V_6$	$-V_2+V_5$

MATRIX ELEMENTS OF THE SECULAR EQUATION

Rep.	$a_{19}=a_{91}$	$a_{1,10}=a_{10,1}$	$a_{1,11}=a_{11,1}$	$a_{1,12}=a_{12,1}$
Δ_1	$2V_3$	$2V_4$	$\sqrt{8}V_4$	$\sqrt{8}V_4$
Δ_5	V_1-V_7	$V_3+V_5-V_8-V_9$	V_6-V_9	V_4-V_{10}
Z_1	$\sqrt{2}(V_3+V_5)$	$2V_4$	V_2+V_6	$2V_4$
Z_3	$\sqrt{2}(V_3-V_5)$	V_3-V_8	$\sqrt{2}(V_4-V_7)$	
Z_4	$\sqrt{2}(V_4-V_7)$	V_3-V_8	V_6-V_8	$\sqrt{2}(V_3-V_5)$
Q_1	V_4+V_5	$\sqrt{2}(V_3+V_4)$	$1/\sqrt{3}(V_3+3V_4+V_5+V_6)$	
Q_2	$-V_4+V_5$	$\sqrt{2}(V_3-V_4)$	$1/\sqrt{3}(V_3-3V_4+V_5+V_6)$	
Λ_1	$\sqrt{6}V_3$	$\sqrt{3}V_4$	V_5	$\sqrt{6}V_4$
Λ_3	$-V_4+V_7$	$-V_3+V_9$	V_1-V_7	V_2-V_8
Σ_1	$2V_3$	$\sqrt{2}V_3$	$2V_4$	$\sqrt{2}V_5$
Σ_3	V_2-V_6	$\sqrt{2}(V_3-V_5)$		

	$a_{1,13}=a_{13,1}$	$a_{1,14}=a_{14,1}$	$a_{1,15}=a_{15,1}$	$a_{1,16}=a_{16,1}$
Δ_1	$2V_4$	$2V_5$	$2V_5$	V_6
Z_1	$\sqrt{2}(V_3+V_5)$	$2V_4$	$2V_4$	V_3+V_8
Λ_1	$\sqrt{3}V_3$	$\sqrt{3}V_4$	$\sqrt{3}V_5$	$\sqrt{3}V_4$
Σ_1	$2V_3$	$\sqrt{2}V_4$	$2V_4$	V_3

MATRIX ELEMENTS OF THE SECULAR EQUATION

Rep.	$a_{26}=a_{62}$	$a_{27}=a_{72}$	$a_{28}=a_{82}$	$a_{29}=a_{92}$
Z_1	$\sqrt{2}(V_2+V_3)$	$2V_4$	$\sqrt{2}(V_3+V_5)$	$\sqrt{2}(V_1+V_4)$
Z_3	$\sqrt{2}(V_4-V_7)$	$\sqrt{2}(V_2-V_3)$	V_3-V_8	$\sqrt{2}(V_8-V_9)$
Z_4	$\sqrt{2}(V_4-V_7)$	V_6-V_8	V_3-V_8	$\sqrt{2}(V_1-V_4)$
W_1	$1/\sqrt{3}(2V_1+V_2+2V_4$ $+V_6+2V_7+2V_8+2V_9)$	$1/\sqrt{3}(V_2+V_3+2V_4$ $+2V_5+2V_7+2V_9+2V_{10})$		
W_2'	$1/\sqrt{3}(-2V_1-V_2-2V_4$ $-V_6+2V_7+2V_8+2V_9)$	$1/\sqrt{3}(V_2+V_3-2V_4$ $+2V_5-2V_7+2V_9-2V_{10})$		
W_3	$2/\sqrt{3}(V_8-V_9)$	$1/\sqrt{3}(V_2-V_3+2V_5-2V_9)$		
Q_1	$1/\sqrt{2}(V_1+V_3+V_4+V_5)$	$1/\sqrt{3}(V_1+V_2+2V_3+2V_4)$	$1/\sqrt{3}(V_1+V_2$ $+2V_4+V_5+V_6)$	V_1+V_3
Q_2	$1/\sqrt{2}(-V_1+V_3-V_4+V_5)$	$1/\sqrt{3}(-V_1+V_2+2V_3-2V_4)$	$1/\sqrt{3}(-V_1+V_2$ $-2V_4+V_5+V_6)$	$-V_1+V_3$
L_1	$V_1+2V_3+2V_7+V_9$	$1/\sqrt{2}(V_2+4V_4+V_5$ $+V_7+4V_8+V_{10})$		
L_2'	$-V_1+2V_3-2V_7+V_9$	$1/\sqrt{2}(V_2-V_5+V_7-V_{10})$		
L_3	$1/\sqrt{2}(V_1-V_3-V_{10}+V_{11})$			
L_3'	$1/\sqrt{2}(V_1-V_3-2V_4+2V_9$ $+V_{10}-V_{11})$			
Λ_1	V_5	$\sqrt{3}V_4$	$\sqrt{3}V_1$	$\sqrt{6}V_4$
Λ_3	$1/\sqrt{2}(-V_2-V_5+2V_8)$	V_1-V_4	$1/\sqrt{2}(2V_1-V_4-V_7)$	V_5-V_8
Σ_1	V_3+V_5	$\sqrt{2}V_1$	$2V_4$	$\sqrt{2}(V_1+V_4)$
Σ_4	$-V_3-V_5+V_6+V_8$	V_1-V_7	$-V_2-V_3+V_8+V_9$	
Σ_3	$V_3-V_5+V_6-V_8$	$\sqrt{2}(V_4-V_7)$	V_1-V_7	$\sqrt{2}(V_3-V_8)$

MATRIX ELEMENTS OF THE SECULAR EQUATION

Rep	a_{22}	$a_{23}=a_{32}$	$a_{24}=a_{42}$	$a_{25}=a_{52}$
Σ_1	$(k+K_1)^2+V_2$	$2V_1$	$\sqrt{2}(V_2+V_3)$	V_1+V_4
Σ_2	$(k+K_8)^2-V_3-V_6+V_9$	$V_1-2V_4+V_7$	$-V_3+V_6+V_9-V_{11}$	$V_1-V_4-V_7+V_{10}$
Σ_3	$(k+K_3)^2-V_2+V_3-V_5$	$\sqrt{2}(V_1-V_4)$	$\sqrt{2}(V_2-V_3)$	V_1-V_7
Σ_4	$(k+K_3)^2+V_2-V_3-V_5$	$\sqrt{2}(V_1-V_4)$	$-V_1+V_7$	$\sqrt{2}(V_1-V_7)$
X_3'	$(k+K_6)^2-2V_3+V_6-V_{13}$ $+2V_{16}-V_{19}$	$\sqrt{2}(V_1-V_4-V_7+V_{12}+V_{15}-V_{18})$		
	$a_{2,10}=a_{10,2}$	$a_{2,11}=a_{11,2}$	$a_{2,12}=a_{12,2}$	$a_{2,13}=a_{13,2}$
Δ_1	$V_2+2V_3+V_5$	$\sqrt{2}(V_2+V_3+V_6+V_8)$	$\sqrt{2}(V_3+V_5+V_8+V_9)$	$V_6+2V_8+V_9$
Δ_5	$V_2+V_3-V_6-V_8$	V_2-V_5	V_1-V_7	
Z_1	V_2+V_3	$2V_4$	V_2+V_6	$\sqrt{2}(V_4+V_7)$
Z_3	V_2-V_6	$\sqrt{2}(V_1-V_4)$		
Z_4	V_2-V_6	V_2-V_3	$\sqrt{2}(V_8-V_9)$	
Q_1	$\sqrt{2}(V_5+V_7)$	$1/\sqrt{3}(V_2+V_3+V_4+2V_7+V_8)$		
Q_2	$\sqrt{2}(V_5-V_7)$	$1/\sqrt{3}(V_2+V_3-V_4-2V_7+V_8)$		
Λ_1	$\sqrt{3}V_2$	V_1	$\sqrt{6}V_3$	$\sqrt{3}V_7$
Λ_3	$+V_1-V_7$	$-V_3+V_9$	$-V_4+V_{10}$	
Σ_1	$2V_4$	$\sqrt{2}(V_2+V_3)$	V_1+V_4	$\sqrt{2}(V_4+V_7)$
Σ_3	$V_2-V_3+V_8-V_9$			
	$a_{2,14}=a_{14,2}$	$a_{2,15}=a_{15,2}$	$a_{2,16}=a_{16,2}$	$a_{2,17}=a_{17,2}$
Δ_1	$V_1+2V_4+V_7$	$V_4+2V_7+V_{10}$	$2V_4$	
Z_1	V_3+V_8	V_6+V_8	$2V_4$	$\sqrt{2}(V_3+V_5)$
Λ_1	$\sqrt{3}V_5$	$\sqrt{3}V_4$	$\sqrt{3}V_6$	
Σ_1	V_2+V_6	$\sqrt{2}(V_3+V_5)$	$\sqrt{2}V_7$	

MATRIX ELEMENTS OF THE SECULAR EQUATION

Rep	a_{33}	$a_{34}=a_{43}$	$a_{35}=a_{53}$	$a_{36}=a_{63}$
Z_1	$(k+K_2)^2+V_2$	$2V_4$	$2^{\frac{1}{2}}(V_1+V_4)$	$2^{\frac{1}{2}}(V_3+V_5)$
Z_3	$(k+K_5)^2-V_2+V_6-V_8$	V_1-V_7	$2^{\frac{1}{2}}(V_3-V_5)$	V_1-V_7
Z_4	$(k+K_5)^2+V_2-V_6-V_8$	V_1-V_7	V_1-V_7	$V_2+V_3-V_8-V_9$
W_1	$(k+K_3)^2+V_1+V_2+2V_4$ $+V_6+V_7+V_8$	$(\frac{2}{3})^{\frac{1}{2}}(V_1+V_2+2V_3+3V_4$ $+V_5+2V_7+V_8+V_9)$	$2^{\frac{1}{2}}(V_1+V_3+V_8+V_{10})$	$(\frac{2}{3})^{\frac{1}{2}}(V_1+V_2+V_3+V_4+V_5$ $+2V_7+V_8+2V_9+2V_{10})$
W'_2	$(k+K_3)^2-V_1+V_2-2V_4$ $+V_6-V_7+V_8$	$(\frac{2}{3})^{\frac{1}{2}}(V_1-V_2+V_4+V_5$ $-V_8-V_9)$	$2^{\frac{1}{2}}(-V_1+V_3+V_8-V_{10})$	$(\frac{2}{3})^{\frac{1}{2}}(V_1+V_2+V_3-V_4$ $-V_5-2V_7+V_8)$
W_3	$(k+K_3)^2-V_2+V_6-V_8$	$(\frac{2}{3})^{\frac{1}{2}}(V_1+V_3-V_5-V_7)$	$2^{\frac{1}{2}}(V_3-V_8)$	$(\frac{2}{3})^{\frac{1}{2}}(V_1+V_2-V_3+V_8-$ $-V_9+V_{10})$
Q_1	$(k+K_3)^2+V_4$	$(\frac{1}{2})^{\frac{1}{2}}(V_1+V_2+V_3+V_4)$	V_1+V_5	$(\frac{1}{2})^{\frac{1}{2}}(V_2+V_3+2V_4)$
Q_2	$(k+K_3)^2-V_4$	$(\frac{1}{2})^{\frac{1}{2}}(-V_1+V_2+V_3-V_4)$	$-V_1+V_5$	$(\frac{1}{2})^{\frac{1}{2}}(V_2+V_3-2V_4)$
L_1	$(k+K_2)^2+2V_3+2V_4+V_7$	$(\frac{1}{4})^{\frac{1}{2}}(2V_1+V_2+V_4+V_5$ $+2V_8+V_7)$	$2^{\frac{1}{2}}(V_1+V_3+V_4+V_6$ $+V_7+V_9)$	$V_2+2V_4+2V_8+V_{10}$
L'_2	$(k+K_2)^2+2V_3-2V_4-V_7$	$(\frac{1}{4})^{\frac{1}{2}}(2V_1+V_2+V_4-V_5$ $-2V_8-V_7)$	$2^{\frac{1}{2}}(V_1-V_3+V_4-V_6$ $+V_7-V_9)$	$V_2-2V_4+2V_8-V_{10}$
L_3	$(k+K_3)^2-V_3-V_7+V_{10}$	$(\frac{1}{2})^{\frac{1}{2}}(2V_2-V_4-V_5-V_7$ $-V_8+2V_{10})$	$V_3-V_4-V_9+V_{10}$	$(\frac{1}{2})^{\frac{1}{2}}(V_1-V_2+V_5-V_7-V_8$ $+V_{10}-V_{12}+V_{13})$
L'_3	$(k+K_3)^2-V_3+V_7-V_{10}$	$(\frac{1}{2})^{\frac{1}{2}}(2V_2+V_4-V_5+V_7$ $-V_8-2V_{10})$	$-V_3-V_4+V_9+V_{10}$	$(\frac{1}{2})^{\frac{1}{2}}(V_1-V_2+V_5-V_7+V_8$ $-V_{10}+V_{12}-V_{13})$
Λ_1	$(k+K_2)^2+2V_3$	$2V_1+V_4$	$2V_2+V_5$	$3^{\frac{1}{2}}V_3$
Λ_3	$(k+K_4)^2-V_3$	$-V_1+V_4$	$-V_4+V_7$	$(\frac{1}{2})^{\frac{1}{2}}(-V_1-V_4+2V_7)$

MATRIX ELEMENTS OF THE SECULAR EQUATION

Rep	$a_{37}=a_{73}$	$a_{38}=a_{83}$	$a_{39}=a_{93}$	$a_{3,10}=a_{10,3}$
Z_1	$2V_1$	$\sqrt{2}(V_2+V_3)$	$\sqrt{2}(V_4+V_7)$	V_6+V_8
Z_3	$V_2-V_3+V_8-V_9$	$\sqrt{2}(V_3-V_8)$	$V_2-V_3+V_8-V_9$	$\sqrt{2}(V_5-V_9)$
Z_4	$\sqrt{2}(V_4-V_7)$	$\sqrt{2}(V_1-V_{10})$	$V_2+V_3-V_8-V_9$	$\sqrt{2}(V_1-V_{10})$
W_1	$\sqrt{2/3}(V_1+V_2+2V_4+V_6+V_7+2V_8+V_9+V_{10}+V_{11}+V_{12})$			
W_2'	$\sqrt{2/3}(-V_1+V_2-2V_4+V_6-V_7+2V_8+V_9-V_{10}+V_{11}-V_{12})$			
W_3	$\sqrt{2/3}(V_2-V_6+2V_8-V_9-V_{11})$			
Q_1	$1/\sqrt{3}(V_1+V_3+2V_4+V_5+V_6)$	$1/\sqrt{3}(V_1+V_2+V_3+V_4+V_7+V_8)$	V_3+V_7	$\sqrt{2}(V_1+V_8)$
Q_2	$1/\sqrt{3}(-V_1+V_3-2V_4+V_5+V_6)$	$1/\sqrt{3}(-V_1+V_2+V_3-V_4-V_7+V_8)$	V_3-V_7	$\sqrt{2}(-V_1+V_8)$
L_1	$1/\sqrt{2}(V_1+2V_3+3V_4+3V_9+2V_{10}+V_{11})$			
L_2'	$1/\sqrt{2}(V_1+2V_3+V_4-V_9-2V_{10}-V_{11})$			
Λ_1	V_1+2V_4	V_1+2V_4	$\sqrt{2}(V_1+V_4+V_7)$	$2V_3+V_6$
Λ_3	V_5-V_8	$1/\sqrt{2}(2V_3-V_6-V_9)$	V_1-V_4	V_2-V_8
Σ_1	$\sqrt{2}V_2$	V_3+V_6	$\sqrt{2}(V_2+V_5)$	V_2+V_8
Σ_3	V_3-V_9	$\sqrt{2}(V_2-V_8)$	V_1-V_{10}	$\sqrt{2}(V_4-V_7)$
Σ_4	$\sqrt{2}(V_2-V_5)$	$\sqrt{2}(-V_4+V_{10})$		

MATRIX ELEMENTS OF THE SECULAR EQUATION

Rep	a_{33}	$a_{34}=a_{43}$	$a_{35}=a_{53}$	$a_{36}=a_{63}$
Σ_1	$(k+K_2)^2+V_3$	$\sqrt{2}(V_1+V_4)$	$2V_3$	$2V_4$
Σ_2	$(k+K_{10})^2-V_2-V_3+V_5$	$-V_7+2V_{10}-V_{12}$	$V_2-V_3-V_8+V_9$	
Σ_3	$(k+K_4)^2-V_6$	V_1-V_4	$\sqrt{2}(V_2-V_8)$	$\sqrt{2}(V_4-V_7)$
Σ_4	$(k+K_7)^2-V_3$	$\sqrt{2}(-V_5+V_8)$	V_2-V_8	$\sqrt{2}(-V_7+V_{10})$
X_3'	$(k+K_7)^2+V_2-V_3-V_6-3V_8$ $+V_9-V_{11}+3V_{13}+V_{14}+V_{17}-V_{19}-V_{20}$			

	$a_{3,11}=a_{11,3}$	$a_{3,12}=a_{12,3}$	$a_{3,13}=a_{13,3}$	$a_{3,14}=a_{14,3}$
Δ_1	$\sqrt{2}(V_3+V_5+V_8+V_9)$	$\sqrt{2}(V_2+V_3+V_6+V_8)$	$V_2+2V_3+V_5$	$V_4+2V_7+V_{10}$
Δ_5	$\sqrt{2}(V_4-V_7)$	$\sqrt{2}(V_3-V_9)$		
Z_1	$2V_4$	V_3+V_8	$\sqrt{2}(V_1+V_4)$	V_2+V_6
Z_3	V_4-V_{10}			
Z_4	$\sqrt{2}(V_4-V_7)$	V_4-V_{10}		
Q_1	$1/\sqrt{3}(V_1+2V_4+V_5+V_8+V_9)$			
Q_2	$1/\sqrt{3}(-V_1-2V_4+V_5+V_8+V_9)$			
Λ_1	$\sqrt{3}V_4$	$\sqrt{2}(V_2+V_5+V_8)$	$2V_4+V_7$	$2V_3+V_9$
Λ_3	$-V_4+V_{10}$	$-V_3+V_9$		
Σ_1	$\sqrt{2}(V_1+V_4)$	$2V_3$	$\sqrt{2}(V_5+V_8)$	$2V_4$

	$a_{3,15}=a_{15,3}$	$a_{3,16}=a_{16,3}$	$a_{3,17}=a_{17,3}$	
Δ_1	$V_1+2V_4+V_7$	$2V_{10}$		
Z_1	V_2+V_3	$2V_7$	$\sqrt{2}(V_8+V_9)$	
Λ_1	V_1+2V_7	V_2+2V_8		
Σ_1	$\sqrt{2}(V_1+V_7)$	$\sqrt{2}V_8$		

MATRIX ELEMENTS OF THE SECULAR EQUATION

Rep.	a_{44}	$a_{45}=a_{54}$	$a_{46}=a_{64}$	$a_{47}=a_{74}$
Z_1	$(k+K_3)^2+V_2$	$2^{\frac{1}{2}}(V_3+V_5)$	$2^{\frac{1}{2}}(V_1+V_4)$	V_6+V_8
Z_3	$(k+K_6)^2+V_2-V_6-V_8$	$2^{\frac{1}{2}}(V_4-V_7)$	$V_2+V_3-V_8-V_9$	V_1-V_7
Z_4	$(k+K_6)^2-V_2+V_6-V_8$	$V_2-V_3+V_8-V_9$	V_1-V_7	$2^{\frac{1}{2}}(V_3-V_5)$
W_1	$(k+K_4)^2+V_2+2V_4+2V_8$ $\frac{2}{3}(2V_1+V_6+2V_7+2V_9+2V_{10})$	$(\frac{1}{3})^{\frac{1}{2}}(V_3+2V_7+V_8+2V_1+2V_5+2V_9+2V_{10})$	$\frac{1}{3}(2V_1+2V_2+4V_3+8V_4+2V_6+2V_7+5V_8+2V_{10}+3V_{11}+4V_{12}+2V_{13})$	
W_2'	$(k+K_4)^2+V_2+\frac{2}{3}(2V_1+ +V_4+V_6-2V_7-V_8-2V_9-2V_{10})$	$(\frac{1}{3})^{\frac{1}{2}}(V_3-2V_7+V_8+2V_1-2V_5-2V_9+2V_{10})$	$\frac{1}{3}(2V_1+2V_2+4V_3+4V_4-2V_6+2V_7-V_8-2V_{10}-3V_{11}-4V_{12}-2V_{13})$	
W_3	$(k+K_4)^2+\frac{1}{3}(4V_1+V_2-4V_4-2V_6-2V_8)$	$(\frac{1}{3})^{\frac{1}{2}}(2V_1+V_3-V_8-2V_{10})$	$\frac{2}{3}(V_1+V_2-V_7-V_8)$	
Q_1	$(k+K_4)^2+V_1/2+3V_4/2+V_5$	$(\frac{1}{2})^{\frac{1}{2}}(V_2+V_3+2V_4)$	$\frac{1}{2}(2V_1+V_2+V_3+V_4+V_5+V_6+V_7)$	$(1/6)^{\frac{1}{2}}(2V_1+V_2+3V_3+2V_4+2V_7+2V_8)$
Q_2	$(k+K_4)^2-V_1/2-3V_4/2+V_5$	$(\frac{1}{2})^{\frac{1}{2}}(V_2+V_3-2V_4)$	$\frac{1}{2}(-2V_1+V_2+V_3-V_4+V_5+V_6-V_7)$	$(1/6)^{\frac{1}{2}}(-2V_1+V_2+3V_3-2V_4-2V_7+2V_8)$
L_1	$(k+K_3)^2+3/2(V_1+V_3+V_7+V_9)+V_{10}$	$(3/2)^{\frac{1}{2}}(V_2+2V_4+V_5+V_7+2V_8+V_{10})$	$(3/4)^{\frac{1}{2}}(V_3+2V_4+V_6+V_7+2V_9+V_{10})$	$(3/2)^{\frac{1}{2}}(V_1+V_2+V_5+V_7+V_8+V_{10}+V_{12}+V_{13})$
L_2'	$(k+K_3)^2+3/2(V_1+V_3-V_7-V_9)-V_{10}$	$(3/2)^{\frac{1}{2}}(V_2+V_5-V_7-V_{10})$	$(3/4)^{\frac{1}{2}}(-V_3+2V_4+V_6-V_7-2V_9+V_{10})$	$(3/2)^{\frac{1}{2}}(V_1+V_2+V_5+V_7-V_8-V_{10}-V_{12}-V_{13})$
L_3	$(k+K_4)^2+V_1-V_3-V_4-V_9-V_{10}+V_{11}+V_{12}$	$2^{\frac{1}{2}}(V_1+V_2-2V_7-2V_8+V_{12}+V_{13})$	$V_1+2V_3-2V_6-V_7-V_9-2V_{10}+2V_{12}+V_{14}$	
L_3'	$(k+K_4)^2-V_1-V_3+V_4-V_9+V_{10}+V_{11}-V_{12}$	$2^{\frac{1}{2}}(V_1-V_2-2V_7+2V_8+V_{12}-V_{13})$	$V_1-2V_6-3V_7+3V_9+2V_{10}-V_{14}$	
Λ_1	$(k+K_3)^2+2V_3$	V_1+2V_4	$3^{\frac{1}{2}}V_4$	$2V_3+V_6$
Λ_3	$(k+K_6)^2-V_3$	V_5-V_8	$(\frac{1}{2})^{\frac{1}{2}}(2V_2-V_5-V_8)$	$-V_7+V_{10}$

MATRIX ELEMENTS OF THE SECULAR EQUATION

Rep.	a_{44}	$a_{45}=a_{54}$	$a_{46}=a_{64}$	$a_{47}=a_{74}$
Σ_1	$(k+K_3)^2+V_2+V_3+V_5$	$\sqrt{2}(V_1+V_4)$	$\sqrt{2}(V_2+V_3)$	$2V_4$
Σ_2	$(k+K_{12})^2-V_3-V_6+V_9$	$-V_4+V_7+V_{10}-V_{12}$		
Σ_3	$(k+K_5)^2-V_2$	$\sqrt{2}(V_4-V_7)$	$\sqrt{2}(V_8-V_9)$	V_7-V_{10}
Σ_4	$(k+K_8)^2-V_3+V_6-V_9$	$\sqrt{2}(-V_3+V_9)$	V_1-V_7	$-V_3+V_6-V_9+V_{11}$
	$a_{48}=a_{84}$	$a_{49}=a_{94}$	$a_{4,10}=a_{10,4}$	$a_{4,11}=a_{11,4}$
Z_1	$\sqrt{2}(V_4+V_7)$	$\sqrt{2}(V_2+V_3)$	$2V_1$	V_3+V_8
Z_3	$\sqrt{2}(V_1-V_{10})$	V_4-V_{10}	$\sqrt{2}(V_1-V_{10})$	$V_2+V_3-V_8-V_9$
Z_4	$\sqrt{2}(V_3-V_8)$	V_4-V_{10}	$\sqrt{2}(V_5-V_9)$	$\sqrt{2}(V_8-V_9)$
Q_1	$1/\sqrt{6}(2V_1+2V_3+3V_4+V_5+V_6+V_7+2V_8)$	$1/\sqrt{2}(V_2+V_4+V_7+V_9)$	$V_2+2V_4+V_9$	$1/\sqrt{6}(V_1+V_2+2V_3+2V_4+2V_7+2V_8+V_9+V_{10})$
Q_2	$1/\sqrt{6}(-2V_1+2V_3-3V_4+V_5+V_6-V_7+2V_8)$	$1/\sqrt{2}(V_2-V_4-V_7+V_9)$	$V_2-2V_4+V_9$	$1/\sqrt{6}(-V_1+V_2+2V_3-2V_4-2V_7+2V_8+V_9-V_{10})$
Λ_1	$2V_2+V_5$	$\sqrt{2}(V_2+V_5+V_8)$	V_1+2V_4	$\sqrt{3}V_3$
Λ_3	$1/\sqrt{2}(-V_4-V_7+2V_{10})$	$-V_2+V_5$	$-V_4+V_{10}$	V_3-V_9
Σ_1	$\sqrt{2}(V_1+V_4)$	$V_1+2V_4+V_7$	$\sqrt{2}(V_1+V_7)$	$V_3+V_5+V_6+V_8$
Σ_3	$\sqrt{2}(V_1-V_4)$	V_5-V_9	$\sqrt{2}(V_6-V_8)$	
Σ_4	$V_1+V_4-V_7-V_{10}$			
	$a_{4,16}=a_{16,14}$	$a_{4,17}=a_{17,4}$		
Δ_1	V_2			
Z_1	V_2+V_6	$\sqrt{2}(V_1+V_4)$		
Λ_1	$2V_4+V_{10}$			
Σ_1	$2V_4$			

MATRIX ELEMENTS OF THE SECULAR EQUATION

Rep.	$a_{4,12}=a_{12,4}$	$a_{4,13}=a_{13,4}$	$a_{4,14}=a_{14,4}$	$a_{4,15}=a_{15,4}$
Δ_1	$\sqrt{8}V_7$	$2V_{10}$	$2V_3$	$2V_9$
Δ_5	$\sqrt{2}(V_8-V_{13})$			
Z_1	$2V_4$	$\sqrt{2}(V_8+V_9)$	$2V_7$	$2V_{10}$
Z_4	$V_2-V_3+V_8-V_9$			
Λ_1	$\sqrt{2}(V_1+V_4+V_7)$	V_5+2V_8	V_1+2V_7	$2V_3+V_9$
Λ_3	V_1-V_7			
Σ_1	$\sqrt{2}(V_4+V_7)$	$V_1+2V_4+V_7$	$\sqrt{2}(V_3+V_8)$	$V_2+V_3+V_8+V_9$

	a_{55}	$a_{56}=a_{65}$	$a_{57}=a_{75}$	$a_{58}=a_{85}$
Z_1	$(k+K_4)^2+V_2+V_6+V_8$	$V_1+2V_4+V_7$	$\sqrt{2}(V_3+V_5)$	$V_1+2V_4+V_7$
Z_3	$(k+K_6)^2-V_2$	$\sqrt{2}(V_1-V_4)$	$\sqrt{2}(V_8-V_9)$	V_3-V_8
Z_4	$(k+K_7)^2-V_2+V_6-V_8$	V_4-V_{10}	$\sqrt{2}(V_8-V_9)$	$\sqrt{2}(V_5-V_9)$
W_1	$(k+K_4)^2+2V_7+V_{13}$	$1/\sqrt{3}(V_2+2V_4+2V_5$ $+2V_7+2V_9+2V_{12}+V_{14})$	$1/\sqrt{3}(2V_2+2V_4+2V_7$ $+V_8+V_{11}+2V_{12}+2V_{14})$	
W_2'	$(k+K_4)^2-2V_7+V_{13}$	$1/\sqrt{3}(-V_2-2V_4+2V_5$ $-V_{14}+2V_7+2V_9-2V_{12})$	$1/\sqrt{3}(2V_2-2V_4-2V_7$ $+V_8+V_{11}-2V_{12}+2V_{14})$	
W_3	$(k+K_4)^2-V_{13}$	$2/\sqrt{3}(V_5-V_9)$	$1/\sqrt{3}(2V_2+V_8-V_{11}-2V_{14})$	
L_1	$(k+K_4)^2+2V_3+2V_4+2V_9$ $+V_1+2V_{10}+V_{11}+V_{12}$	$\sqrt{2}(V_1+V_2+V_7+V_8+V_{12}+V_{13})$	$V_1+2V_3+2V_7+V_6+2V_9$ $+V_{10}+2V_{12}+V_{14}$	
L_2'	$(k+K_4)^2-V_1+2V_3-2V_4$ $+2V_9-2V_{10}+V_{11}-V_{12}$	$\sqrt{2}(V_1-V_2+V_7-V_8$ $+V_{12}-V_{13})$	$V_1+V_6-V_{10}-V_{14}$	
L_3	$(k+K_5)^2-V_4-V_{11}+V_{15}$	$1/\sqrt{2}(+V_1+V_4-V_5-V_8$ $-V_{10}-V_{12}+V_{13}+V_{16})$		
L_3'	$(k+K_5)^2+V_4-V_{11}-V_{15}$	$1/\sqrt{2}(-V_1+V_4-V_5+V_8$ $-V_{10}+V_{12}-V_{13}+V_{16})$		

MATRIX ELEMENTS OF THE SECULAR EQUATION

Rep.	a_{55}	$a_{56}=a_{65}$	$a_{57}=a_{75}$	$a_{58}=a_{85}$
Q_1	$(k+K_4)^2+V_7$	$1/\sqrt{2}(V_1+V_3+V_4+V_8)$	$1/\sqrt{3}(V_2+2V_4+V_5$ $+V_6+V_7)$	$1/\sqrt{3}(2V_1+V_3+V_7$ $+V_8+V_9)$
Q_2	$(k+K_4)^2-V_7$	$1/\sqrt{2}(-V_1+V_3-V_4+V_8)$	$1/\sqrt{3}(V_2-2V_4+V_5$ $+V_6-V_7)$	$1/\sqrt{3}(-2V_1+V_3-V_7)$ $+V_8+V_9)$
Λ_1	$(k+K_4)^2+2V_3$	$\sqrt{3}V_2$	$2V_1+V_4$	$2V_4+V_7$
Λ_3	$(k+K_7)^2-V_3$	$1/\sqrt{2}(2V_3-V_6-V_9)$	$-V_1+V_4$	$1/\sqrt{2}(-V_1-V_4+2V_7)$
Σ_1	$(k+K_4)^2+V_6$	V_1+V_4	$\sqrt{2}V_5$	$2V_3$
Σ_2	$(k+K_{14})^2-V_2-V_{11}+V_{13}$			
Σ_3	$(k+K_8)^2+V_3-V_6-V_9$	V_1-V_7	$\sqrt{2}(V_2-V_8)$	$V_3+V_6-V_9-V_{11}$
Σ_4	$(k+K_9)^2-V_{11}$	$\sqrt{2}(-V_4+V_{10})$	$\sqrt{2}(V_3-V_9)$	$\sqrt{2}(-V_1+V_{12})$

	$a_{59}=a_{95}$	$a_{5,10}=a_{10,5}$	$a_{5,11}=a_{11,5}$	$a_{5,12}=a_{12,5}$
Z_1	$V_2+V_3+V_8+V_9$	$\sqrt{2}(V_4+V_7)$	$\sqrt{2}(V_3+V_8)$	$\sqrt{2}(V_1+V_{10})$
Z_3	$\sqrt{2}(V_2-V_3)$	V_8-V_{11}	$\sqrt{2}(V_{10}-V_{12})$	
Z_4	V_1-V_7	$\sqrt{2}(V_3-V_8)$	$\sqrt{2}(V_3-V_5)$	$V_6-V_8+V_{11}-V_{13}$
Q_1	V_4+V_8	$\sqrt{2}(V_3+V_7)$	$1/\sqrt{3}(V_2+V_3+V_4$ $+V_6+2V_{10})$	
Q_2	$-V_4+V_8$	$\sqrt{2}(V_3-V_7)$	$1/\sqrt{3}(V_2+V_3-V_4$ $+V_6-2V_{10})$	
Λ_1	$\sqrt{2}(V_1+V_4+V_7)$	V_5+2V_8	$\sqrt{3}V_7$	$\sqrt{2}(V_3+V_6+V_9)$
Λ_3	V_9-V_{11}	$-V_4+V_{10}$	V_2-V_8	V_4-V_{10}
Σ_1	$\sqrt{2}(V_2+V_8)$	$2V_5$	$\sqrt{2}(V_4+V_7)$	V_3+V_9
Σ_3	$\sqrt{2}(V_1-V_{10})$	$V_1-V_4-V_7+V_{10}$		

MATRIX ELEMENTS OF THE SECULAR EQUATION

Rep.	$a_{5,13}=a_{13,5}$	$a_{5,14}=a_{14,5}$	$a_{5,15}=a_{15,5}$	$a_{5,16}=a_{16,5}$
Δ_1	$2(V_4+V_7)$	$2(V_3+V_9)$	$2(V_3+V_9)$	$2V_8$
Z_1	$V_2+V_3+V_8+V_9$	$\sqrt{2}(V_1+V_{10})$	$\sqrt{2}(V_4+V_7)$	$\sqrt{2}(V_5+V_9)$
Λ_1	V_1+2V_4	V_2+2V_8	$2V_4+V_{10}$	$2V_3+V_9$
Σ_1	$\sqrt{2}(V_2+V_8)$	V_1+V_{10}	$\sqrt{2}(V_4+V_7)$	$\sqrt{2}V_5$
	$a_{610}=a_{10,6}$	$a_{6,11}=a_{11,6}$	$a_{6,12}=a_{12,6}$	$a_{6,13}=a_{13,6}$
Δ_1	$2V_{10}$	$\sqrt{8}V_7$	$\sqrt{8}V_4$	$2V_1$
Δ_5	$V_8+V_9-V_{11}-V_{13}$	$V_{13}-V_{16}$	$V_{10}-V_{15}$	
Z_1	$\sqrt{2}(V_3+V_5)$	$\sqrt{2}(V_1+V_{10})$	$\sqrt{2}(V_3+V_8)$	$V_4+2V_7+V_{10}$
Z_3	$\sqrt{2}(V_4-V_{12})$	$V_6+V_8-V_{11}-V_{13}$		
Z_4	$\sqrt{2}(V_4-V_{12})$	$\sqrt{2}(V_{10}-V_{12})$	V_1-V_7	
Q_1	$V_1+V_6+V_7+V_8$	$1/\sqrt{6}(2V_1+V_3+2V_4+3V_8+2V_9+2V_{10})$		
Q_2	$-V_1+V_6-V_7+V_8$	$1/\sqrt{6}(-2V_1+V_3-2V_4+3V_8+2V_9-2V_{10})$		
Λ_1	$\sqrt{3}V_9$	V_{10}	$\sqrt{6}V_8$	$\sqrt{3}V_1$
Λ_3	$\sqrt{2}(-V_1+2V_{12}-V_7)$	$\sqrt{2}(2V_2-V_8-V_{13})$	$\sqrt{2}(2V_1-V_7-V_{12})$	
Σ_1	$2V_4$	$\sqrt{2}(V_8+V_9)$	V_7+V_{10}	$\sqrt{2}(V_1+V_4)$
Σ_3	$V_2-V_3+V_8-V_9$			
	$a_{6,14}=a_{14,6}$	$a_{6,15}=a_{15,6}$	$a_{6,16}=a_{16,6}$	$a_{6,17}=a_{17,6}$
Δ_1	$2V_9$	$2V_3$	V_{13}	
Z_1	$\sqrt{2}(V_5+V_9)$	$\sqrt{2}(V_8+V_9)$	$\sqrt{2}(V_1+V_{10})$	$V_2+V_3+V_8+V_9$
Λ_1	$\sqrt{3}V_6$	$\sqrt{3}V_7$	$\sqrt{3}V_5$	
Σ_1	V_5+V_9	$\sqrt{2}(V_6+V_8)$	$\sqrt{2}V_1$	

MATRIX ELEMENTS OF THE SECULAR EQUATION

Rep.	a_{66}	$a_{67}=a_{76}$	$a_{68}=a_{86}$	$a_{69}=a_{96}$
Z_1	$(k+K_5)^2+V_2+V_6+V_8$	$\sqrt{2}(V_4+V_7)$	$V_2+V_3+V_8+V_9$	$V_1+2V_4+V_7$
Z_3	$(k+K_7)^2+V_2-V_6-V_8$	V_4-V_{10}	$\sqrt{2}(V_1-V_{10})$	V_1-V_7
Z_4	$(k+K_8)^2+V_2-V_6-V_8$	$\sqrt{2}(V_1-V_4)$	$\sqrt{2}(V_1-V_{10})$	$V_6+V_8-V_{11}-V_{13}$
W_1	$(k+K_5)^2+1/3(4V_1$ $+2V_2+2V_6+2V_8+4V_9$ $+8V_{10}+4V_{12}+5V_{13}+2V_{15})$	$1/3(2V_1+5V_3+6V_4$ $+2V_7+3V_8+2V_9+6V_{12}$ $+2V_{13}+2V_{14}+2V_{15}+4V_{16})$		
W_2'	$(k+K_5)^2+1/3(4V_1$ $+2V_2+2V_6+2V_8-4V_9$ $-4V_{12}-3V_{13}-2V_{15})$	$1/3(-2V_1+5V_3-6V_4$ $-2V_7+3V_8+2V_9-6V_{12}$ $+2V_{13}+2V_{14}-2V_{15}+4V_{16})$		
W_3	$(k+K_5)^2+1/3(2V_1-2V_{10}$ $-2V_2+2V_6-2V_8-V_{13})$	$2/3(5V_3-3V_8+2V_9$ $-2V_{13}+2V_{14}-4V_{16})$		
Q_1	$(k+K_5)^2+1/2(3V_4$ $+V_7+2V_8)$	$1/\sqrt{6}(2V_1+2V_2+V_3$ $+V_4+3V_7+V_8+2V_9)$	$1/\sqrt{6}(V_1+V_2+V_3+2V_4$ $+2V_5+V_6+2V_7+V_9-V_{10})$	$1/\sqrt{2}(V_3+V_4+V_8+V_{10})$
Q_2	$(k+K_5)^2-1/2(3V_4$ $+V_7-2V_8)$	$1/\sqrt{6}(-2V_1+2V_2+V_3$ $-V_4-3V_7+V_8+2V_9)$	$1/\sqrt{6}(-V_1+V_2+V_3-2V_4$ $+2V_5+V_6-2V_7+V_9-V_{10})$	$1/\sqrt{2}(V_3-V_4+V_8-V_{10})$
L_1	$(k+K_5)^2+2V_4+2V_{11}+V_{15}$	$1/\sqrt{2}(V_1+V_4+2V_5+2V_8$ $+2V_{10}+2V_{12}+V_{13}+V_{16})$		
L_2'	$(k+K_5)^2-2V_4+2V_{11}-V_{15}$	$1/\sqrt{2}(-V_1+V_4+2V_5-2V_8$ $+2V_{10}-2V_{12}-V_{13}+V_{16})$		
L_3	$(k+K_6)^2-V_4+V_9+V_{10}$ $-V_{14}+V_{18}-1/2(V_3+V_7$ $+V_{11}+V_{15})$			
L_3'	$(k+K_6)^2-V_4-V_9+V_{10}$ $+V_{14}-V_{18}-1/2(V_3-V_7$ $+V_{11}-V_{15})$			

MATRIX ELEMENTS OF THE SECULAR EQUATION

Rep	a_{66}	$a_{67}=a_{76}$	$a_{68}=a_{86}$	$a_{69}=a_{96}$
Λ_1	$(k+K_5)^2$	$\sqrt{3}V_1$	$\sqrt{3}V_7$	$\sqrt{6}V_4$
Λ_3	$(k+K_8)^2-V_3-V_9+V_{11}$	$\sqrt{2}(V_4-2V_7+V_{10})$	$V_1-V_4-V_{10}+V_{12}$	$\sqrt{2}(-V_3+2V_9-V_6)$
Σ_1	$(k+K_5)^2+V_2$	$\sqrt{2}V_7$	$2V_1$	$\sqrt{2}(V_4+V_7)$
Σ_3	$(k+K_{10})^2-V_2+V_3-V_5$	$\sqrt{2}(V_1-V_4)$	V_7-V_{12}	$\sqrt{2}(V_3-V_8)$
Σ_4	$(k+K_{10})^2+V_2-V_3-V_5$	$-V_7+V_{12}$	$V_2+V_3-V_8-V_9$	
	$a_{7,11}=a_{11,7}$	$a_{7,12}=a_{12,7}$	$a_{7,13}=a_{13,7}$	$a_{7,14}=a_{14,7}$
Δ_1	$\sqrt{2}(V_1+V_4+V_7+V_{10})$	$\sqrt{2}(V_4+V_7+V_{10}+V_{12})$	$2(V_{10}+V_{12})$	$2(V_2+V_8)$
Δ_5	$\sqrt{2}(V_1-V_4)$	$\sqrt{2}(V_2-V_8)$		
Z_1	V_3+V_8	$2V_7$	$\sqrt{2}(V_2+V_3)$	$2V_4$
Z_3	V_1-V_7			
Z_4	$V_{13}-V_{14}$	$\sqrt{2}(V_2-V_3)$		
Q_1	$1/3(V_1+2V_3+V_4+2V_5$ $+V_6+4V_7+3V_8+2V_{10}$ $+V_{11}+V_{12})$			
Q_2	$1/3(-V_1+2V_3-V_4+2V_5$ $+V_6-4V_7+3V_8-2V_{10}$ $+V_{11}-V_{12})$			
Λ_1	$\sqrt{3}V_9$	$\sqrt{2}(V_4+V_7+V_{10})$	$2V_2+V_5$	$2V_4+V_{10}$
Λ_3	$-V_4+V_{10}$	$-V_8+V_{13}$		
Σ_1	$2V_1$	$\sqrt{2}V_2$	$2V_9$	$\sqrt{2}V_4$
	$a_{7,15}=a_{15,7}$	$a_{7,16}=a_{16,7}$	$a_{7,17}=a_{17,7}$	$a_{5,17}=a_{17,5}$
Δ_1	$2(V_8+V_{13})$	$2V_3$		
Z_1	$2V_1$	V_8+V_{11}	$\sqrt{2}(V_{10}+V_{12})$	$V_4+2V_7+V_{10}$
Λ_1	$2V_9+V_3$	$2V_7+V_1$		
Σ_1	$2V_4$	V_{11}		

MATRIX ELEMENTS OF THE SECULAR EQUATION

Rep.	a_{77}	$a_{78}=a_{87}$	$a_{79}=a_{97}$	$a_{7,10}=a_{10,7}$
Z_1	$(k+K_6)^2 +V_2$	$\sqrt{2}(V_1 +V_4)$	$\sqrt{2}(V_8 +V_9)$	$2V_{10}$
Z_3	$(k+K_8)^2 -V_2 +V_6 -V_8$	$\sqrt{2}(V_5 -V_9)$	$V_6 -V_8 +V_{11} -V_{13}$	$\sqrt{2}(V_3 -V_8)$
Z_4	$(k+K_9)^2 -V_2$	$V_3 -V_8$	$\sqrt{2}(V_{10} -V_{12})$	$V_8 -V_{11}$
W_1	$(k+K_6)^2 +1/3(2V_1 +V_2$ $+2V_6 +4V_7 +4V_9 +8V_{10}$ $+6V_{13} +4V_{18} +2V_{19})$			
W_2'	$(k+K_6)^2 +1/3(-2V_1 +V_2$ $+2V_6 -4V_7 +4V_9 -8V_{10}$ $+6V_{13} -4V_{18} +2V_{19})$			
W_3	$(k+K_6)^2 +1/3(-V_2 +2V_6$ $+4V_9 -6V_{13} -2V_{19})$			
Q_1	$(k+K_6)^2 +V_1 +2/3(V_4$ $+V_5 +V_7 +V_8 +V_9 +V_{10})$	$1/3(V_1 +V_2 +3V_3$ $+5V_4 +V_7 +4V_8 +V_9$ $+2V_{10})$	$1/\sqrt{3}(V_1 +V_2 +V_4$ $+V_6 +V_7 +V_9)$	$\sqrt{2/3}(V_2 +V_4 +V_8$ $+V_9 +2V_{10})$
Q_2	$(k+K_6)^2 -V_1 +2/3(-V_4$ $+V_5 -V_7 +V_8 +V_9 -V_{10})$	$1/3(-V_1 +V_2 +3V_3$ $-5V_4 -V_7 +4V_8 +V_9 -2V_{10})$	$1/\sqrt{3}(-V_1 +V_2 -V_4$ $+V_6 -V_7 +V_9)$	$\sqrt{2/3}(V_2 -V_4 +V_8$ $+V_9 -2V_{10})$
L_1	$(k+K_6)^2 +V_3 +2V_4 +V_7$ $+V_9 +V_{10} +V_{11} +2V_{14}$ $+V_{15} +V_{18}$			
L_2'	$(k+K_6)^2 +V_3 +2V_4 -V_7$ $-V_9 +V_{10} +V_{11} -2V_{14} -V_{15} -V_{18}$			
Λ_1	$(k+K_6)^2 +2V_3$	$V_5 +2V_8$	$\sqrt{2}(V_2 +V_5 +V_8)$	$2V_7 +V_{10}$
Λ_3	$(k+K_9)^2 -V_3$	$1/\sqrt{2}(2V_2 -V_5 -V_8)$	$V_{10} -V_{12}$	$V_3 -V_9$
Σ_1	$(k+K_6)^2$	$\sqrt{2}V_8$	$2V_3$	$\sqrt{2}V_6$
Σ_3	$(k+K_{11})^2 -V_6$	$\sqrt{2}(V_8 -V_{13})$	$V_1 -V_{10}$	$\sqrt{2}(V_4 -V_7)$
Σ_4	$(k+K_{12})^2 -V_3 +V_6 -V_9$	$-V_4 -V_7 +V_{10} +V_{12}$		

MATRIX ELEMENTS OF THE SECULAR EQUATION

Rep.	a_{88}	$a_{89}=a_{98}$	$a_{8,10}=a_{10,8}$	$a_{8,11}=a_{11,8}$
X_1	$(k+K_7)^2+V_2+V_3+V_6+3V_8+V_9+V_{11}+3V_{13}+V_{14}+V_{17}+V_{19}+V_{20}$			
Δ_1	$(k+K_7)^2+2V_6+V_{11}$	$2(V_3+V_9)$	$V_4+2V_7+V_{10}$	$\sqrt{2}(V_1+V_4+V_{10}+V_{12})$
Δ_2'	$(k+K_{12})^2-2V_2+V_3$	$V_1-2V_4+V_7$		
Δ_5	$(k+K_{10})^2+V_2-V_{13}-V_{14}$	$V_1+V_4-V_{10}-V_{12}$	$V_2+V_3-V_{14}-V_{16}$	$V_8+V_9-V_{11}-V_{13}$
Z_1	$(k+K_7)^2+V_2+V_6+V_8$	$V_4+2V_7+V_{10}$	$\sqrt{2}(V_8+V_9)$	$\sqrt{2}(V_1+V_{10})$
Z_3	$(k+K_{10})^2-V_{13}$	$\sqrt{2}(V_5-V_9)$	V_2-V_{14}	$\sqrt{2}(V_4-V_{12})$
Z_4	$(k+K_{11})^2-V_{13}$	$\sqrt{2}(V_4-V_{12})$	V_2-V_{14}	V_8-V_{11}
Q_1	$(k+K_7)^2+V_7+2/3(V_1+V_5+V_8+V_9+2V_{10})$	$1/\sqrt{3}(V_1+V_2+V_7+V_8+V_9+V_{10})$	$\sqrt{2/3}(V_3+2V_4+V_5+V_{11}+V_{12})$	$1/3(2V_1+2V_2+V_3+2V_4+2V_7+4V_9+2V_{10}+V_{12}+2V_{13})$
Q_2	$(k+K_7)^2-V_7+2/3(-V_1+V_5+V_8+V_9-2V_{10})$	$1/\sqrt{3}(-V_1+V_2-V_7+V_8+V_9-V_{10})$	$\sqrt{2/3}(V_3-2V_4+V_5+V_{11}-V_{12})$	$1/3(2V_2-2V_1+V_3-2V_4-2V_7+4V_9-2V_{10}-V_{12}+2V_{13})$
Λ_1	$(k+K_7)^2+2V_3$	$\sqrt{2}(V_3+V_6+V_9)$	$2V_1+V_4$	$\sqrt{3}V_2$
Λ_3	$(k+K_{11})^2-V_3-V_9+V_{11}$	$\sqrt{2}(2V_7-V_{10}-V_{12})$	$2(-V_8+2V_2-V_{13})$	$\sqrt{2}(-V_1-V_7+2V_{12})$
Σ_1	$(k+K_7)^2+V_3$	$\sqrt{2}(V_5+V_8)$	V_2+V_8	$\sqrt{2}(V_7+V_{10})$
Σ_3	$(k+K_{12})^2+V_3-V_6-V_9$	$\sqrt{2}(V_4-V_{12})$	$V_4-V_7+V_{10}-V_{12}$	
Σ_4	$(k+K_{14})^2+V_2-V_{11}-V_{13}$			

	$a_{8,16}=a_{16,8}$	$a_{8,17}=a_{17,8}$	$a_{9,17}=a_{17,9}$	$a_{13,17}=a_{17,13}$
Δ_1	$2V$			
Z_1	$\sqrt{2}(V_4+V_{12})$	$V_6+V_8+V_{11}+V_{13}$	$V_1+2V_4+V_7$	$V_{10}+2V_{12}+V_{15}$
Λ_1	V_4+2V_{10}			
Σ_1	$\sqrt{2}V_2$			

MATRIX ELEMENTS OF THE SECULAR EQUATION

Rep	$a_{8,12}=a_{12,8}$	$a_{8,13}=a_{13,8}$	$a_{8,14}=a_{14,8}$	$a_{8,15}=a_{15,8}$
Δ_1	$\sqrt{2}(V_1+V_4+V_{10}+V_{12})$	$V_4+2V_7+V_{10}$	$V_2+2V_8+V_{13}$	$V_2+2V_8+V_{13}$
Δ_5	$V_4+V_7-V_{12}-V_{15}$			
Z_1	$\sqrt{2}(V_5+V_9)$	$V_1+2V_4+V_7$	$\sqrt{2}(V_3+V_8)$	$\sqrt{2}(V_3+V_5)$
Z_4	$\sqrt{2}(V_5-V_9)$			
Λ_1	$\sqrt{2}(V_1+V_4+V_7)$	$2V_9+V_{11}$	$2V_4+V_{10}$	V_2+2V_8
Λ_3	$\sqrt{2}(-V_3-V_9+2V_{14})$			
Σ_1	$2V_9$	$\sqrt{2}(V_2+V_5)$	$2V_7$	$\sqrt{2}(V_4+V_{10})$

	a_{99}	$a_{9,10}=a_{10,9}$	$a_{9,11}=a_{11,9}$	$a_{9,12}=a_{12,9}$
Δ_1	$(k+K_8)^2+2V_3+V_6$	$2(V_{10}+V_{12})$	$\sqrt{2}(V_4+V_7+V_{10}+V_{12})$	$\sqrt{2}(V_1+V_4+V_7+V_{10})$
Δ_2'	$(k+K_{14})^2-2V_6+V_{11}$			
Δ_5	$(k+K_{13})^2-V_{11}$	$V_4+V_7-V_{12}-V_{15}$	$V_{10}-V_{15}$	V_6-V_{17}
Z_1	$(k+K_8)^2+V_2+V_6+V_8$	$\sqrt{2}(V_1+V_4)$	$\sqrt{2}(V_5+V_9)$	$\sqrt{2}(V_1+V_{10})$
Z_3	$(k+K_{12})^2-V_2+V_6-V_8$	$\sqrt{2}(V_9-V_{13})$	$V_{10}-V_{15}$	
Z_4	$(k+K_{12})^2+V_2-V_6-V_8$	$\sqrt{2}(V_1-V_{10})$	$\sqrt{2}(V_1-V_4)$	$V_{10}-V_{15}$
Q_1	$(k+K_8)^2+V_4$	$\sqrt{2}(V_7+V_{13})$	$1/\sqrt{3}(V_1+V_4+V_5+V_{11}+V_{12}+V_{13})$	
Q_2	$(k+K_8)^2-V_4$	$\sqrt{2}(-V_7+V_{13})$	$1/\sqrt{3}(V_5-V_1-V_4+V_{11}-V_{12}+V_{13})$	
Λ_1	$(k+K_8)^2+2V_3+2V_9+V_{11}$	$\sqrt{2}(V_4+V_7+V_{10})$	$\sqrt{6}V_8$	$V_1+2V_4+2V_{10}+V_{12}$
Λ_3	$(k+K_{12})^2-V_3$	V_4-V_{10}	$-V_8+V_{13}$	$-V_4+V_{10}$
Σ_1	$(k+K_8)^2+V_3+V_6+V_9$	$\sqrt{2}(V_3+V_9)$	$V_1+2V_4+V_7$	$\sqrt{2}(V_2+V_8)$
Σ_3	$(k+K_{13})^2-V_{13}$	$\sqrt{2}(V_5-V_9)$		

MATRIX ELEMENTS OF THE SECULAR EQUATION

Rep.	$a_{9,13}=a_{13,9}$	$a_{9,14}=a_{14,9}$	$a_{9,15}=a_{15,9}$	$a_{9.16}=a_{16,9}$
Δ_1	$2(V_1+V_4)$	$2(V_8+V_{13})$	$2(V_2+V_8)$	$2V_{14}$
Z_1	$V_6+V_8+V_{11}+V_{13}$	$\sqrt{2}(V_4+V_{12})$	$\sqrt{2}(V_{10}+V_{12})$	$\sqrt{2}(V_3+V_8)$
Λ_1	$\sqrt{2}(V_3+V_6+V_9)$	$\sqrt{2}(V_1+V_7+V_{12})$	$\sqrt{2}(V_2+V_8+V_{13})$	$\sqrt{2}(V_1+V_7+V_{12})$
Σ_1	$V_3+V_6+V_9+V_{11}$	$\sqrt{2}(V_1+V_{10})$	$V_1+V_4+V_7+V_{10}$	V_9
	$a_{10,10}$	$a_{10,11}=a_{11,10}$	$a_{10,12}=a_{12,10}$	$a_{10,13}=a_{13,10}$
Δ_1	$(k+K_9)^2+2V_2+V_3$	$\sqrt{2}(V_3+V_5+V_8+V_9)$	$\sqrt{2}(V_8+V_9+V_{11}+V_{13})$	$V_{13}+2V_{14}+V_{16}$
Δ_5	$(k+K_{11})^2+V_2-V_{13}-V_{14}$	$V_3+V_5-V_8-V_9$	$V_1+V_4-V_{10}-V_{12}$	
Z_1	$(k+K_9)^2+V_2$	$2V_7$	V_3+V_8	$\sqrt{2}(V_{10}+V_{12})$
Z_3	$(k+K_{15})^2-V_{13}$	$\sqrt{2}(V_1-V_{10})$		
Z_4	$(k+K_{13})^2-V_{13}$	V_3-V_8	$\sqrt{2}(V_9-V_{13})$	
Q_1	$(k+K_9)^2+V_1+V_9+V_{10}$	$1/\sqrt{6}(V_1+V_2+2V_3+2V_4$ $+V_7+V_9+2V_{12}+V_{13}+V_{14})$		
Q_2	$(k+K_9)^2-V_1+V_9-V_{10}$	$1/\sqrt{6}(-V_1+V_2+2V_3-2V_4$ $-V_7+V_9-2V_{12}+V_{13}+V_{14})$		
Λ_1	$(k+K_9)^2+2V_3$	$\sqrt{3}V_1$	$\sqrt{2}(V_2+V_5+V_8)$	$V_{10}+2V_{12}$
Λ_3	$(k+K_{13})^2-V_{11}$	$-V_4+V_{15}$	$-V_5+V_{16}$	
Σ_1	$(k+K_9)^2+V_{11}$	$\sqrt{2}(V_4+V_{10})$	$2V_8$	$\sqrt{2}(V_3+V_9)$
Σ_3	$(k+K_{14})^2-V_2+V_{11}-V_{13}$			
	$a_{10,14}=a_{14,10}$	$a_{10,15}=a_{15,10}$	$a_{10,16}=a_{16,10}$	$a_{10,17}=a_{17,10}$
Δ_1	$V_1+2V_4+V_7$	$V_{10}+2V_{12}+V_{15}$	$2V_1$	
Z_1	V_8+V_{11}	$V_{13}+V_{14}$	$2V_4$	$\sqrt{2}(V_2+V_3)$
Λ_1	V_3+2V_9	$2V_4+V_{10}$	$2V_8+V_{13}$	
Σ	$2V_7$	$\sqrt{2}(V_1+V_{12})$	$\sqrt{2}V_6$	

MATRIX ELEMENTS OF THE SECULAR EQUATION

Rep.	$a_{11,11}$	$a_{11,12}=a_{12,11}$	$a_{11,13}=a_{13,11}$	$a_{11,14}=a_{14,11}$
Δ_1	$(k+K_{10})^2+V_2+V_3+2V_8+V_{11}+V_{13}+V_{14}$	$V_2+V_3+V_5+2V_9+V_{13}+V_{14}+V_{16}$	$\sqrt{2}(V_8+V_9+V_{11}+V_{13})$	$\sqrt{2}(V_1+V_4+V_{10}+V_{12})$
Δ_5	$(k+K_{12})^2-V_3$	V_1-V_7		
Z_1	$(k+K_{10})^2+V_{13}$	$2V_7$	$\sqrt{2}(V_5+V_9)$	$2V_7$
Z_3	$(k+K_{16})^2+V_2-V_6-V_8$			
Z_4	$(k+K_{14})^2-V_2$	$\sqrt{2}(V_{14}-V_{16})$		
Q_1	$(k+K_{10})^2+1/3(V_1+2V_5+2V_8+3V_7+4V_{12}+2V_{14}+V_{15})$			
Q_2	$(k+K_{10})^2+1/3(-V_1+2V_5-3V_7+2V_8-4V_{12}+2V_{14}-V_{15})$			
Λ_1	$(k+K_{10})^2$	$\sqrt{6}V_4$	$\sqrt{3}V_{13}$	$\sqrt{3}V_7$
Λ_3	$(k+K_{14})^2-V_{11}$	V_1-V_{12}		
Σ_1	$(k+K_{10})^2+V_2+V_3+V_5$	$\sqrt{2}(V_1+V_4)$	$V_7+2V_{10}+V_{12}$	$\sqrt{2}(V_3+V_8)$

	$a_{11,15}=a_{15,11}$	$a_{11,16}=a_{16,11}$	$a_{11,17}=a_{17,11}$
Δ_1	$\sqrt{2}(V_4+V_7+V_{12}+V_{15})$	$\sqrt{8}V_7$	
Z_1	$2V_7$	V_2+V_{14}	$\sqrt{2}(V_4+V_{12})$
Λ_1	$\sqrt{3}V_6$	$\sqrt{3}V_{10}$	
Σ_1	$V_2+V_3+V_8+V_9$	$2V_{12}$	

	$a_{12,16}=a_{16,12}$	$a_{12,17}=a_{17,12}$	$a_{16,16}$	$a_{16,17}=a_{17,16}$
Δ_1	$\sqrt{8}V_{12}$		$(k+K_{15})^2$	
Z_1	$2V_7$	$\sqrt{2}(V_5+V_9)$	$(k+K_{15})^2+V_{13}$	$\sqrt{2}(V_1+V_{10})$
Λ_1	$\sqrt{2}(V_3+V_9+V_{14})$		$(k+K_{15})^2+2V_{11}$	
Σ_1	$\sqrt{2}V_{13}$		$(k+K_{15})^2$	

MATRIX ELEMENTS OF THE SECULAR EQUATION

Re	$a_{12,12}$	$a_{12,13}=a_{13,12}$	$a_{12,14}=a_{14,12}$	$a_{12,15}=a_{15,12}$
Δ_1	$(k+K_{11})^2+V_2+V_3$ $+2V_8+V_{11}+V_{13}+V_{14}$	$\sqrt{2}(V_3+V_5+V_8+V_9)$	$\sqrt{2}(V_4+V_7+V_{12}+V_{15})$	$\sqrt{2}(V_1+V_4+V_{10}+V_{12})$
Δ_5	$(k+K_{14})^2-V_{11}$			
Z_1	$(k+K_{11})^2+V_{13}$	$\sqrt{2}(V_4+V_{12})$	V_2+V_{14}	V_8+V_{11}
Z_4	$(k+K_{16})^2-V_2+V_6-V_8$			
Λ_1	$(k+K_{11})^2+2V_3+2V_9+V_{11}$	$\sqrt{2}(V_7+V_{10}+V_{12})$	$\sqrt{2}(V_2+V_8+V_{13})$	$\sqrt{2}(V_1+V_7+V_{12})$
Λ_3	$(k+K_{15})^2-V_{11}$			
Σ_1	$(k+K_{11})^2+V_6$			
	$a_{13,13}$	$a_{13,14}-a_{14,13}$	$a_{13,15}-a_{15,13}$	$a_{13,16}-a_{16,13}$
Δ_1	$(k+K_{12})^2+2V_2+V_3$	$V_{10}+2V_{12}+V_{15}$	$V_1+2V_4+V_7$	$2V_{18}$
Z_1	$(k+K_{12})^2+V_2+V_6+V_8$	$\sqrt{2}(V_1+V_{10})$	$\sqrt{2}(V_1+V_4)$	$\sqrt{2}(V_9+V_{13})$
Λ_1	$(k+K_{12})^2+2V_3$	V_4+2V_{10}	$2V_8+V_{13}$	$2V_4+V_{10}$
Σ_1	$(k+K_{12})^2+V_3+V_6+V_9$	$\sqrt{2}(V_4+V_{12})$	$V_4+V_7+V_{10}+V_{12}$	$2V_3$
	$a_{14,14}$	$a_{14,15}=a_{15,14}$	$a_{14,16}=a_{16,14}$	$a_{14,17}=a_{17,14}$
Δ_1	$(k+K_{13})^2+V_{11}+2V_6$	$V_6+2V_{11}+V_{17}$	$2V_5$	
Z_1	$(k+K_{13})^2+V_{13}$	V_3+V_8	$2V_{10}$	$\sqrt{2}(V_9+V_{13})$
Λ_1	$(k+K_{13})^2+2V_{11}$	$2V_4+V_{15}$	$2V_5+V_{16}$	
Σ_1	$(k+K_{13})^2+V_{13}$	$\sqrt{2}(V_5+V_9)$	$\sqrt{2}V_{10}$	
	$a_{15,15}$	$a_{15,16}=a_{16,15}$	$a_{15,17}=a_{17,15}$	$a_{17,17}$
Δ_1	$(k+K_{14})^2+2V_6+V_{11}$	$2V_{16}$		
Z_1	$(k+K_{14})^2+V_2$	$2V_{12}$	$\sqrt{2}(V_{14}+V_{16})$	$(k+K_{16})^2+V_2+V_6+V_8$
Λ_1	$(k+K_{14})^2+2V_{11}$	V_1+2V_{12}		
Σ_1	$(k+K_{14})^2+V_2+V_{11}+V_{13}$	$2V_{10}$		

CONVERGENCE OF $E' = E-V_0$ Group Γ, $k = 2\pi(000)$

$\lambda = 0.25$ $V_0' = -100$

Γ_1

3x3	-0.23261	118.99319	161.53269	
4x4	-0.25392	118.98930	161.53210	319.24283
5x5	-0.28312	118.96833	161.52965	319.21509
6x6	-0.28999	118.96730	161.51067	319.20505
E	-8.09954	111.15776	153.70113	311.39551

Γ_{15}

3x3	115.65358	158.25105	317.51576
4x4	115.65196	158.20383	317.47597
5x5	115.64962	158.19457	317.45961
E	107.84008	150.38503	309.65007

Γ_{25}'

3x3	118.93180	315.45184	436.51803
4x4	118.91309	315.44606	436.24236
E	111.10355	307.63652	428.43282

Γ_{12}

2x2	156.57050	314.89810
3x3	156.47526	314.84611
E	148.66572	307.03657

Γ_2'

2x2	122.33410	436.58290
3x3	122.29443	436.50317
E	114.48489	428.69363

CONVERGENCE OF $E' = E-V_0$ Group Δ ,$k=2\pi(\frac{1}{2}00)$

$\lambda=0,25$ $V_0' = -100$

Δ_1

5x5	9.60913	84.98725	91.95703	165.98332	170.83750
7x7	9.59795	84.93284	91.95177	165.89151	170.71804
9x9	9.58409	84.92286	91.89145	165.88123	170.70083
12x12	9;56323	84.91044	91.87694	165.85687	170.66808
14x14	9.55398	84.90478	91.86767	165.85635	170 .65907
E	1. 74444	77.09524	84. 05813	158.04681	162.84953

Δ_2

4x4	166.36696	245.41650
5x5	166.32594	245.41128
E	158.51640	

Δ_2'

5x5	90.98338	170.02478
7x7	90.95164	170.00279
9x9	90.95104	169.96997
E	83.14150	162.16043

Δ_5

5x5	87.78865	163.91088	170.79522
8x8	87.77786	163.86373	170.74684
10x10	87.76343	163.84406	170.73742
12x12	87.76207	163.84255	170.71980
E	79.95253	156.03301	162.91026

Group X $k=2\pi(100)$

X_1

4x4	38.09019	78.73327	199.71062
6x6	38.05081	78.73301	199.68726
8x8	38.03262	78.71185	199.68574
E	30.22308	70.90231	191.87620

X_4'

4x4	40.04392	198.35872
6x6	40.03307	198.34182
E	32.22353	190.53228

CONVERGENCE OF $E' = E-V_0$

Group X $k=2\pi(100)$

$\lambda = 0,25$ $V'_0 = -100$

X_2

3x3	193.99178	393.43812
4x4	193.97280	393.43574
E	186.16326	

X_3

4x4	81.09584	239.28415
5x5	81.09582	239.26640
E	73.28628	

X'_3

3x3	197.98906	511.67554
E	190.17952	

X_5

3x3	197.37645	236.29385
5x5	197.37776	236.25594
E	189.52822	

X'_5

3x3	77.96110	196.44392	236.56138
5x5	77.93677	196.38760	236.52143
7x7	77.92538	196.37818	236.47524
E	70.11584	188.56864	

Group Z $k=2\pi(1\frac{1}{4}0)$

Z_1

5x5	40.38301	61.39585	100.56607	159.69181	199.49306
7x7	40.37263	61.38342	100.44147	159.65753	199.38150
9x9	40.35593	61.34545	100.43739	159.64711	199.38085
11x11	40.34903	61.33721	100.42833	159.57542	199.36822
13x13	40.33209	61.33408	100.41825	159.56359	199.33506
15x15	40.32102	61.28888	100.40392	159.56339	199.29852
E	32.51148	53.52334	92. 59438	151.75385	191.48898

Z_3

5x5	42.56492	160.94441	200.68420
7x7	42.50726	160.90214	200.61087
9x9	42.50374	160.89991	200.59676
E	34.69420	153.09037	192.78722

CONVERGENCE OF $E' = E - V_o$

$\lambda = 0.25 \quad V_o' = -100$

Z_4

4x4	62.25140	101.85612	198.92882
6x6	62.20422	101.81984	198.87271
8x8	62.19242	101.81745	198.83539
10x10	62.18922	101.77077	198.81035
E	54.37968	93.96123	191.00081

GROUP W $k=2\pi(1\frac{1}{2}0)$

W_1

4x4	44.90646	126.28616	206.44700
5x5	44.90342	126.26263	206.43476
6x6	44.86990	126.25402	206.43401
E	37.06036	118.44448	198.62447

W_2'

4x4	51.87715	126.11006	207.22253
5x5	51.86486	126.10715	207.14124
6x6	51.86211	126.09791	207.11461
E	44.05257	118.28837	199.30507

W_3

4x4	49.98102	129.07770	208.23958
5x5	49.97795	129.07514	208.23253
6x6	49.97792	129.07512	208.20271
E	42.16838	121.26558	200.39317

GROUP Q $k=2\pi(\frac{11}{24})$

Q_1

5x5	32.48352	72.39977	114.27637	153.80954	192.55789
7x7	32.48085	72.39892	114.26436	153.79770	192.54677
9x9	32.46582	72.39456	114.25973	153.79657	192.54337
E	24.65628	64.58502	106.45019	145.98703	184.73383

Q_2

5x5	36.17273	75.60538	112.89730	153.47321	192.55718
7x7	36.16933	75.58287	112.88125	153.41069	192.51058
9x9	36.16662	75.56050	112.87634	153.38914	192.46090
E	28.35708	67.75096	105.06680	145.57960	184.65136

CONVERGENCE OF $E' = E - V_0$

GROUP L $k=2\pi(\frac{1}{2}\frac{1}{2}\frac{1}{2})$

$\lambda = 0.25$ $V_0' = -100$

L_1

4x4	27.59008	107.462 8	190.46338
5x5	27.55143	107.44860	190.46338
6x6	27.53792	107.44824	190.46124
E	19.72838	99.63870	182.65170

L_2'

4x4	31.15607	112.92840	187.55404
5x5	31.15607	112.92149	187.50572
6x6	31.15599	112.88985	187.48658
E	23.34645	105.08031	179.67704

	L_3			L_3'	
3x3	110.19297	185.99786	3x3	105.13145	187.54888
4x4	110.15618	185.97525	3x3	105.09074	187.54830
5x5	110.13327	185.96680	5x5	105.08782	187.54829
E	102.32373	178.15726	E	97.27828	179.73875

GROUP Λ $k=2\pi(\frac{1}{4}\frac{1}{4}\frac{1}{4})$

Λ_1

4x4	7.23676	66.47956	107.40376	127.89964		
6x6	7.15437	66.45080	107.35618	127.87853	147.17608	185.16644
8x8	7.13880	66.38060	107.35511	127.83450	147.01529	184.78065
10x10	7.12331	66.36341	107.33046	127.83308	147.00302	184.75976
12x12	7.11357	66.34459	107.32137	127.81790	146.99430	184.75973
14x14	7.10517	66.34153	107.30930	127.80414	146.99133	184.71390
E	-0.70437	58.53199	99.49976	119.99460	139.18179	176.90436

Λ_3

4x4	104.89821	125.10894	145.04140	204.19574
6x6	104.80738	125.10104	145.02964	204.16909
8x8	104.80659	125.04092	145.01802	204.16742
10x10	104.80448	125.02741	144.99091	204.15726
E	96.99494	117.21787	137.18137	196.34772

CONVERGENCE OF $E' = E - V_0$

GROUP Σ $k = 2\pi$([illegible]0)

$\lambda = 0.25$ $V_0' = -100$

Σ_1

6x6	10.83697	69.35442	110.70085	130.31803	169.31461	188.13818
8x8	10.82929	69.29008	110.68932	130.26847	169.26413	187.83283
10x10	10.81735	69.27103	110.68384	130.23943	169.24170	187.80526
12x12	10.80841	69.26758	110.66386	130.21881	169.23235	187.80511
14x14	10.79934	69.26315	110.65250	130.21512	169.21202	187.79170
E	2.98980	61.45361	102.84296	122.40558	161.40248	179.98216

Σ_3

5x5	70.86062	130.10442	168.89601	189.83359
7x7	70.82248	130.09804	168.88752	189.83358
9x9	70.81677	130.07795	168.86597	189.77460
E	63.00723	122.26841	161. 05643	181.96506

Σ_4

3x3	108.39456	127.92228
5x5	108.35677	127.87941
7x7	108.30725	127.84872
E	100.49771	120.03918

Σ_2

3x3	130.06669	266.58469
4x4	130.02892	266.58082
E	122.21938	

GROUP K $k = 2\pi$($\frac{3}{4}$0)

K_1

8x8	41.17259	46.32686	84.89607	123.42122	163.59058	202.62694
10x10	41.16352	46.30436	84.89287	123.39861	163.56058	202.58990
12x12	41.16054	46.28822	84.86456	123.28591	163.52200	202.56238
14x14	41.15242	46.28412	84.85472	123.28147	163.51640	202.53664
E	33.34288	38.47458	77.04518	115.47193	155.70686	194.72710

K_3

5x5	45.02092	163.39419	202.35770
7x7	44.97117	163.38234	202.33004
9x9	44.96587	163.36606	202.30484
E	37.15633	155.55652	194.49530

K_4

3x3	82.96918	160.79693
5x5	82.94096	160.72918
7x7	82.86345	160.69798
E	75.05391	152.88844

K_2

3x3	163.32182	238.44379
4x4	163.29141	238.44196
E	155.48187	

CONVERGENCE OF $E' = E - V_0$ Group Γ, $k = -2\pi(000)$

$\lambda = 0.50$ $V_0' = -500$

		Γ_1		
3x3	-0.06638	126.58689	165.14653	
4x4	-0.20161	126.58345	165.12613	320.49896
5x5	-0.26021	126.51030	165.12074	320.48403
6x6	-0.26743	126.50906	165.05224	320.47432
E	-11.83693	114.93956	153.48274	308.90482
		Γ_{15}		
3x3	116.09754	158.60860	320.82778	
4x4	115.93862	158.59685	320.82494	
5x5	115.93177	158.52274	320.81945	
E	104.36227	146.95324	309.24995	
		Γ_{25}'		
3x3	116.47262	316.64352		
4x4	116.46594	316.58731		
E	104.89644	305.01781		
		Γ_{12}		
2x2	153.71154	312.45864		
3x3	153.67610	312.45253		
E	142.10660	300.88303		
		Γ_2'		
2x2	121.65436	437.51981		
3x3	121.56168	437.26278		
E	109.99218	425.69328		

CONVERGENCE OF $E'=E-V_0$

GROUP Δ $k=2\pi(\frac{1}{4}00)$

$\lambda=0.50$ $V_0'=-500$

Δ_1

6x6	2.39932	103.30785	120.69063	144.43381	163.76716	200.35323
8x8	2.30281	103.30690	120.67642	144.42978	163.74721	200.32196
10x10	2.25102	103.21586	120.64607	144.41633	163.74032	200.31109
12x12	2.22662	103.1993L	120.58461	144.39618	163.70323	200.28765
14x14	2.19939	103.17281	120.56922	144.32194	163.69048	200.24583
E	-9.37011	91.60331	108.99972	132.75244	152.12098	188.67633

Δ_5

5x5	99.08147	138.39437	161.17611
7x7	99.05738	138.36171	161.13917
9x9	99.01830	138.30588	161.09097
11x11	99.00082	138.25272	160.99874
E	[illegible].43132	126.68322	149.42924

Δ_2'

4x4	101.64840	141.48186
6x6	101.59771	141.45018
8x8	101.56268	141.43125
E	89.99318	129.86175

Δ_2

3x3	156.17754	274.64639
4x4	156.15807	274.61072
5x5	156.14983	274.60024
E	144.58033	

GROUP X $k=2\pi(100)$

X_1

5x5	39.67229	81.84466	202.13368
6x6	39.62239	81.83531	202.11632
7x7	39.60875	81.83434	202.11615
E	28.03925	70.26484	190.54665

X_4'

3x3	38.78206	199.58093
4x4	38.76007	199.58059
5x5	38.70569	199.55690
E	27.13619	187.98740

X_2

2x2	191.78269	395.13811
3x3	191.78181	394.97039
E	180.21231	

X_3

3x3	79.51915	237.98447
4x4	79.50360	237.94228
E	67.93410	

X_3'

2x2	194.58098	509.18767
E	183.01148	

CONVERGENCE OF $E' = E - V_o$

$\lambda = 0.50 \quad V_o' = -500$

X_5'			X_5		
4x4	76.93481	198.92877	3x3	195.86231	235.87311
5x5	76.89718	198.92121	4x4	195.84795	235.41358
6x6	76.87066	198.91993			
E	65.30116	187.35042	E	184.27844	

GROUP Z $k=2\pi(1\frac{1}{4}0)$

Z_1

5x5	42.18719	62.21190	101.90734	160.75866	199.85251
7x7	42.15331	62.12525	101.75936	160.73336	199.53214
9x9	42.10734	62.06818	101.67365	160.65451	199.50984
12x12	42.07741	62.03759	101.64603	160.60263	199.47653
14x14	42.02952	62.03474	101.64585	160.58472	199.44946
E	30.46002	50.46524	90.07635	149.01522	187.87996

Z_3

5x5	41.27969	159.61929	199.54748
7x7	41.23650	159.52963	199.52898
9x9	41.22485	159.50156	199.43993
E	29.65535	147.93206	187.87043

Z_4

4x4	60.98416	100.53185	201.57452
6x6	60.94428	100.47773	201.45903
8x8	60.93493	100.45545	201.40785
10x10	60.89984	100.42822	201.33160
E	49.33034	88.85872	189.76210

GROUP W $k=2\pi(1\frac{1}{2}0)$

W_1

4x4	47.86041	130.70362	207.28986
5x5	47.84472	130.65699	207.28944
6x6	47.77734	130.64428	207.28737
E	36.20784	119.07478	195.71787

W_2'

4x4	51.43707	126.91806	206.65858
5x5	51.42631	126.91377	206.58144
6x6	51.40061	126.89807	206.58043
E	39.83111	115.32857	195.01093

CONVERGENCE OF $E'=E-V_0$

$\lambda = 0.50 \quad V_0' = -500$

W_3

4x4	48.72843	127.67846	206.98900
5x5	48.68494	127.65362	206.90627
6x6	48.67990	127.65361	206.89482
E	37.11040	116.08411	195.32532

GROUP Q $k=2\pi(\frac{3}{4}\frac{1}{2}\frac{1}{4})$

Q_1

6x6	33.58924	73.00003	114.35896	154.53259	192.03942
7x7	33.56335	72.95291	114.33599	154.51065	192.01224
8x8	33.49745	72.94859	114.33418	154.49690	192.00405
E	21.92795	61.37909	102.76468	142.92740	180.43455

Q_2

6x6	35.24911	74.72807	112.61824	152.72483	193.21786
7x7	35.24460	74.71143	112.61539	152.66833	193.21705
8x8	35.24286	74.71119	112.60651	152.66246	193.18737
E	23.67336	63.14169	101.03701	141.09296	181.61787

GROUP L $k=2\pi(\frac{1}{2}\frac{1}{2}\frac{1}{2})$

L_1

4x4	28.63889	111.15282	192.74565
5x5	28.48136	111.15274	192.74370
6x6	28.45994	111.15074	192.73892
E	16.89044	99.58124	181.16942

L_2'

4x4	30.29491	113.27101	190.14960
5x5	30.28125	113.25802	190.11570
6x6	30.27994	113.15921	190.09186
E	18.71044	101.58971	178.52236

	L_3			L_3'	
4x4	108.39833	183.79590	4x4	104.68410	187.24361
5x5	108.37631	183.79576	5x5	104.66758	187.21745
E	96.80681	172.22626	E	93.09808	175.64795

CONVERGENCE OF $E'=E-V_0$

$\lambda = 0.50$ $V_0' = -500$

GROUP Λ k=2π([illegible])

Λ_1

4x4	7.35557	66.56941	109.90551	129.72512		
6x6	7.33475	66.43516	109.66029	129.64388	149.61579	185.29634
8x8	7.28513	66.39633	109.63199	129.47041	149.59174	185.18585
10x10	7.20768	66.36954	109.57445	129.46255	149.58635	185.13623
12x12	7.18917	66.30347	109.55630	129.41111	149.57103	185.12471
E	-4.38033	54.73397	97.98680	117.84161	138.00153	173.55521

Λ_3

4x4	103.97978	123.87487	143.78700	203.06676
6x6	103.94621	123.85480	143.75224	203.02093
8x8	103.91840	123.82946	143.68952	203.01841
E	92.34890	109.94606	132.12002	191.44891

GROUP Σ k=2π([illegible]0)

Σ_1

6x6	11.03037	70.58881	111.49144	132.67296	168.89338	189.67931
8x8	10.95364	70.54690	111.47053	132.62268	168.61471	189.56388
10x10	10.87711	70.53072	111.45091	132.59440	168.60379	189.53294
12x12	10.86074	70.48590	111.39612	132.57577	168.58789	189.50836
E	-0.70876	58.91640	99.82662	121.00627	157.01839	177.93886

Σ_3

5x5	69.59534	130.00090	169.40202	188.37645
7x7	69.57226	129.95660	169.34202	188.37244
E	58.00276	118.38710	157.77252	176.80294

	Σ_4			Σ_2	
4x4	107.49689	127.83548			
6x6	107.46786	127.75770	3x3	127.62332	265.48171
E	95.89836	116.18820	E	116.05382	

GROUP K k=2π([illegible]0)

K_1

8x8	43.27477	45.63246	85.71976	123.49133	166.09754	201.96687
10x10	43.19468	45.61235	85.70075	123.35672	166.06534	201.95586
12x12	43.12124	45.60140	85.62836	123.32143	166.03118	201.92189

K_3

5x5	43.73737	163.31469	202.79454
7x7	43.70616	163.21918	202.58762
E	32.13666	151.64968	191.01812

	K_4			K_2	
4x4	81.87736	160.90914			
6x6	81.82902	160.73925	3x3	160.85713	236.26088
E	70.25952	149.16975	E	149.28763	

CONVERGENCE OF $E'-E-V_0$ GROUP $k=2\pi(000)$

$\lambda=0.75$ $V'=-2000$

Γ_1

3x3	-0.04486	123.12466	160.11370	
4x4	-0.06331	123.12036	160.11015	317.94938
5x5	-0.06431	123.11583	160.10563	317.93578
6x6	-0.06644	123.11142	160.08485	317.92542
E	-5.85084	117.32702	154.30045	312.14102

Γ_{15}

3x3	119.01708	158.54704	316.78246
4x4	118.98053	158.54677	316.77413
5x5	118.98007	158.54149	316.76169
E	113.19567	152.75709	310.97729

Γ_{25}'

3x3	116.41126	317.52514
4x4	116.40673	317.47219
E	110.62233	311.68779

Γ_{12}

2x2	155.83627	313.44401
3x3	155.81359	313.39799
E	150.02919	307.61359

Γ_2'

2x2	117.92804	437.02843
3x3	117.92552	437.02540
E	112.14112	431.24100

CONVERGENCE OF $E'=E-V_0$

$\lambda = 0.75 \quad V_0' = -2000$

GROUP $k=2\pi(\lambda 00)$

Δ_1

5x5	2.42625	103.68734	120.89097	143.40049	161.20775	
7x7	2.41453	103.68530	120.86011	143.38103	161.16669	199.92334
9x9	2.40289	103.67915	120.85471	143.37937	161.15726	199.89527
11x11	2.40235	103.66074	120.85140	143.37283	161.15029	199.88566
E	-3.38205	97.87635	115.06700	137.58843	155.36589	194.10126

Δ_5

6x6	100.39901	139.95258	161.02929
7x7	100.39823	139.95043	161.01950
8x8	100.37544	139.94825	161.01937
E	94.59104	134.16385	155.23497

Δ_2' Δ_2

3x3	99.88799	139.39575	3x3	158.30248	276.77251
5x5	99.88586	139.38014	4x4	158.29026	276.74890
E	94.10146	133.59574	E	152.50586	

GROUP X $k=2\pi(100)$

X_1

4x4	40.35995	81.58620	198.11726
5x5	40.35818	81.58474	198.07045
6x6	40.35729	81.58217	198.07041
E	34.57289	75.79777	192.28601

X_4' X_5'

3x3	38.49100	198.15237	4x4	78.22110	199.32328
4x4	38.46970	198.1493 2	5x5	78.19804	199.32314
E	32.68530	192.36492	E	72.41364	193.53874

X_3 X_5

3x3	77.68866	235.75677	2x2	196.68669	236.87711
4x4	77.68661	235.70321	3x3	196.68040	236.86311
E	71.90221		E	190.89600	

X_2 X_3'

E	190.80291	E	188.26720

CONVERGENCE OF $E' = E - V_0$

$\lambda = 0.75 \quad V_0' = -2000$

GROUP Z $k = 2\pi(1\frac{1}{4}0)$

Z_1

6x6	42.83140	62.57641	102.21990	161.38216	199.84374
8x8	42.81654	62.57529	102.17936	161.36131	199.83535
10x10	42.81544	62.56426	102.17232	161.32254	199.81379
12x12	42.81486	62.56375	102.17145	161.32110	199.80745
14x14	42.81392	62.56133	102.17092	161.31973	199.79486
E	37.02952	56.77693	96.38652	155.53533	194.01046

Z_3

5x5	40.96056	160.26680	198.57414
7x7	40.95045	160.26390	198.56447
9x9	40.93591	160.25706	198.54972
E	35.15151	154.47266	192.76532

Z_4

4x4	62.25141	101.85635	198.92858
6x6	62.20423	101.82007	198.87247
8x8	62.19243	101.81768	198.83515
10x10	62.18923	101.77100	198.81011
E	56.40483	95.98660	193.02571

GROUP W $k = 2\pi(1\frac{1}{2}0)$

W_1

4x4	50.94426	129.07347	206.88447
5x5	50.94425	129.07347	206.87220
6x6	50.94407	129.07269	206.86999
E	45.15967	123.28829	201.08559

W_2'

4x4	49.53993	129.47908	207.60366
5x5	49.53885	129.47853	207.60233
6x6	49.53736	129.47250	207.57489
E	43.75296	123.68810	201.79049

W_3

4x4	48.36333	127.29748	206.00395
5x5	48.35498	127.29279	205.98909
6x6	48.35131	127.29203	205.98906
E	42.56691	121.50763	200.20466

CONVERGENCE OF $E' = E - V_0$

$\lambda = 0.75 \quad V_0' = -2000$

GROUP Q $k = 2\pi(\frac{3}{4}\frac{1}{2}\frac{1}{4})$

Q_1

4x4	34.82553	74.38551	113.36876	152.72141	
6x6	34.80989	74.37801	113.35984	152.69344	192.01309
8x8	34.80273	74.36727	113.35771	152.68793	192.00975
E	29.01833	68.58287	107.57331	146.90555	186.22535

Q_2

4x4	34.15289	73.64192	113.61469	152.69571	
6x6	34.14718	73.63160	113.59173	152.64754	193.00160
8x8	34.13598	73.62292	113.58718	152.63655	192.99868
E	28.35158	67.83852	107.80278	146.85215	187.21428

GROUP L $k = 2\pi(\frac{1}{2}\frac{1}{2}\frac{1}{2})$

L_1

4x4	29.88681	110.59620	188.23595
5x5	29.88073	110.59590	188.23572
6x6	29.87888	110.59368	188.23545
E	24.09448	104.80928	182.45105

L_2'

4x4	29.20234	109.33833	189.60625
5x5	29.18942	109.33611	189.60446
6x6	29.18902	109.32314	189.60416
E	23.40462	103.53874	183.81976

	L_3			L_3'	
4x4	107.34485	186.48016	4x4	108.29365	187.17213
5x5	107.34469	186.46701	5x5	108.28676	187.16822
E	101.56029	180.68261	E	102.50236	181.38382

GROUP Λ $k = 2\pi(\frac{1}{4}\frac{1}{4}\frac{1}{4})$

Λ_1

4x4	7.37167	66.54400	107.55281	127.28992		
6x6	7.36811	66.52621	107.46589	127.28752	146.98761	185.15507
8x8	7.34768	66.52352	107.46575	127.25695	146.97706	185.12142
10x10	7.33828	66.51303	107.46234	127.25615	146.97524	185.12046
12x12	7.33762	66.50353	107.46139	127.24977	146.97187	185.11596
14x14	7.33378	66.50043	107.45276	127.24748	146.97151	185.10930
E	1.54938	60.71603	101.66836	121.46308	141.18711	179.32490

CONVERGENCE OF $E'=E-V_0$

$\lambda=0.75$ $V_0'=-2000$

Λ_3

4x4	105.33952	125.11227	144.92922	204.12460
6x6	105.33427	125.09304	144.92327	204.09335
8x8	105.32359	125.08813	144.91396	204.08602
10x10	105.32216	125.08577	144.90587	204.07662
E	99.53776	119.30137	139.12147	198.29222

GROUP Σ $k=2\pi(\frac{3}{8}\frac{3}{8}0)$

Σ_1

6x6	11.06189	71.19559	110.48988	130.88348	168.40877	189.83959
8x8	11.05086	71.19312	110.46915	130.88212	168.37157	189.79918
10x10	11.04034	71.19229	110.46245	130.88143	168.35993	189.79027
12x12	11.03935	71.16983	110.45434	130.87699	168.35248	189.78855
14x14	11.03401	71.16736	110.45015	130.87536	168.34744	189.78769
E	5.24961	65.38296	104.66575	125.09096	162.56304	184.00329

Σ_3

5x5	69.32386	129.58205	169.63593	187.79857
7x7	69.32243	129.57820	169.63224	187.79340
9x9	69.31336	129.56639	169.61503	187.78973
E	63.52896	123.78199	163.83063	182.00533

Σ_4

5x5	109.03051	130.16486
7x7	109.02841	130.15188
E	103.24401	124.36748

Σ_2

3x3	127.50732	267.71802
4x4	127.50721	267.69317
E	121.72281	

GROUP K $k=2\pi(\frac{3}{4}\frac{3}{4}0)$

K_1

8x8	44.14044	45.52274	84.58165	123.42300	164.19049	201.68908
10x10	44.13066	45.51941	84.57496	123.40188	164.18882	201.66697
12x12	44.12259	45.49703	84.56515	123.38420	164.17760	201.64243
14x14	44.11619	45.49674	84.56231	123.38398	164.17595	201.63722
E	38.33179	39.71234	78.77791	117.59958	158.39155	195.85282

K_3

5x5	43.42283	162.88930	202.90039
7x7	43.42101	162.87964	202.89082
9x9	43.41209	162.86577	202.87680
E	37.62769	157.08137	197.09240

K_4

5x5	83.14886	163.45605
7x7	83.14574	163.42902
E	77.36134	157.64462

K_2

3x3	160.80389	239.79157
4x4	160.80380	239.78847
E	155.01940	

CONVERGENCE OF E'-E-V$_o$ Group Γ,k=2π(000)

λ =0.25 V$_0^!$ = -500

		Γ_1		
3x3	-5.78640	121.73938	180.12012	
4x4	-6.21621	121.52291	180.11741	333.42513
5x5	-7.08137	121.30902	179.93718	332.76912
6x6	-7.29494	121.27050	179.51951	332.32157
7x7	-7.33464	121.06978	179.39922	331.97790
E	-46.38234	82.02208	140.35152	292.9302
		Γ_{15}		
3x3	95.82174	167.00399	325.57384	
4x4	95.80704	165.73230	324.52175	
5x5	95.78931	165.45127	324.09254	
6x6	95.72734	165.32008	323.85739	
E	56.67964	126.27238	284.80969	
		Γ_{25}'		
3x3	118.30084	315.93906	445.84111	
4x4	118.28251	315.87640	438.51412	
E	79.23481	276.82870	399.46642	
		Γ_{12}		
3x3	147.71277	311.32608	427.74706	
4x4	147.66410	311.25114	425.98630	
E	108.61640	272.20344	386.93860	
		Γ_2'		
2x2	137.27660	446.83300		
3x3	136.20517	444.61294		
E	97.15747	405.56524		

CONVERGENCE OF $E' = E - V_0$

$\lambda = 0\,25$ $V_0' = -500$

GROUP Δ $k = 2\pi(\frac{1}{2}00)$

Δ_1

9x9	2.79788	68.96354	101.71004	160.07943	181.45228
11x11	2.35111	68.80706	101.35899	159.53959	180.83373
14x14	1.81564	68.74274	101.15900	159.29230	180.08796
15x15	1.72037	68.73998	101.13322	159.28797	180.02641
16x16	1.70735	68.73220	100.92422	159.28552	180.02347
E	-37.34035	29.6845	61.87652	120.23782	140.97577

Δ_5

8x8	77.68786	149.90648	181.87271
10x10	77.43786	149.22819	181.59578
12x12	77.40371	149.13895	181.13848
E	38.35601	110.09125	142.09078

	Δ_2'			Δ_2	
5x5	97.11748	178.65321	3x3	159.71197	241.40784
7x7	96.23124	177.93815	4x4	158.05896	239.87440
9x9	96.22906	177.00344	5x5	157.04853	239.62343
E	57.18136	137.95574	E	118.00083	

GROUP X $k = 2\pi(100)$

X_1

4x4	23.33574	84.66729	209.67006
6x6	22.46019	84.50953	209.28643
8x8	21.77483	84.26300	209.26294
E	-17.27287	45.21530	170.21524

	X_4'			X_5'	
4x4	38.19935	197.50650	5x5	68.64478	193.62411
6x6	37.99472	197.03365	7x7	68.45548	193.15889
E	-1.05298	157.98595	E	29.40778	154.11119

	X_3			X_5	
4x4	86.76609	248.72368	4x4	186.86658	242.11068
5x5	86.76207	248.19058	5x5	186.11664	241.97239
E	47.71437		E	147.06894	

	X_2			X_3'	
3x3	177.83901	390.00226	3x3	198.71595	501.53678
4x4	177.33574	389.99853			
E	138.28804		E	159.66825	

CONVERGENCE OF $E' = E - V_0$

$\lambda = 0.25 \quad V_0' = -500$

GROUP Z $k = 2\pi(1\frac{1}{4}0)$

Z_1

9x9	23.94101	60.79058	98.71034	157.13606	197.25065
11x11	23.80862	60.48730	98.28592	155.51167	197.15343
13x13	23.47120	60.35642	97.98147	154.91368	196.73254
15x15	23.21664	60.35241	97.86249	154.83898	195.63936
17x17	22.96240	60.26184	97.84484	154.47776	195.63678
E	-16.08530	21.21414	58.79714	115.43006	156.58908

Z_3

7x7	40.59253	158.33552	200.62384
9x9	40.46279	158.29538	200.42513
11x11	40.41400	157.10924	200.35205
E	1.36630	118.06154	161.30435

Z_4

8x8	58.64273	102.97372	195.93568
10x10	58.63377	101.58612	195.51396
12x12	58.63330	101.41262	195.36148
E	19.58560	62.36492	156.31378

GROUP W $k = 2\pi(1\frac{1}{2}0)$

W_1

4x4	24.31287	120.40686	203.02274
5x5	24.19247	119.89877	202.77689
6x6	23.51460	119.54173	202.72417
7x7	23.09012	119.46479	202.68792
E	-15.95758	80.41709	163.64022

W_2'

4x4	55.75491	118.27295	210.14199
5x5	55.44934	117.95493	208.32284
6x6	55.42119	117.52887	207.81847
7x7	55.39705	117.52043	207.81847

W_3

4x4	50.10236	132.44340	212.36096
5x5	50.02726	132.36212	212.19472
6x6	50.02610	132.35940	211.35068
7x7	49.98778	132.35600	211.31308
E	10.94008	93.30830	172.26538

→ E	16.34935	78.47273	168.77077

CONVERGENCE OF $E'=E-V_0$

GROUP Q $k=2\pi(\frac{311}{424})$

$\lambda=0.25$ $V_0'=-500$

Q_1

7x7	18.73571	68.79729	118.19705	157.09368	193.82687
9x9	18.44085	68.59690	118.05888	157.06567	193.75220
11x11	17.88884	68.58781	117.43618	157.06077	193.50590
E	-21.15886	29.54011	78.38848	118.01307	154.45820

Q_2

7x7	40.10872	76.37336	113.23349	155.39918	194.67731
9x9	39.97905	76.01448	112.86382	154.89597	193.74741
11x11	39.97372	75.96653	112.13474	154.56326	193.54438
E	0.92602	36.91883	73.08704	115.51556	154.49668

GROUP L $k=2\pi(\frac{111}{222})$

L_1

4x4	14.83617	106.41319	200.37451
5x5	14.12004	105.75276	200.37105
6x6	13.78264	105.67207	200.26493
7x7	13.44874	105.51265	200.23750
E	-25.59896	66.46495	161.18980

L'_2

4x4	32.62929	130.69366	187.76465
5x5	32.61592	130.49334	186.70052
6x6	32.61303	129.68152	186.18577
7x7	32.54309	129.55893	186.17847
E	-6.50461	90.51123	147.13077

	L_3			L'_3	
4-4	114.25361	176.96335	4x4	87.05438	189.90088
5 5	113.55968	176.82844	5x5	87.00728	189.89275
6x6	113.44850	176.62762	6x6	86.99058	189.15360
E	74.40080	137.57992	E	47.94288	150.10590

GROUP Λ $k=2\pi(\frac{111}{444})$

Λ_1

6x6	1.19665	63.02946	110.50478	142.26758	154.69772	187.85893
8x8	0.88841	60.60080	110.46854	141.15307	150.88422	184.46951
10x10	0.53531	60.21947	109.60614	141.04984	150.74940	183.93566
12x12	0.24288	59.97186	109.05135	140.64508	150.57462	183.90994
14x14	0.00887	59.91436	108.79423	140.14722	150.32990	182.95083
16x16	-0.18665	59.84796	108.63318	139.73596	149.86497	182.93591
E	-39.23435	20.80026	69.58548	100.68826	110.81727	143.88821

CONVERGENCE OF $E'=E-V_0$

$\lambda=0.25$ $V_0'=-500$

Λ_3

6x6	90.14255	124.38898	144.61361	204.53332
8x8	89.99069	123.40778	143.71991	204.51811
10x10	89.97858	123.00946	142.98362	204.41621
12x12	89.85810	122.58128	142.93247	203.93107
E	50.81040	83.53358	103.88477	164.88337

GROUP Σ $k=2\pi(\frac{3}{8}\frac{3}{8}0)$

Σ_1

8x8	4.25357	60.92745	115.72921	134.40567	171.71080	181.95052
10x10	4.05206	60.48165	115.18496	133.85413	171.04404	181.39762
12x12	3.80424	60.29709	114.74028	133.12142	170.88662	181.31554
14x14	3.57089	60.18993	114.34433	133.05436	170.43243	180.92961
16x16	3.35832	60.13694	113.40626	132.87965	170.41549	180.19531
E	-35.68938	21.08924	74.35856	93.83195	131.36779	141.14761

Σ_3

6x6	67.45391	127.01437	173.25077	197.59342
8x8	67.00807	125.85138	173.04098	196.59723
10x10	66.88128	125.71997	172.42434	196.33560
E	27.83358	86.67227	133.37664	157.28790

	Σ_4			Σ_2	
6x6	91.38840	126.89840	4x4	129.75673	260.70597
8x8	90.95956	126.13695	5x5	129.43530	259.36309
E	51.91186	87.08925	E	90.38760	

GROUP K $k=2\pi(\frac{3}{4}\frac{3}{4}0)$

K_1

8x8	23.38612	48.98416	92.17014	124.64134	168.64408	205.14560
10x10	23.23726	48.54239	91.94620	123.80754	168.00016	204.22465
12x12	23.22587	47.72755	91.20487	121.17594	167.50610	204.04054
14x14	23.00757	47.65430	90.85360	121.01420	167.40938	203.35793
16x16	22.74586	47.63493	89.95737	120.76150	167.28848	203.23832
E	-16.30184	8.58723	50.90967	81.71380	128.24078	164.19062

K_3

6x6	43.63742	159.30686	207.78025
8x8	42.92000	158.31090	207.49465
10x10	42.78765	158.14592	206.45124
E	3.73995	119.09822	167.40354

	K_4			K_2	
6x6	73.46592	152.15021	4x4	161.72341	226.91420
8x8	72.85859	151.75756	5x5	161.17308	225.69279
E	33.81089	112.70986	E	122.12538	

The Compatibility Relations

Having calculated the energy values for each irreducible representation we are faced with the problem how to connect these values and form the energy bands.

The principle which is followed is that the symmetry of any type along an axis must be contained in the symmetry of the type at the end of the axis. Representations which obey this law are called compatible and may be found applying the following rule; the sum of the characters of the compatible representations along the axis must be equal to the character of the representation at the end point.

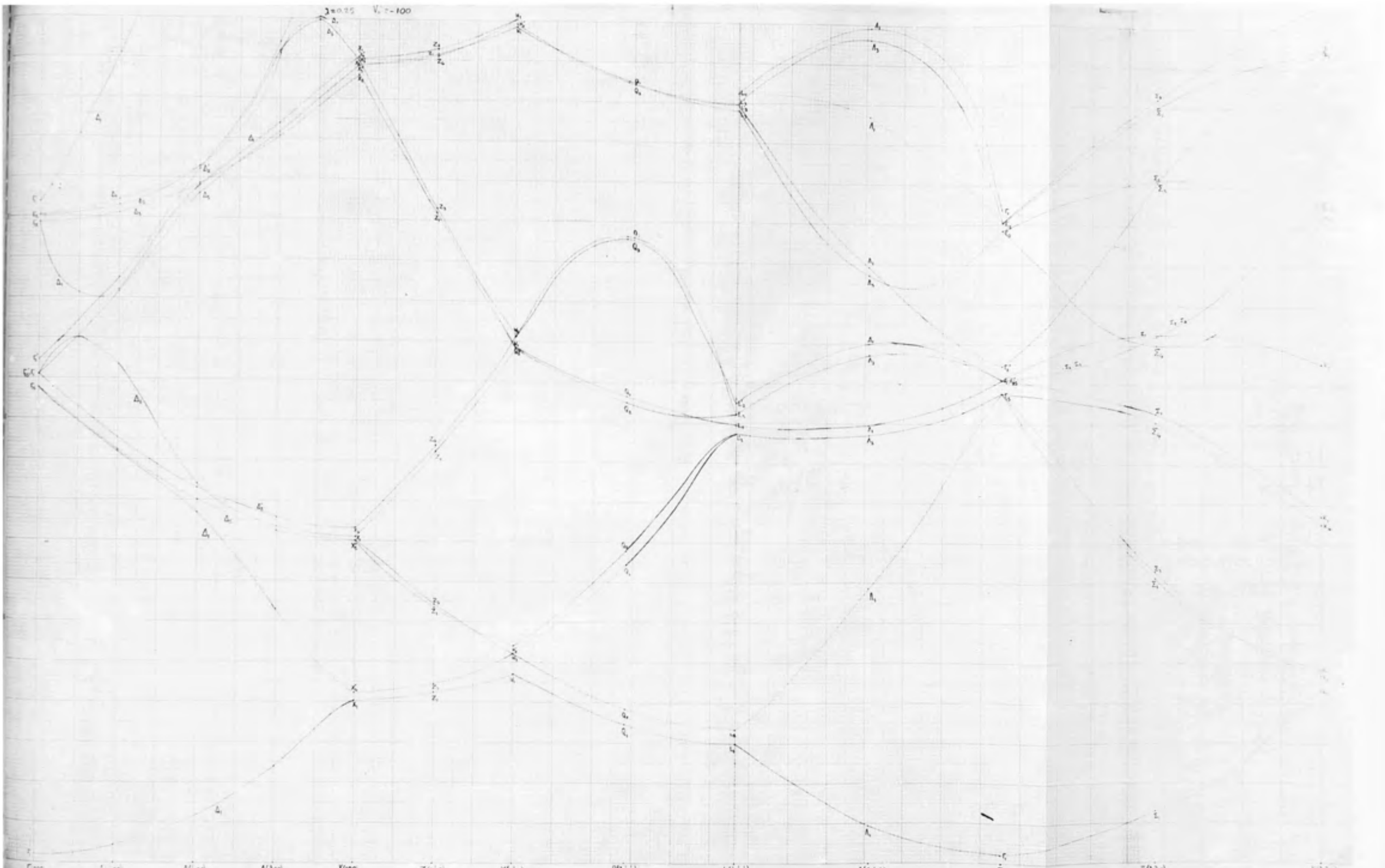
We give below a complete table with the compatibility relations used to plot our graphs. From this table we see that, for example, Γ_{12} joins to Δ_1 and Δ_2. Indeed if we inspect the basis functions for these representations we notice that the symmetries of Δ_1 and Δ_2 are contained in the symmetry of Γ_{12}.

Compatibility Relations for Group O_h^5

Γ_1	Γ_2'	Γ_{12}	Γ_{15}	Γ_{25}'
Δ_1	Δ_2'	$\Delta_1\Delta_2$	$\Delta_1\Delta_5$	$\Delta_2'\Delta_5$
Λ_1	Λ_1	Λ_3	$\Lambda_1\Lambda_3$	$\Lambda_1\Lambda_3$
Σ_1	Σ_3	$\Sigma_1\Sigma_4$	$\Sigma_1\Sigma_3\Sigma_4$	$\Sigma_1\Sigma_2\Sigma_3$

X_1	X_2	X_3	X_5	X_3'	X_4'	X_5'
Δ_1	Δ_2	Δ_2'	Δ_5	Δ_2	Δ_1	Δ_5
Z_1	Z_1	Z_4	Z_2Z_3	Z_3	Z_3	Z_1Z_4

L_1	L_2'	L_3	L_3'		W_1	W_2'	W_3
Λ_1	Λ_1	Λ_3	Λ_3		Z_1	Z_1	Z_3Z_4
Q_1	Q_2	Q_1Q_2	Q_1Q_2		Q_1	Q_2	Q_1Q_2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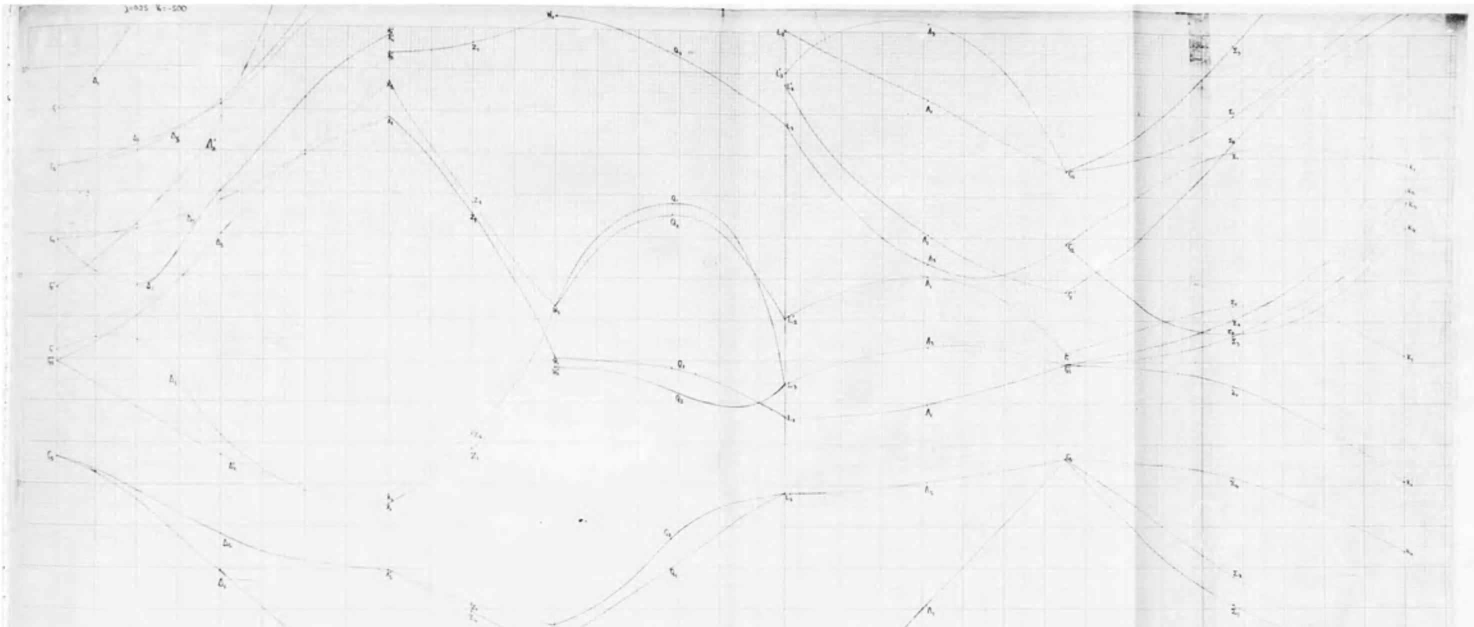
Γ(000)
X(100)
L
Λ
Γ
Σ
K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Δ
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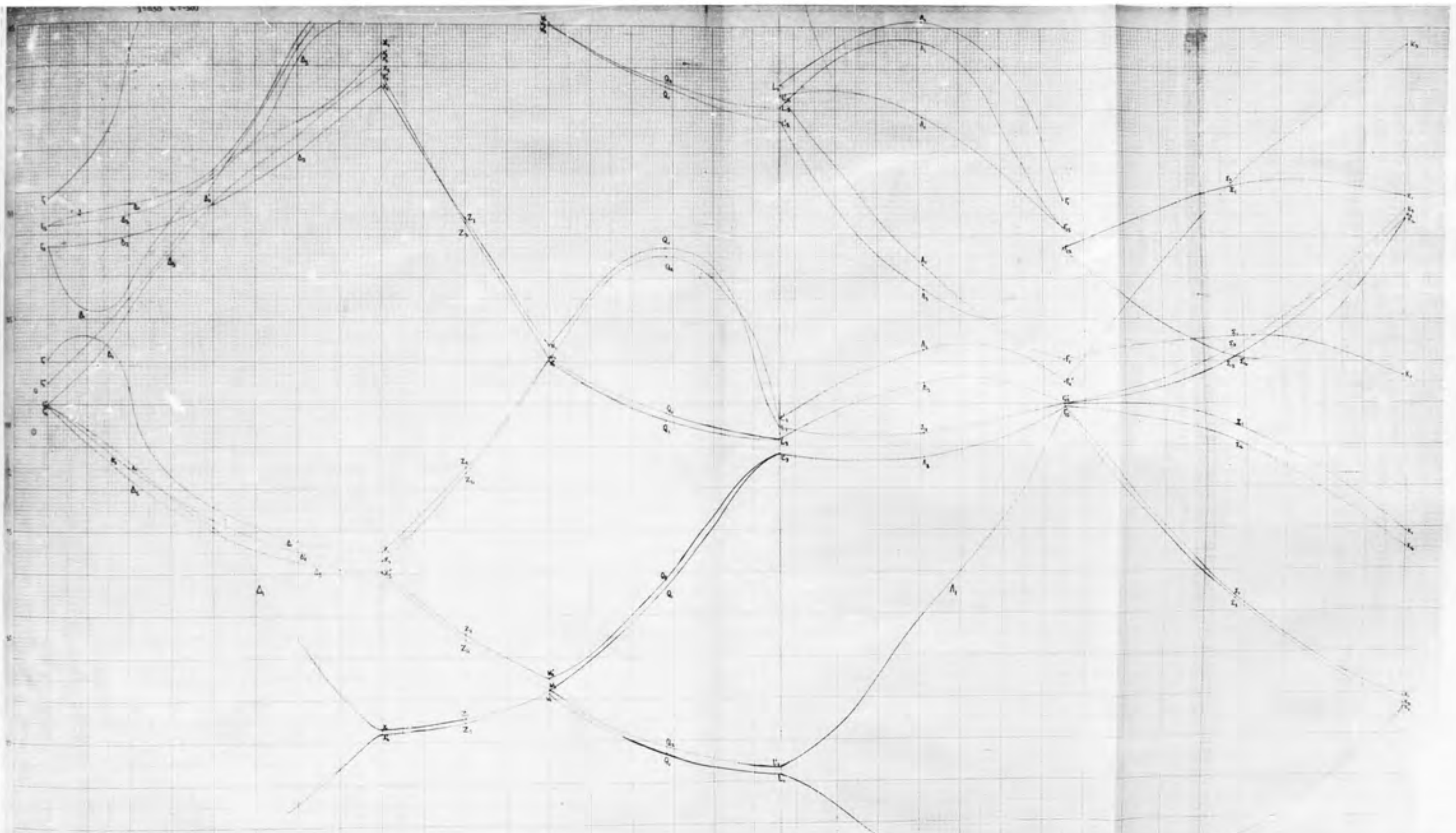
Γ(000)
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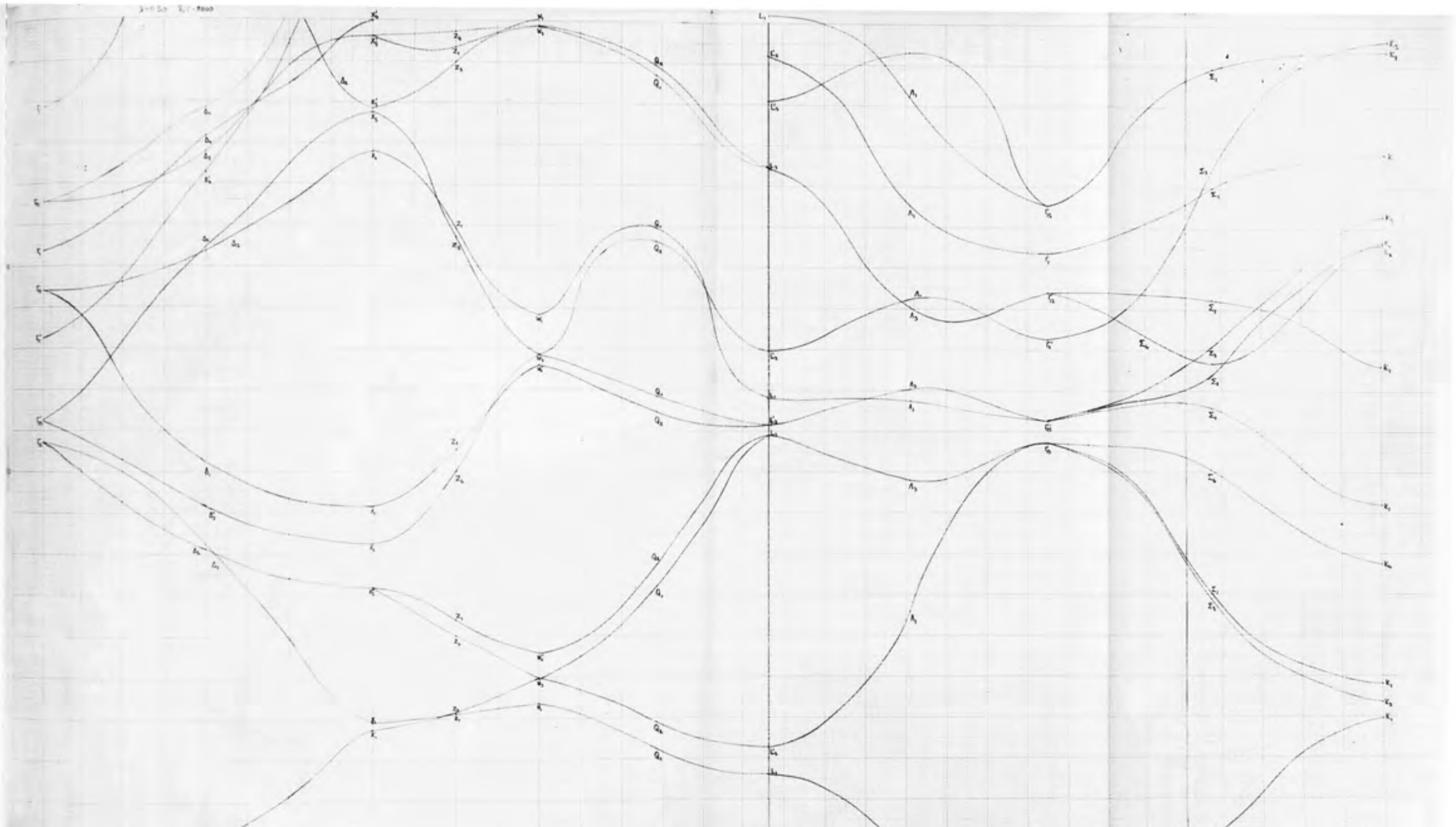Γ(000)
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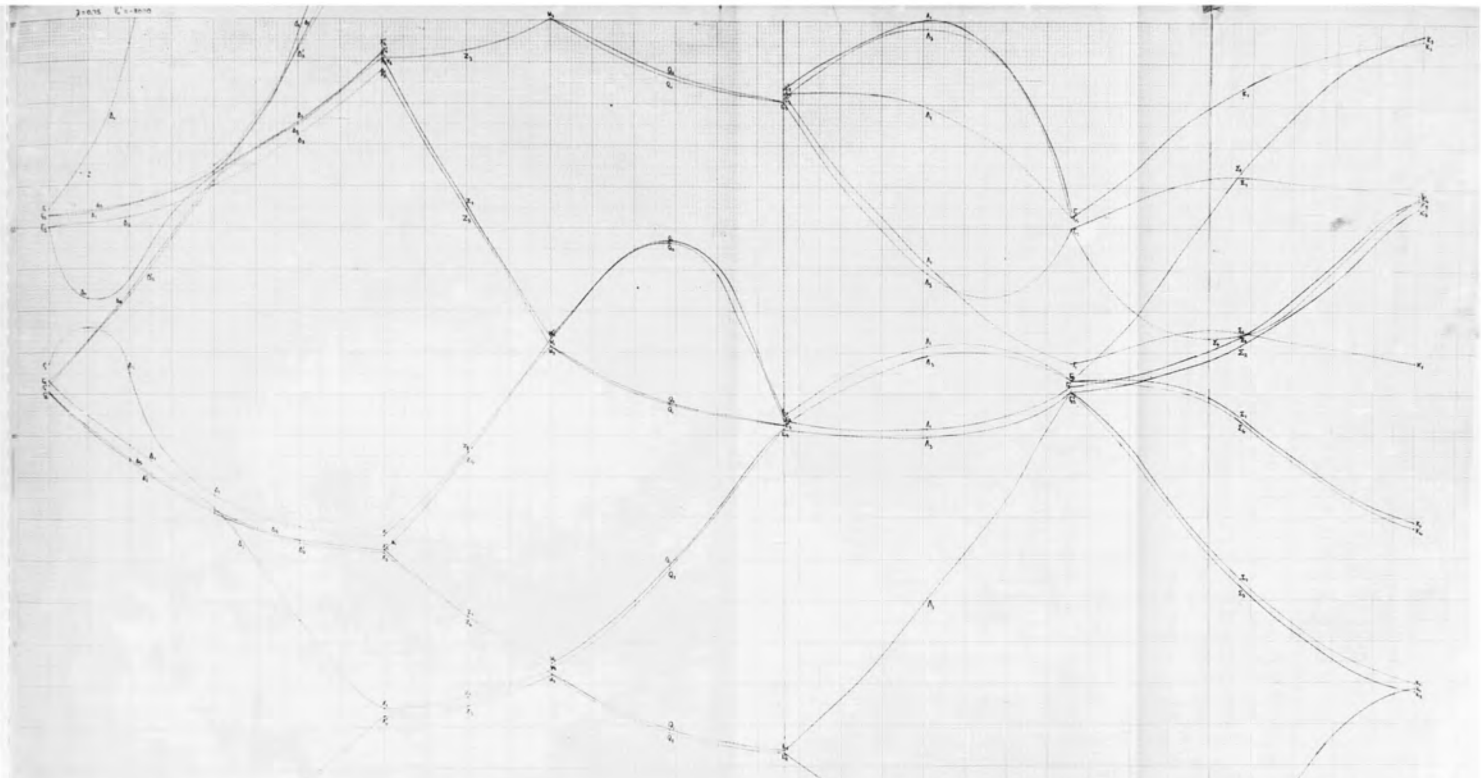
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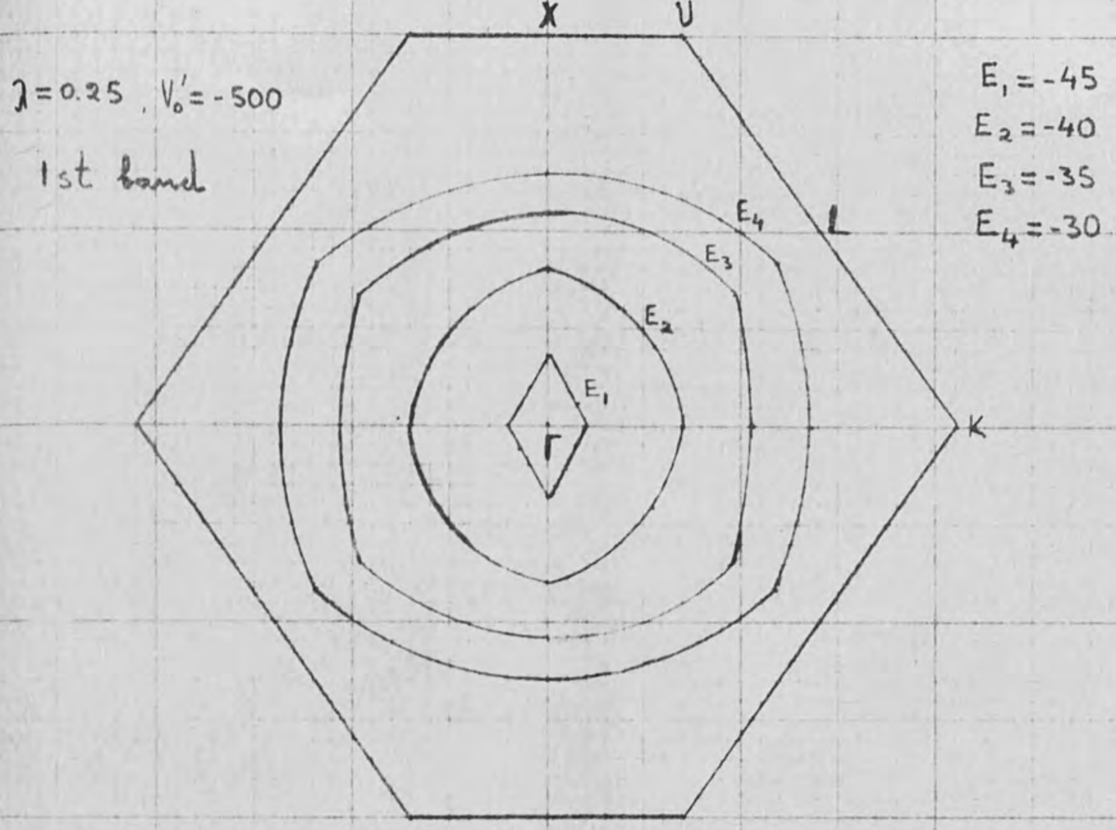
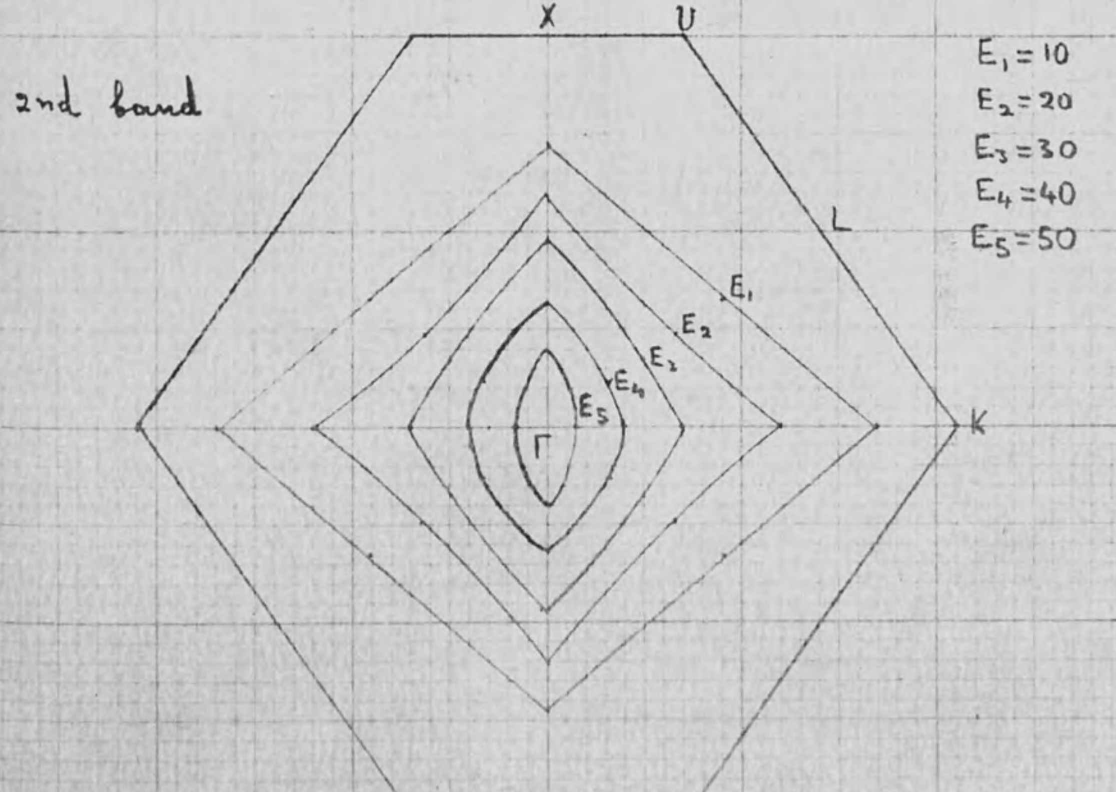
Λ
Γ(000)
Σ
K





Constant energy contours

4. The Free-electron Limit

In the case of the free-electron limit the potential may be taken equal to zero (empty lattice) and so the eigenvalues are found from the expression: $W_1(\underline{k}') = \frac{\hbar^2}{2m}\left|\underline{k}'+\underline{K}'_1\right|^2$ or by using the transformations of section 3, we have:

$$E(\underline{k}) = \left|k+K_i\right|^2$$

in dimensionless units.

As an example the energy values, for face-centred cubic lattice at $k = 2\pi(100)$, are given below:

$\underline{K}_o = 2\pi(000)$ ...: $E_o = 4\pi^2$ non-degenerate

$\underline{K}_1 = 2\pi(\pm1\pm1\pm1)$: $E_1 = 4\pi^2\left[(1+1)^2 +2\right] = 24\pi^2$ 4-times degenerate

$E'_1 = 4\pi^2\left[(1-1)^2 +2\right] = 8\pi^2$ 4-times degenerate

$\underline{K}_2 = 2\pi(\pm200)$: $E_2 = 4\pi^2\,(1+2)^2 = 36\pi^2$ non-degenerate

$E'_2 = 4\pi^2\,(1^2+4) = 20\pi^2$ 4-times degenerate

$E''_2 = 4\pi^2\,(1-2)^2 = 4\pi^2$ non-degenerate

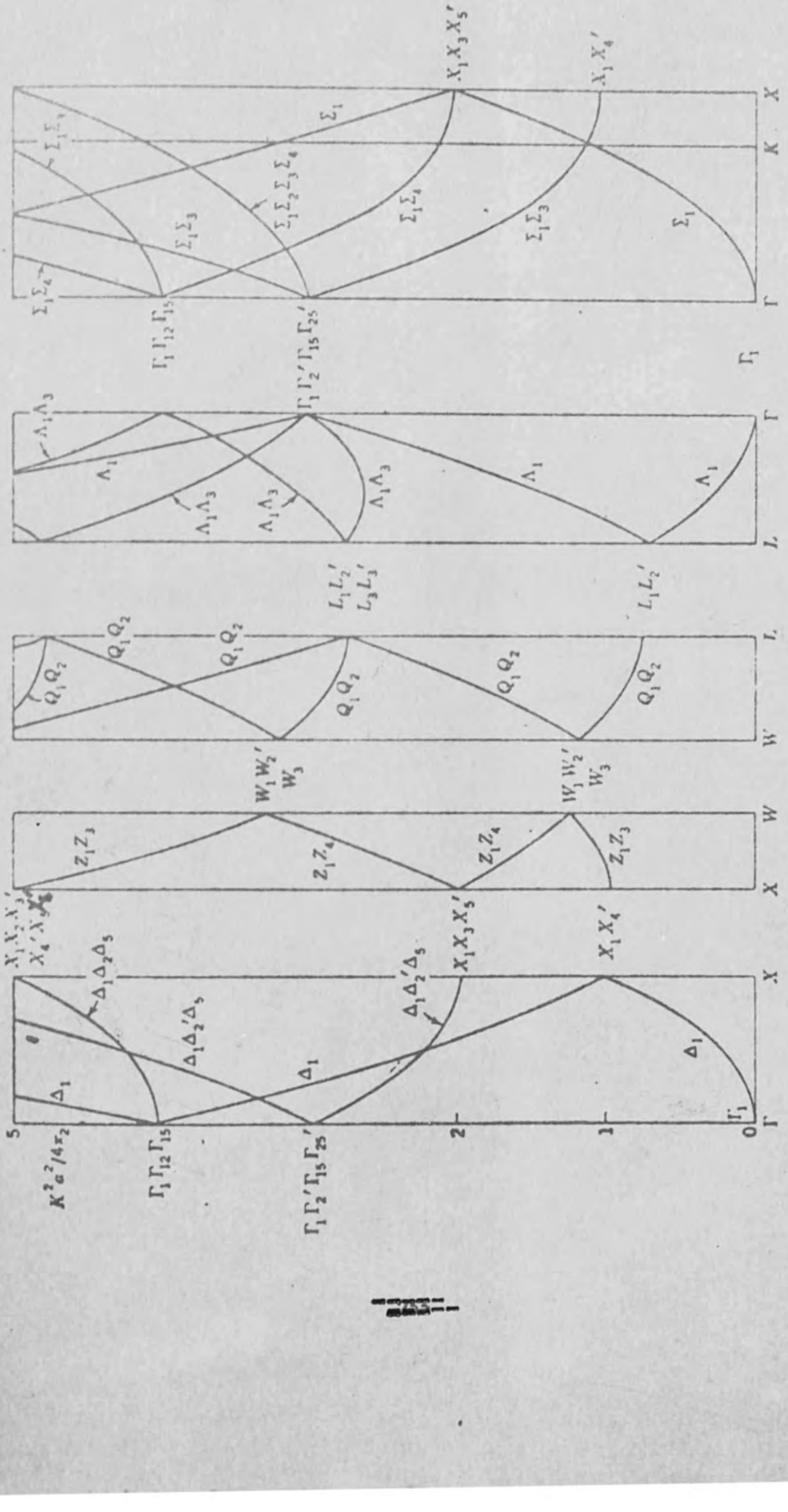
$\underline{K}_3 = 2\pi(\pm2\pm20)$: $E_3 = 4\pi^2\left[(1+2)^2 +4\right] = 52\pi^2$ 4-times degenerate

$E'_3 = 4\pi^2\left[(1-2)^2 +4\right] = 20\pi^2$ 4-times gegenerate

$E''_3 = 4\pi^2(1^2+8) = 36\pi^2$ 4-times degenerate

For many metals the energy bands found this way were very well approximated. One of the few exceptions is iron which shows a different band structure from the one the free-electron approach suggests.

The E - k curves for the free-electron limit in the face-centred cubic lattice are presented in the next page in order to make the comparison with our calculations. We also give tables of the energy levels at the free-electron limit which have been used to substitute for the values of the terms (k+K) in our secular equation.



[redacted] Free-electron energy bands, face-centered cubic structure.

ENERGY LEVELS AT THE FREE ELECTRON LIMIT

$$E = \left| \underline{k} + \underline{K}_n \right|^2$$

	Γ	Δ	Δ	Δ
$k+K_n$	$k=2\pi(000)$	$k=2\pi(\frac{1}{4}00)$	$k=2\pi(\frac{1}{2}00)$	$k=2\pi(\frac{3}{4}00)$
$k+K_0$	0	2.4674	9.8698	22.2066
$k+K_1$	118.43490	101.1634	88.8264	81.4242
$k+K_2$	157.91340	120.9026	88.8264	61.6850
$k+K_3$	315.82728	140.6418	167.7832	199.8594
$k+K_4$	434.25517	160.3810	167.7832	180.1202
$k+K_5$	473.73960	199.8594	246.7400	298.5554
$k+K_6$	631.65361	278.8162	246.7400	219.5986
$k+K_7$		318.2946	325.6968	338.0338
$k+K_8$		357.7730	404.6536	456.4690
$k+K_9$		377.5122	325.6968	278.8162
$k+K_{10}$		416.9906	404.6536	397.2514
$k+K_{11}$		456.4690	483.6104	515.6866
$k+K_{12}$		495.9474	562.5672	634.1218
$k+K_{13}$		436.7298	404.6536	377.5122
$k+K_{14}$		515.6866	562.5672	614.3826
$k+K_{15}$		555.1650	483.6104	416.9906

ENERGY LEVELS AT THE FREE ELECTRON LIMIT

$$E = \left| \underline{k} + \underline{K}_n \right|^2$$

$k+K_n$	$k=2\pi(100)$ X	$k=2\pi(1\frac{1}{4}0)$ Z	$k=2\pi(1\frac{1}{2}0)$ W	$k=2\pi(\frac{3}{4}\frac{1}{2}\frac{1}{4})$ Q
$k+K_0$	39.4784	41.9458	49.3480	34.5436
$k+K_1$	78.9568	61.6850	128.3048	74.0220
$k+K_2$	197.3920	101.1634	207.2616	113.5004
$k+K_3$	236.8704	160.3810	286.2184	152.9788
$k+K_4$	355.3056	199.8594	365.1752	192.4572
$k+K_5$	394.7840	219.5986	444.1320	231.9356
$k+K_6$	513.2192	239.3378	523.0888	271.4140
$k+K_7$	552.6976	259.0770		310.8924
$k+K_8$		318.2946		350.3708
$k+K_9$		338.0338		389.8492
$k+K_{10}$		357.7730		429.3276
$k+K_{11}$		377.5122		
$k+K_{12}$		397.2514		
$k+K_{13}$		416.9906		
$k+K_{14}$		456.4690		
$k+K_{15}$		476.2082		
$k+K_{16}$		495.9474		

ENERGY LEVELS AT THE FREE ELECTRON LIMIT

$$E = \left|\underline{k}+\underline{K}_n\right|^2$$

$k+K_n$	$k=2\pi(\frac{1}{2}\frac{1}{2}\frac{1}{2})$ L	$k=2\pi(\frac{1}{4}\frac{1}{4}\frac{1}{4})$ Λ	$k=2\pi(\frac{3}{8}\frac{3}{8}0)$ Σ	$k=2\pi(\frac{3}{4}\frac{3}{4}0)$ K
$k+K_0$	29.6088	7.4022	11.1033	44.4132
$k+K_1$	108.5656	66.6198	70.3209	44.4132
$k+K_2$	187.5224	106.0982	109.7993	83.8916
$k+K_3$	266.4792	125.8374	129.5385	162.8484
$k+K_4$	345.4360	145.5766	169.0169	202.3268
$k+K_5$	424.3928	185.0550	188.7561	281.2836
$k+K_6$	503.3496	204.7942	208.4953	123.3700
$k+K_7$	582.3064	244.2726	228.2345	320.7620
$k+K_8$		323.2294	267.7129	241.8052
$k+K_9$		342.9686	326.930$_5$	360.2404
$k+K_{10}$		362.7078	326.9305	241.8052
$k+K_{11}$		382.4470	366.4089	281.2836
$k+K_{12}$		402.1862	386.1481	478.6756
$k+K_{13}$		421.9254	386.1481	360.2404
$k+K_{14}$		441.6646	386.1481	360.2404
$k+K_{15}$		461.4038	445.3657	597.1108

5. The bound electron limit.

In this case the wavefunctions about different atoms do not overlap and the problem becomes an atomic one. Now Schrodinger equation is similar to that of the hydrogen atom, and considering the radial part of it we have :

$$d^2R/dr^2 + 2dR/rdr + \left[2m/\hbar^2\left\{E - V(r)\right\} - \ell(\ell+1)/r^2\right]R = 0 \qquad (5.1)$$

Introducing the transofrmation $\psi = Rr$ we obtain:

$$d\psi/dr = rdR/dr + R$$

and $$d^2\psi/dr^2 = rd^2R/dr^2 + 2dR/dr \qquad (5.2)$$

Using the equations (5.2) equation (5.1) for $l = 0$ becomes:

$$d^2\psi/dr^2 + 2m/\hbar^2\left[E - V(r)\right]\psi = 0 \qquad (5.3)$$

It has been shown (section 1) that the pseudopotential used has a minimum value at $r = R\sqrt{\lambda}$

Now if we let $r - R\sqrt{\lambda} = x$ equation (1.4) gives:

$$\begin{aligned}(\lambda+1)V/C &= -\lambda R/x+R\sqrt{\lambda} - (x+R\sqrt{\lambda})/R + \lambda + 1\\ &= -\sqrt{\lambda}/\left(1+\frac{x}{R\sqrt{\lambda}}\right) - x/R - \sqrt{\lambda} + \lambda + 1\\ &= -\sqrt{\lambda}(1+x/R\sqrt{\lambda})^{-1} - x/R - \sqrt{\lambda} + \lambda + 1\\ &= -\sqrt{\lambda}(1 - x/R\sqrt{\lambda} + x^2/R^2\lambda - \ldots\ldots) - x/R - \sqrt{\lambda} + \lambda + 1\end{aligned}$$

If the well is very deep the wave function is confined near $x = 0$. So we may neglect the higher order terms and we have :

$$(\lambda+1)V/C = -2\sqrt{\lambda} + \lambda + 1 - x^2/R^2\sqrt{\lambda}$$

or $$V = C\left[1 - 2\sqrt{\lambda}/\lambda+1 - x^2/R^2(\lambda+1)\sqrt{\lambda}\right] \qquad (5.4)$$

Substituting **V** in equation (5.3) we obtain :

$$d^2\psi/dr^2 + 2m/\hbar^2\left[E - C(1-2\sqrt{\lambda}/\lambda+1) + Cx^2/R^2(\lambda+1)\sqrt{\lambda}\right]\psi = 0 \qquad (5.5)$$

Now let $E - C(1-2\sqrt{\lambda}/\lambda+1) = W$ (5.6)

W is the energy measured from the bottom of the well.

Also let $C/R^2(\lambda+1)\sqrt{\lambda} = -4\beta^2$ = negative (5.7)

Substituting (5.6) and (5.7) into (5.5) we have :

$$d^2\psi/dx^2 + 2m/\hbar^2\left[W - 4\beta^2x^2\right]\psi = 0 \qquad (5.8)$$

This is the equation of the linear harmonic oscillator.

So the eigenvalues are :

$$W_n = 4\beta(n+\tfrac{1}{2})\hbar/\sqrt{2m} \qquad (5.9)$$

Substituting for β from equation (5.7), equation (5.9) becomes :

$$W_n = 2(n+\tfrac{1}{2})\sqrt{-C\hbar}/R\lambda^{1/4}(\lambda+1)^{1/2}(2m)^{1/2} \qquad (5.10)$$

or using $R/a = b$ and $2ma^2C/\hbar^2 = V_0'$

$$W_n = 2(n+\tfrac{1}{2})\hbar^2\sqrt{-V_0'}/2a^2mb\lambda^{1/4}(\lambda+1)^{1/2} \qquad (5.11)$$

Multiplying equation (5.11) by $2a^2m/\hbar^2$ and using the substitution $2ma^2W/\hbar^2 = E$ we have :

$$E_n = 2(n+\tfrac{1}{2})\sqrt{-V_0'}/b\lambda^{1/4}(\lambda+1)^{1/2} \qquad (5.12)$$

which gives the energy values in dimensionless units.

If $1 \neq 0$ equation (5.5) becomes in first approximation:

$$d^2\psi/dr^2 + \left\{2m/\hbar^2\left[E - C(1-2\sqrt{\lambda}/\lambda+1) + Cx^2/R^2(\lambda+1)\sqrt{\lambda}\right] - \ell(\ell+1)/\lambda R^2\right\} = 0 \qquad (5.13)$$

Following the same procedure as above we obtain the expression :

$$E_n = 2(n+\tfrac{1}{2})\sqrt{-V_0'}/b\lambda^{1/4}(\lambda+1)^{1/2} + \ell(\ell+1)/\lambda b^2 \qquad (5.14)$$

which gives the energy in dimensionless units measured from the bottom of the well.

The following table gives the values found using equation (5.14):

TABLE

$\lambda = 0.25$ $V_0' = -500$

	n = 0	n = 1	n = 2
l	E_0	E_1	E_2
0	80	240	400
1	144	304	464
2	272	432	592
3	464	624	784

$\lambda = 0.50$ $V_0' = -2000$

	n = 0	n = 1	n = 2
l	E_0	E_1	E_2
0	122	366	610
1	154	398	642
2	218	462	706
3	314	558	802

$\lambda = 0.75$ $V_0' = -2000$

	n = 0	n = 1	n = 2
l	E	E	E
0	103	309	515
1	124	330	536
2	167	373	579
3	231	437	643

The detailed calculations which we have performed are closer to the free-electron limit and therefore comparison with the bound-electron limit is not possible.

In order to compare with the bound-electron limit we have calculated the Γ point for the values $\lambda = 0.25$ and $V_0' = -2000$. In this case the convergence is unsatisfactory. Nevertheless, as the following table shows, we are able to compare these results and conclude that for these parameters we approach the bound-electron limit.

TABLE

$\lambda = 0.25 \quad V_0' = -2000$

Energies measured from the origin

	From plane-waves calculation		Using equation (5.12) and $V_{min} = -400$
s-like	Γ_1	-246	-240
p-like	Γ_{15}	-166	-176

But still the energy found from the plane wave calculation is below the energy found from equation (5.12).

Further attempt to increase the potential and justify the approximation of the harmonic oscillator fails because convergence in the plane wave method can not be achieved including a reasonable number of waves.

6. Discussion on the graphs of energy bands

The graphs for the energy bands have been drawn along the path Γ-X-W-L-Γ-K in k space. If we take the length ΓX as unity then, from the Geometry, we find :

$XW = 0.5 \quad WL=0.71 \quad \Gamma L=0.87 \quad \Gamma K=1.06$

We now examine the main features of the calculated energy bands for the five different cases considered.

(a) $\lambda = 0.25 \quad V_0' = -100$

For the s-like first band we observe the following ordering of levels: $\Gamma_1, L_1, X_1, K_1, W_1$. i.e. the first band has its minimum at k=o and its maximum atW.

The second band (p-like) contains two branches in the Γ-X direction, three branches in the X-W direction two of which cross, three branches in the W-L direction, two branches in the Γ-L direction and three branches in the Γ-K direction two of which cross. The ordering of levels is : $L_2', X_4', K_3, K_1, W_3, W_2', X_5', K_4, L_3', \Gamma_{15}$ i.e. the mimimum of the second band is at L and the maximum at k=o.

We note that the minimum of the second band L_2' lies below X_1 of the first band. Also X_4' (2nd. band) lies below K_1 (1st. band).

The energy gaps between first and second bands expressed in our dimension less units are as follows:

$$X_1 X_4' = 2 \quad W_1 W_3 = 5 \quad L_1 L_2' = 3.5 \quad K_1 K_3 = 3.7$$

The third band (d-like) includes four branches in the Γ-X direction. Two of them cross with an s-like band and the other two with an f-like band. In the X-W direction the s-like band lies below the d-like and in the W-L direction we observe again crossing of s and d-like bands. Finally in the Γ- L direction the s-like band is above a d-like band and in the Γ- K direction we note again crossing of these bands. The minimum of the d-like band is at X , but for the maximum no reliable value is obtained from our **calculation**.

(b) $\lambda = 0.25$ $V_0' = -500$

The increase of V_0' does not affect the ordering of levels for each band. But now the first band is well separated, that is all their points lie below the points of the second band.

In the second band we notice that the branches $X_5' Z_4 W_3$ and $X_5' Z_1 W_2$ do not cross any more.

The energy gaps are now wider and between first and second bands we find:

$X_1 X_4' = 16.2$ $W_1 W_3 = 27$ $L_1 L_2' = 19$ $K_1 K_3 = 20.2$

In the third band the d-like levels Γ_{25}' and Γ_{12} are now closer to each other.

This calculation gives for the first and second bands the same qualitative results as a calculation on Argon performed by Mattheiss (1964), using the augmented plane-wave method and a potential approximated by a superposition of atomic potentials involving the Slater free - electron exchange potential.

The third band resembles the conduction band of copper as calculated by Segall (1962) using the integral equation approach and two different potentials, the Chodorow potential and an l-dependent one. The same band structure was found by Burdick (1963) using the APW method.

(c) $\lambda = 0.50$ $V_0' = -500$

The increase of λ causes an interchange of the levels X_1 and X_4' . As a consequence of this first and second bands cross in the X - W direction.

The extremes of both the first and second bands remain at the same points as in the previous cases. But we again observe a similar situatiom as in the (a) case, that is L_2' the minimum point of the second band lies below the points X_4' K_1 and W_1 of the first band.

In addition we note that the two branches of the second band in the (100) - direction cross while we have no crossing in the (110) direction.

The energy gaps are now narrower than in case (a). We have: $X_4' X_1 = 1$ $W_1 W_3 = 1$ $L_1 L_2' = 1.7$ $K_1 K_3 = 0.7$

In the third band we have interchange of the levels (X_1 ,X_3) , (W_1 ,W_3) and (L_1 , L_3). Also we note interchange of the s and f - like levels Γ_1 and Γ_2'. The gaps between second and third bands are of about the same order of width as in case (a).

(d) $\lambda = 0.50$ $V_0' = -2000$

The increase of V_0' produces an interchange of the levels L_3 and L_3' . So L_3 is now the second maximum of the second band. The extrene points in all three bands remain unchanged.

The energy gaps are now wider than in case (c) but not as large as in case (b).

We have: $X_4' X_1 = 1.7$ $W_1 W_3 = 6$ $L_1 L_2' = 6.7$ $K_1 K_3 = 4$

These energy gaps are comparable with those found in case (a).

In the third band we note that Γ_{12} is now below Γ_1 and L_3 below L_3'.

(e) $\lambda = 0.75 \quad V_0' = -2000$

The further increase in λ reveals an interchange between the levels (L_2', L_1), (W_3, W_1) and (K_3, K_1) respectively. So the maximum of the first band is now at W_3 and not at W_1, and the minimum of the second at L_1 instead of L_2'.

Now we have no crossing of the first and second bands in the X - W direction but crossing appears in the (110) - direction.

For the second band we note that it crosses the third one since Γ_{25}' is now below Γ_{15}.

The energy gaps are now smaller than in case (d) except for X. We have: $X_4' \; X_1 = 1.9 \quad W_3 \; W_2' = 1.2 \quad L_2' \; L_1 = 0.7 \quad K_1 \; K_3 = 0.7$

This calculation is in good qualitative agreement with Segall's (1961) calculation on aluminium. Segall found the energy bands of aluminium using the Green's function method. His potential was a modification on that used by Heine (1957) in his work on aluminium using the orthogonalised plane wave method.

The Fermi level

In the free-electron limit the Fermi surface is a sphere of radius

$$k_F = (3\pi^2 n/\Omega)^{1/3} \qquad (6.1)$$

where n is the number of electrons in a unit cell and Ω the volume of this cell.

The Fermi level is then

$$W_F = \hbar^2 k_F^2/2m = \hbar^2/2m\ (3\pi^2 n/\Omega)^{2/3} \qquad (6.2)$$

Since for the face-centred cubic structure we have put $\Omega = a^3/4$ equation (6.2) becomes:

$$W_F = \hbar^2/2ma^2\ (3\pi^2 4n)^{2/3} \qquad (6.3)$$

or multiplying (6.3) by $2ma^2/\hbar^2$ we obtain the expression

$$E_F = (3\pi^2 4n)^{2/3} \qquad (6.4)$$

in our dimensionless units.

Our parameters $\lambda = 0.75$ and $V_0' = -2000$ produce, as it is discussed above, energy bands very similar to those found for aluminium. Since there are three conduction electrons in aluminium, equation (6.4) for n = 3, gives $E_F = 50.14$. This value places the Fermi level just above the point W_2' in our graph and this is in complete agreement with Segall's calculation.

Conclusions

The qualitative features of the energy bands do not depend on the details of the potential but only on the symmetry of the crystal.

We found that for the first band, the minimum is for all potentials at k = 0. The maximum is at W, but not always of the same irreducible representation. Also the shape of the whole first band remains almost unchanged.

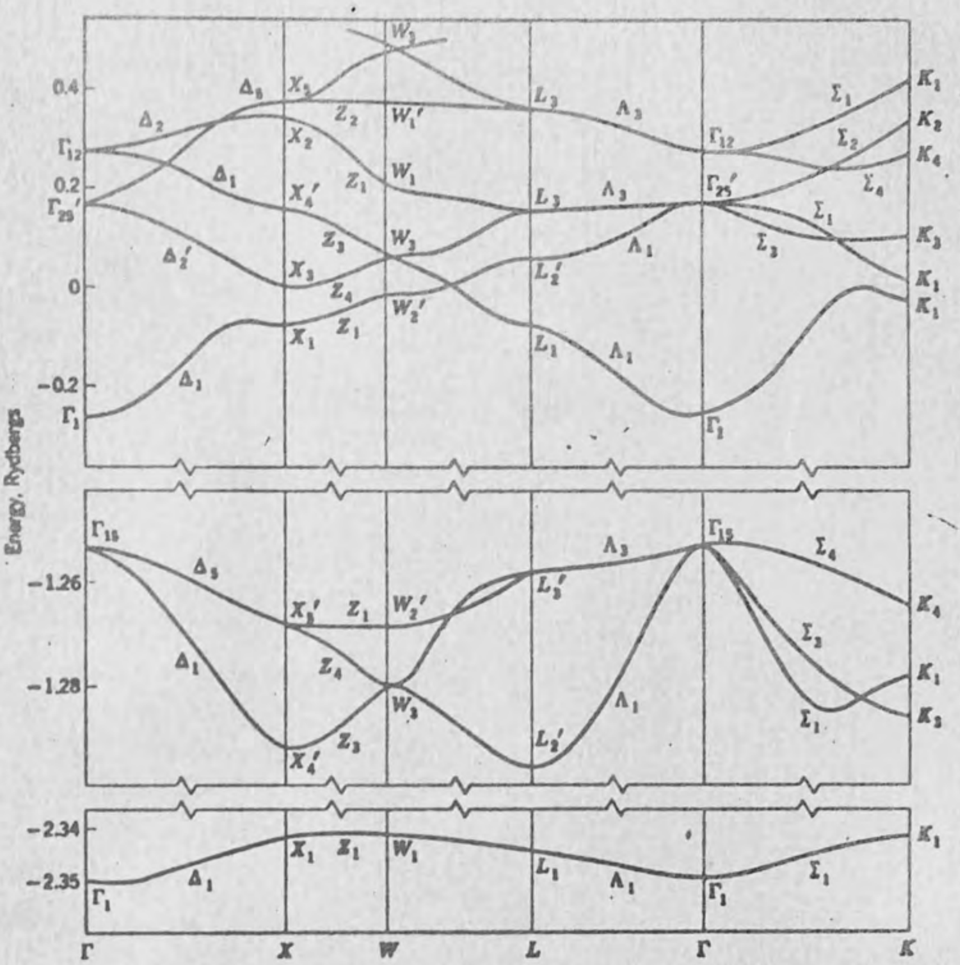
For the second band the minimum is at the point L for all parameters, but again we may have variations of the irreducible representation. Themaximum of this band is always at k = 0. The shape of this band is affected by changes in the ordering of levels.

For the third band we observe a minimum always at X and changes in the ordering of levels.

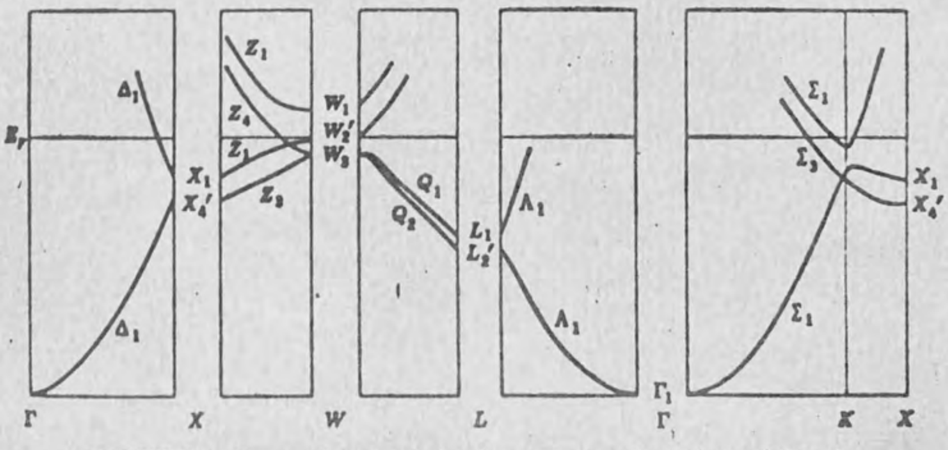
The most sensitive terms seem to be (X_1, X_4'), (L_2', L_1) and (W_3, W_1) which interchange between first and second bands.

The comparison with bands of actual elements shows that the results of our model are in good qualitative agreement with light elements, as aluminium and argon. Especially the first two bands of argon are almost identical with those given by one of our caluulations. Therefore we can conclude that our pseudopotential reproduces the complicated crystal potential of solid argon. For heavier elements as copper, we observe some similarity only in the outer bands.

Finally we point out the agreement of the extrema of our bands with those found by Pincherle and Lee (1961) using a "square well" potential.



[redacted] Energy bands of argon, as calculated by Mattheiss. Note energy gaps and changes of scale.



[redacted] Energy bands of aluminum, from calculations of Segall.

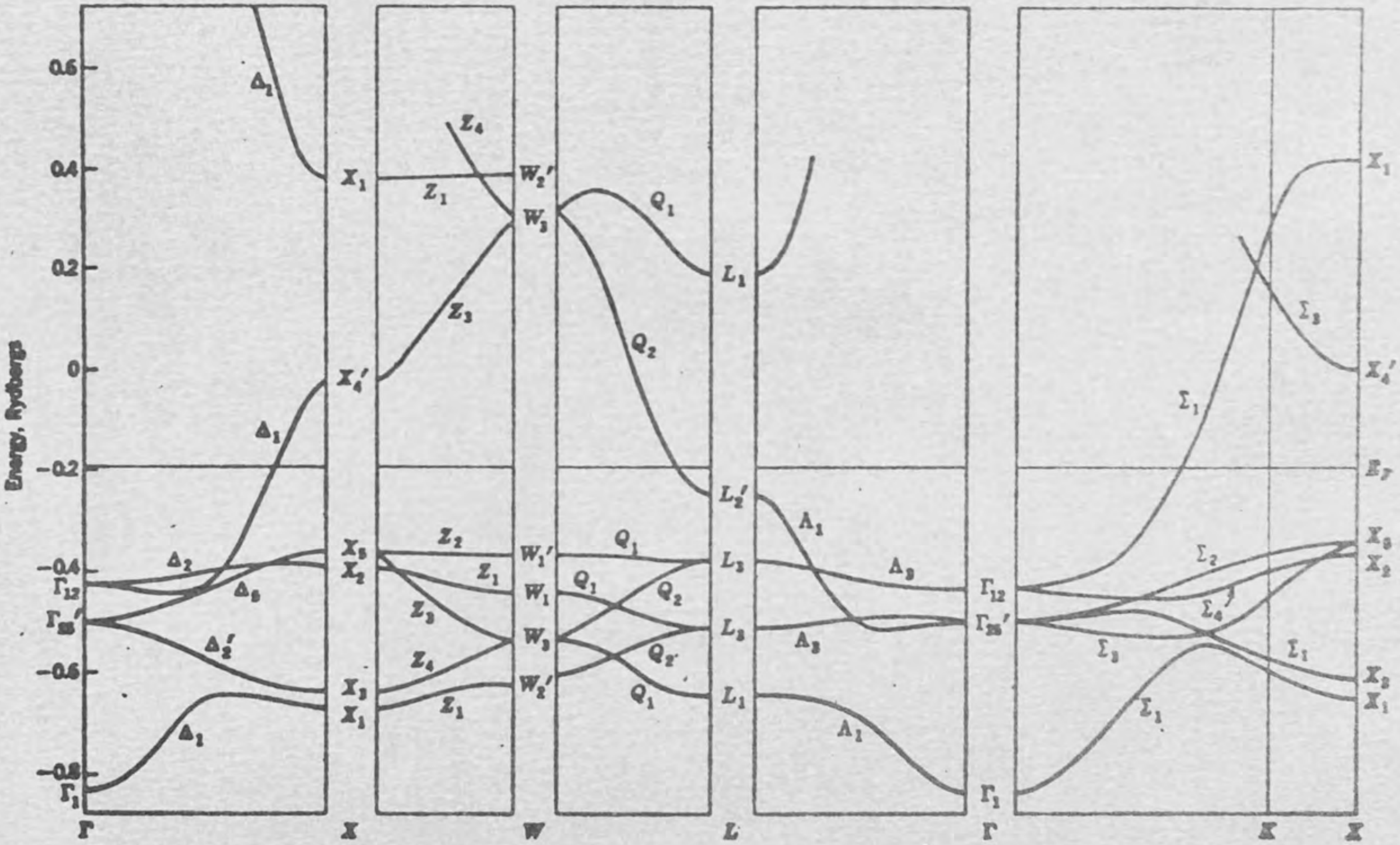
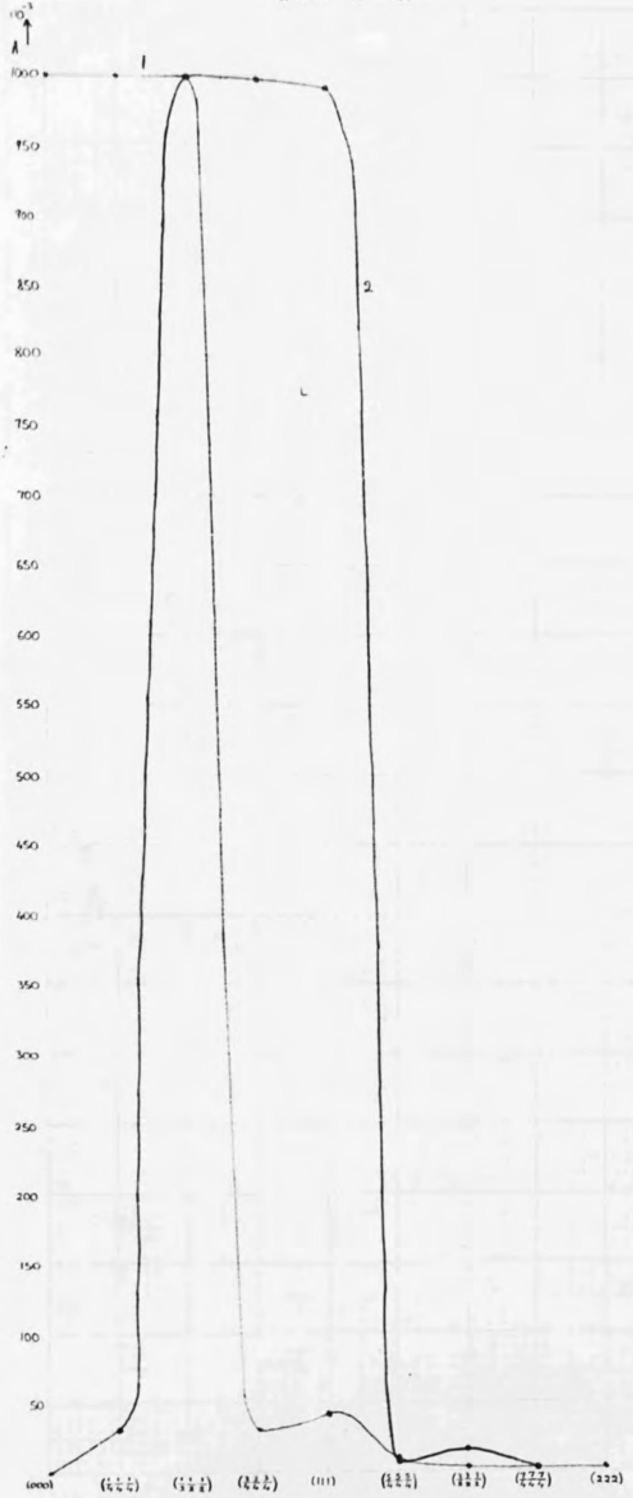
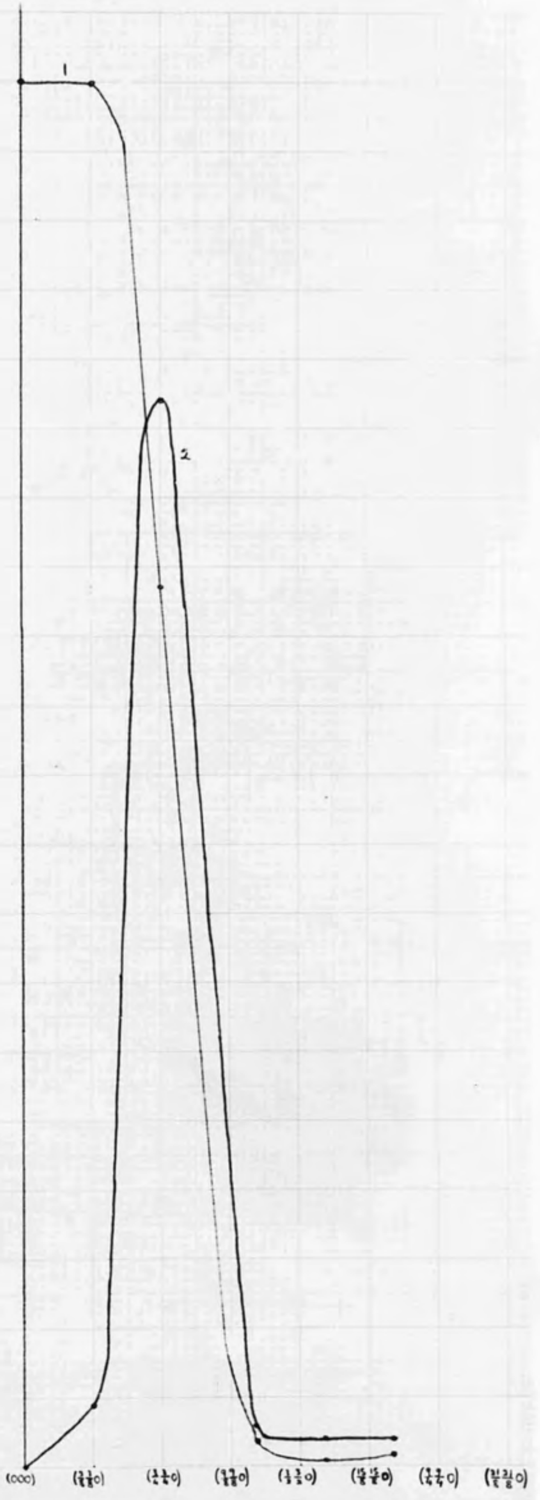
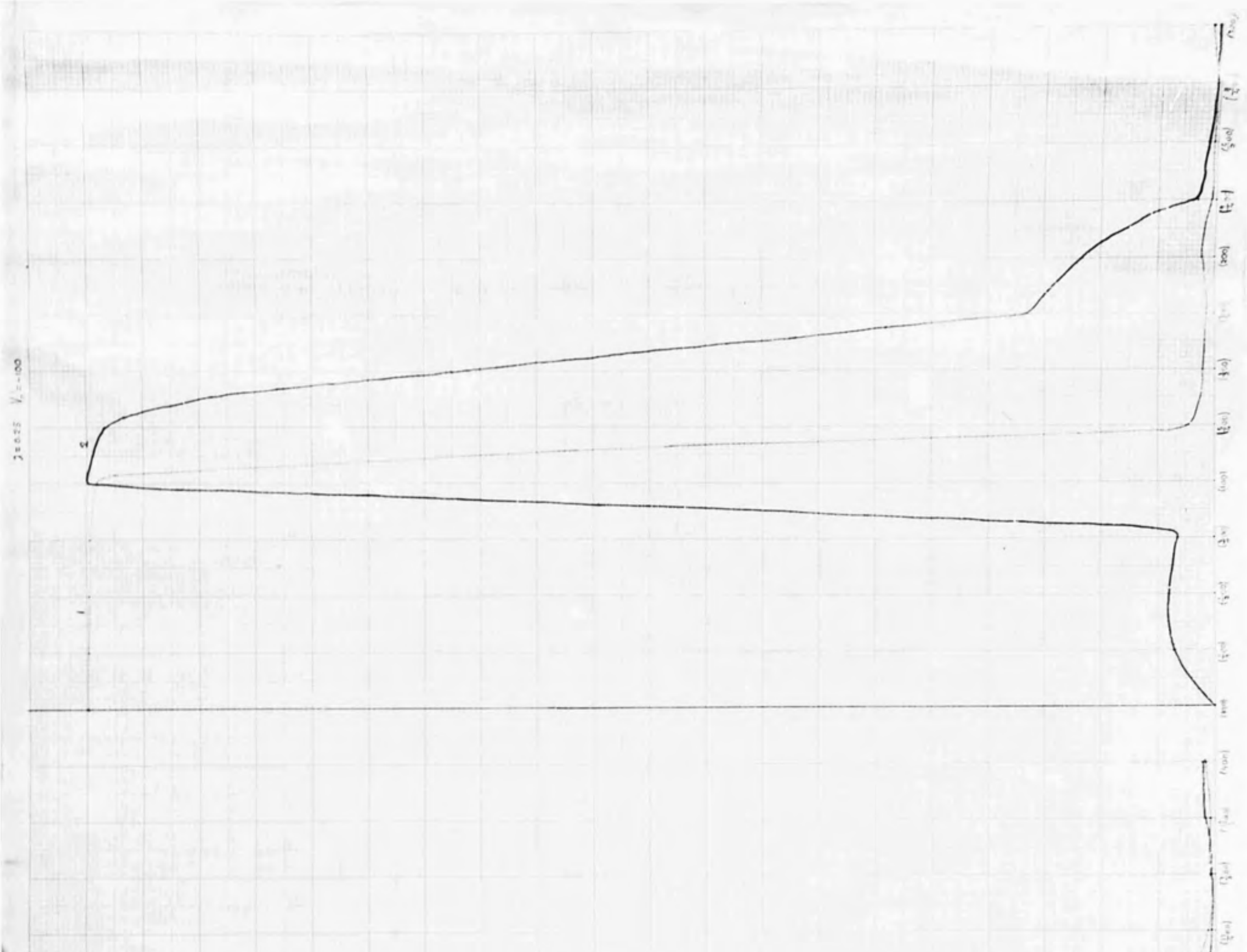


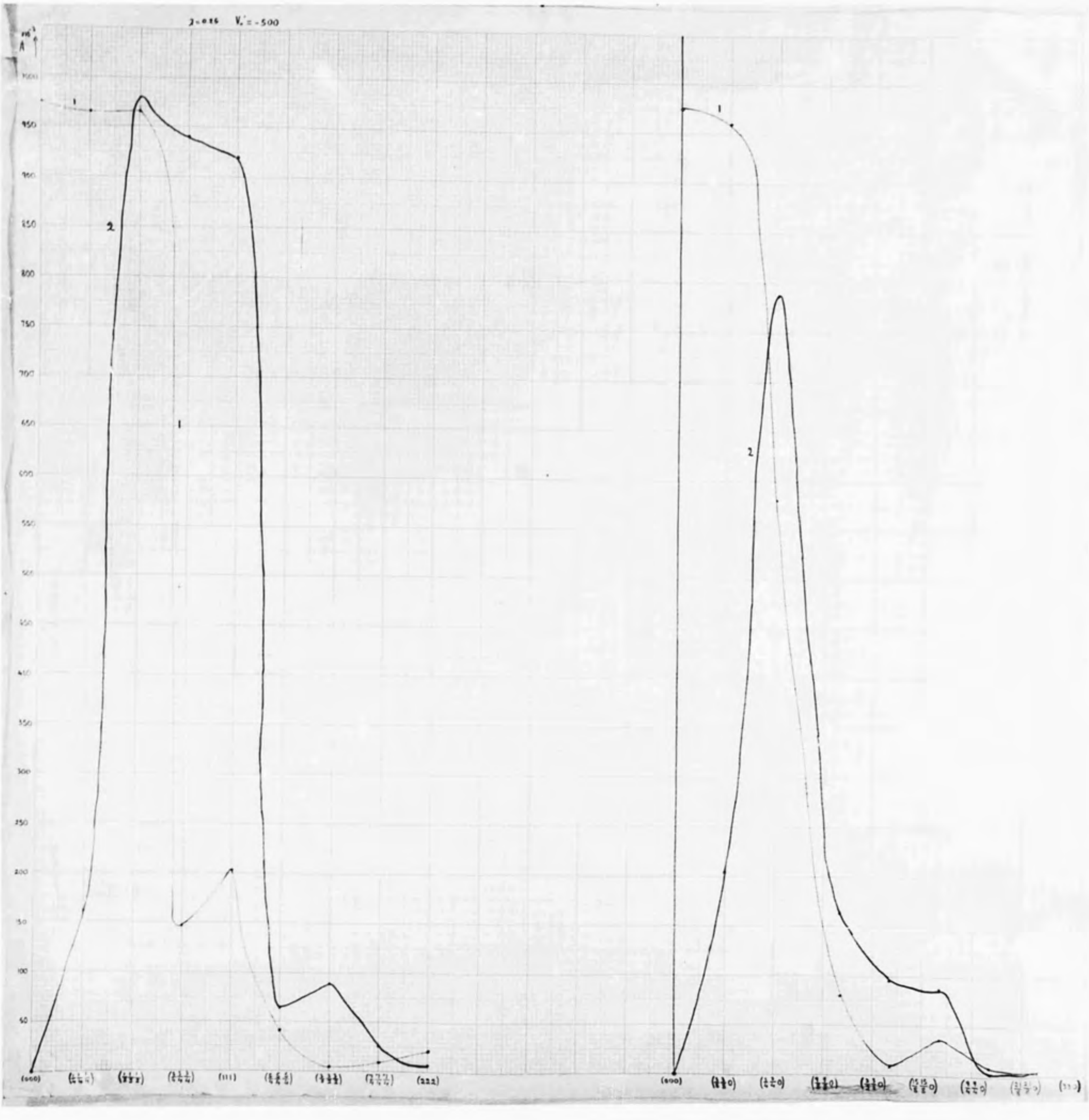
FIG. 10-22 Energy bands of copper, as calculated by Burdick and Segall.

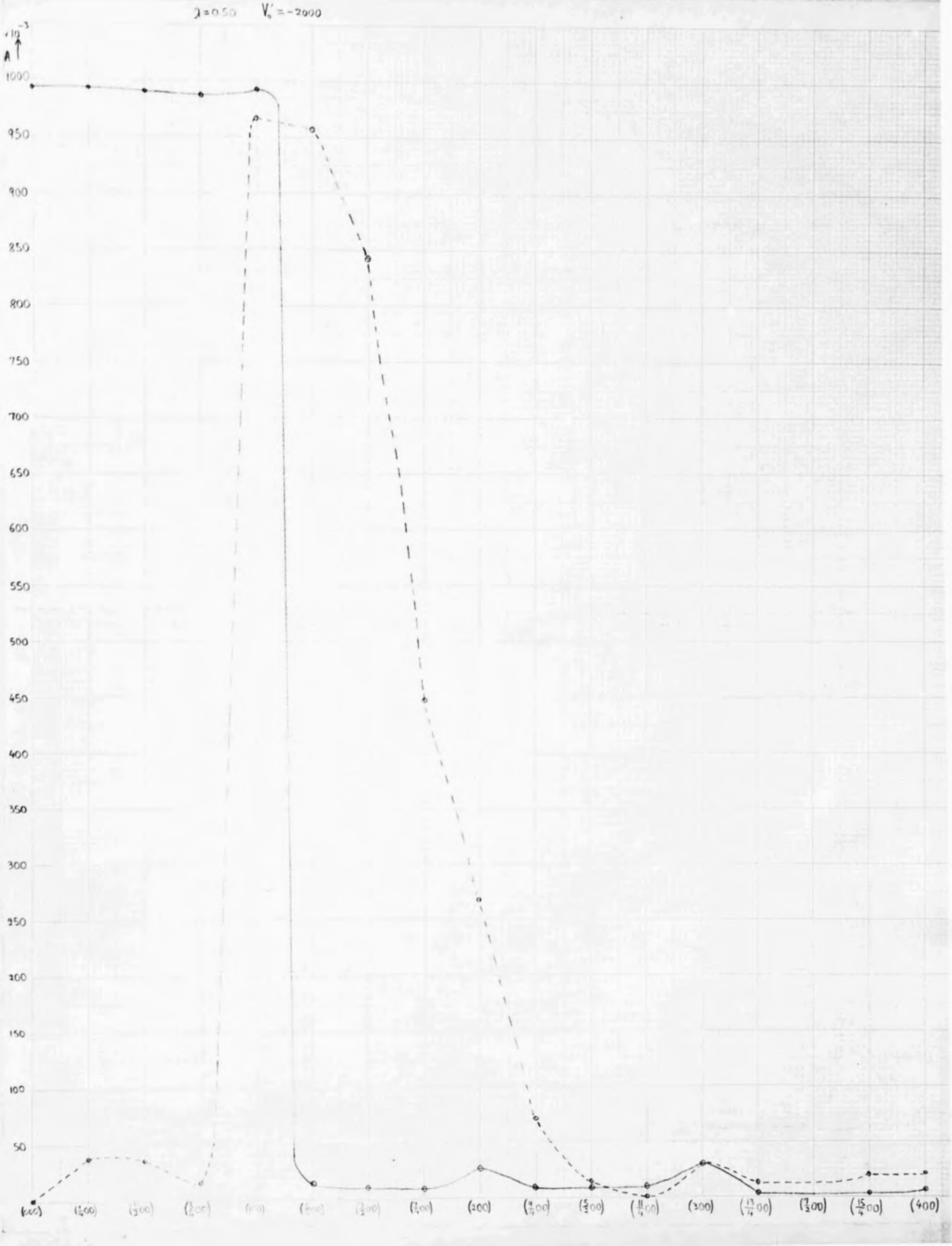
$\lambda = 0.25 \quad V_0' = -100$

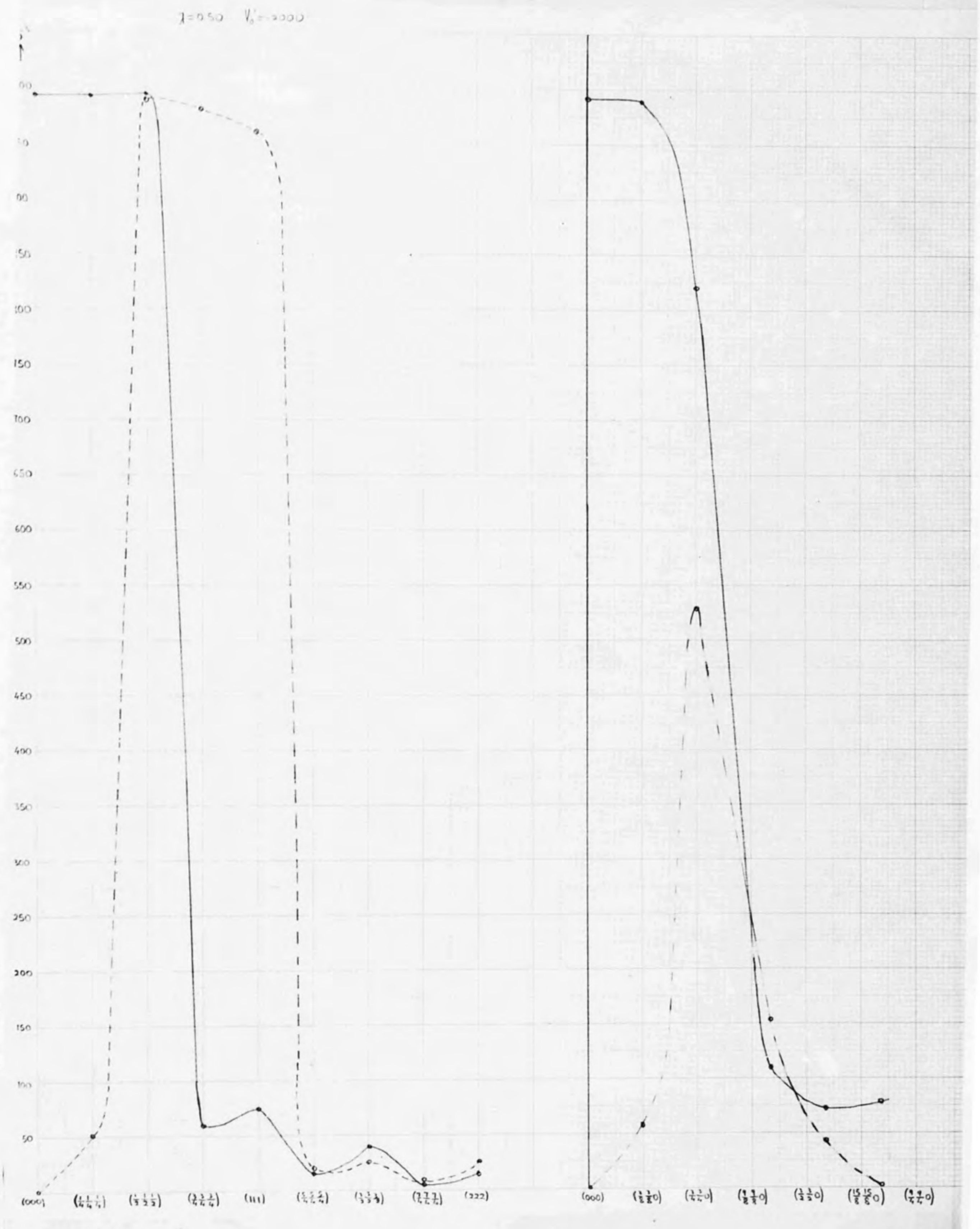





J=0.25 V₁=-100
1
2
3


J=0.16 $V_0'=-500$
$\times 10^3$
A
1000
950
900
850
800
750
700
650
600
550
500
450
400
350
300
250
200
150
100
50
1
2
1
(000)
$(\frac{1}{4}\frac{1}{4}\frac{1}{4})$
$(\frac{1}{2}\frac{1}{2}\frac{1}{2})$
$(\frac{3}{4}\frac{3}{4}\frac{3}{4})$
(111)
$(\frac{5}{4}\frac{5}{4}\frac{5}{4})$
$(\frac{3}{2}\frac{3}{2}\frac{3}{2})$
$(\frac{7}{4}\frac{7}{4}\frac{7}{4})$
(222)
1
2
(000)
$(\frac{3}{8}\frac{3}{8}0)$
$(\frac{3}{4}\frac{3}{4}0)$
$(\frac{9}{8}\frac{9}{8}0)$
$(\frac{3}{2}\frac{3}{2}0)$
$(\frac{15}{8}\frac{15}{8}0)$
$(\frac{9}{4}\frac{9}{4}0)$
$(\frac{21}{8}\frac{21}{8}0)$
(330)


$\lambda = 0.50$ $V_0' = -2000$
$\times 10^{-3}$
A
1000
950
900
850
800
750
700
650
600
550
500
450
400
350
300
250
200
150
100
50
(000)
($\frac{1}{4}$00)
($\frac{1}{2}$00)
($\frac{3}{4}$00)
(100)
($\frac{5}{4}$00)
($\frac{3}{2}$00)
($\frac{7}{4}$00)
(200)
($\frac{9}{4}$00)
($\frac{5}{2}$00)
($\frac{11}{4}$00)
(300)
($\frac{13}{4}$00)
($\frac{7}{2}$00)
($\frac{15}{4}$00)
(400)


$\lambda = 0.50$ $V_0' = -2000$
900
850
800
750
700
650
600
550
500
450
400
350
300
250
200
150
100
50
(000)
$(\frac{1}{4}\frac{1}{4}\frac{1}{4})$
$(\frac{1}{2}\frac{1}{2}\frac{1}{2})$
$(\frac{3}{4}\frac{3}{4}\frac{3}{4})$
(111)
$(\frac{5}{4}\frac{5}{4}\frac{5}{4})$
$(\frac{3}{2}\frac{3}{2}\frac{3}{2})$
$(\frac{7}{4}\frac{7}{4}\frac{7}{4})$
(222)
(000)
$(\frac{3}{8}\frac{3}{8}0)$
$(\frac{3}{4}\frac{3}{4}0)$
$(\frac{9}{8}\frac{9}{8}0)$
$(\frac{3}{2}\frac{3}{2}0)$
$(\frac{15}{8}\frac{15}{8}0)$
$(\frac{9}{4}\frac{9}{4}0)$

MOMENTUM EIGENFUNCTIONS

	$\lambda=0.25$ $V_0'=-100$		$\lambda=0.25$ $V_0'=-500$		$\lambda=0.50$ $V_0'=-2000$	
(xoo)	1st band	2nd band	1st band	2nd band	1st band	2nd band
(000)	0.99896	0	0.97474	0	0.99247	0
($\frac{1}{4}$00)	0.99887	0.03565	0.97257	0.13327	0.99226	0.03668
($\frac{1}{2}$00)	0.99856	0.03986	0.96356	0.18736	0.99093	0.03126
($\frac{3}{4}$00)	0.99755	0.03252	0.93319	0.26594	0.98802	0.01564
(100)	0.99224	0.99947	0.89652	0.98506	0.99341	0.96713
($\frac{5}{4}$00)	0.02289	0.98451	0.15920	0.85622	0.01422	0.95728
($\frac{3}{2}$00)	0.01082	0.67679	0.07243	0.69226	0.01070	0.84208
($\frac{7}{4}$00)	0.00694	0.16449	0.04292	0.46940	0.00919	0.44784
(200)	0.01236	0.11688	0.07009	0.38260	0.02673	0.26828
($\frac{9}{4}$00)	0.00390	0.01648	0.01998	0.10247	0.01028	0.07097
($\frac{5}{2}$00)	0.00315	0.00818	0.01377	0.04890	0.00972	0.01369
($\frac{11}{4}$00)	0.00257	0.00218	0.00791	0.02516	0.00965	0.00061
(300)	0.00717	0.00086	0.03328	0.01068	0.03032	0.03048
($\frac{13}{4}$00)			0.00677	0.00349	0.00293	0.01332
($\frac{7}{2}$00)			0.00521	0.00436		
($\frac{15}{4}$00)			0.00403	0.00892	0.00246	0.02063
(400)			0.00789	0.01068	0.00565	0.02156

MOMENTUM EIGENFUNCTIONS

	$\lambda = 0.25$ $V_0' = -100$		$\lambda = 0.25$ $V_0' = -500$		$\lambda = 0.50$ $V_0' = -2000$	
(xx0)	1st band	2nd band	1st band	2nd band	1st band	2nd band
(000)	0.99896	0	0.97474	0	0.99247	0
$(\frac{3}{8}\frac{3}{8}0)$	0.99839	0.04307	0.96088	0.20582	0.98974	0.05687
$(\frac{3}{4}\frac{3}{4}0)$	0.63616	0.77038	0.58236	0.78703	0.82069	0.52979
$(\frac{5}{4}\frac{5}{4}0)$	0.01776	0.02926	0.07954	0.16344	0.11156	0.15290
$(\frac{13}{8}\frac{13}{8}0)$	0.00355	0.01860	0.00958	0.09637	0.07252	0.04253
(220)	0.00821	0.01869	0.03680	0.08678		
$(\frac{19}{8}\frac{19}{8}0)$			0.00883	0.00198		
$(\frac{11}{4}\frac{11}{4}0)$			0.00542	0.00489		
(xxx)						
(000)	0.99896	0	0.97474	0	0.99247	0
$(\frac{1}{4}\frac{1}{4}\frac{1}{4})$	0.99862	0.03108	0.96634	0.15970	0.99141	0.05126
$(\frac{1}{2}\frac{1}{2}\frac{1}{2})$	0.99836	0.99924	0.96770	0.97942	0.99347	0.98668
$(\frac{3}{4}\frac{3}{4}\frac{3}{4})$	0.03008	0.99724	0.14718	0.93907	0.05899	0.97942
(111)	0.04221	0.99296	0.20292	0.91972	0.07458	0.95952
$(\frac{5}{4}\frac{5}{4}\frac{5}{4})$	0.00974	0.00687	0.04265	0.06408	0.01354	0.01970
$(\frac{3}{2}\frac{3}{2}\frac{3}{2})$	0.00233	0.01499	0.00484	0.08850	0.04054	0.02425
$(\frac{7}{4}\frac{7}{4}\frac{7}{4})$	0.00176	0.00579	0.00895	0.02600	0.00591	0.00698
(222)	0.00380		0.02082	0.00705	0.01522	0.02569

7. Discussion on the "Momentum Eigenfunction" graphs

The momentum eigenfunctions A (k) are plotted for the first and second bands along the directions (100) (110), and (111). The idea of the extended zone scheme is used so that results corresponding to the first, second and third Brillouin Zones are included.

We now explain how we choose the required values of the momentum eigenfunctions fromthe results obtained by the computer.

The solutions are given by the computer as follows:

Γ_1 (000) 7 × 7 matrix

E_0

$A_0(000)$ $A_0(111)$ $A_0(200)$ $A_0(220)$ $A_0(311)$ $A_0(222)$ $A_0(400)$

E_1

$A_1(000)$ $A_1(111)$ $A_1(200)$ $A_1(220)$ $A_1(311)$ $A_1(222)$ $A_1(400)$

etc.

Δ_1 ($\frac{1}{4}$00) 16 x 16 matrix

E_0

$A_0(\frac{1}{4}00)$ $A_0(\frac{3}{4}11)$ $A_0(7/400)$ $A_0(5/411)$ $A_0(\frac{1}{4}20)$ $A_0(9/400)$ etc.

E_1

$A_1(\frac{1}{4}00)$ $A_1(\frac{3}{4}11)$ $A_1(7/400)$ $A_1(5/411)$ $A_1(\frac{1}{4}20)$ $A_1(9/400)$ etc.

etc.

$\underline{\Delta_1(\frac{1}{2}00)}$ 16 x 16 matrix

E_0

$A_0(\frac{1}{2}00)$ $A_0(\frac{1}{2}11)$ $A_0(3/200)$ $A_0(3/211)$ $A_0(\frac{1}{2}20)$ $A_0(5/200)$ etc.

E_1

$A_1(\frac{1}{2}00)$ $A_1(\frac{1}{2}11)$ $A_1(3/200)$ $A_1(3/211)$ $A_1(\frac{1}{2}20)$ $A_1(5/200)$ etc.

etc.

$\underline{\Delta_1(\frac{3}{4}00)}$ 16 x 16 matrix

E_0

$A_0(\frac{3}{4}00)$ $A_0(\frac{1}{4}11)$ $A_0(5/400)$ $A_0(7/411)$ $A_0(\frac{3}{4}20)$ $A_0(11/400)$ etc.

E_1

$A_1(\frac{3}{4}00)$ $A_1(\frac{1}{4}11)$ $A_1(5/400)$ $A_1(7/411)$ $A_1(\frac{3}{4}20)$ $A_1(11/400)$ etc.

etc.

$\underline{X_1(100)}$ 8 x 8 matrix

E_0

$A_0(100)$ $A_0(011)$ $A_0(120)$ $A_0(211)$ $A_0(300)$ etc.

E_1

$A_1(100)$ $A_1(011)$ $A_1(120)$ $A_1(211)$ $A_1(300)$ etc.

etc.

Suppose that we want to plot A v. $\underline{k}$ along the (100) - Direction for the first band. From Γ_1 we obtain the values $A_0(000)$, $A_0(200)$ $A_0(400)$; from $\Delta_1(\frac{1}{4}00)$ the values $A_0(\frac{1}{4}00)$, $A_0(7/400)$, $A_0(9/400)$; from $\Delta_1(\frac{1}{2}00)$ the values $A_0(\frac{1}{2}00)$, $A_0(3/200)$; $A_0(5/200)$; from $\Delta_1(\frac{3}{4}00)$ the values

$A_0(300)$, $A_0(5/400)$, $A_0(11/400)$; and from $X_1(100)$ the values $A_0(100)$, $A_0(300)$.

Following this procedure we constructed the table of pages 147, 148 and plotted the graphs on which we now comment.

(100) - direction

(a) $\lambda = 0.25 \quad V_0' = -100$

For the first band at k=o the momentum eigenfunction has a maximum which is nearly equal to the normalizing factor 1. A (k) decreases slightly approaching the end of the first Brillouin Zone. Entering the second B.Z. the momentum eigenfunction drops to very small values. The decrease of A continues in the higher Zones but we observe secondary maxima at the boundaries of the Zones.

In the second band the momentum eigenfunction increases from 0 at k = 0 to a maximum of approximately 1 just outside the first zone. Then A decreases smoothly tending to zero. A secondary maximum appears in the middle of the first zone.

(b) $\lambda = 0.25 \quad V_0' = -500$

For the first band the increase of the potential causes a more noticeable decrease of the momentum eigenfunction within the first zone. Also the fall to small values in the second zone is now smoother.

For the second band the rise from 0 to the maximum and then the fall to small values are smoother than in the previous case.

(c) $\lambda = 0.50 \quad V_0' = -2000$

These parameters give graphs very similar to the case (a). There is only one difference to be mentioned; due to the interchange of the levels X_1, X_4' (shown in the energy graphs) we have for the first band a maximum at k = (100) instead of k = 0.

Other directions

Observation of the graphs for the (111) direction reveals the same general pattern as in the (100) - direction confirming that our calculations are near to the free-electron limit.

In the (110) - direction, we observe a striking difference. We see that the maximum of the second band does not approach unity, but it is much lower.

Finally, it is interesting to notice the similarity of our graphs with graphs plotted for one-dimensional cases (Slater 1952, Papaconstantopoulos 1963).

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