QUANTITATIVE STUDIES

IN THE

THERMAL SCATTERING OF X RAYS

BY CRYSTALS

Thesis submitted by

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Introduction

The purpose of this paper is the calculation of the thermal scattering of X-rays. The theory of this effect has been given by its discoverer Laval (1938/39,1942) and by several other physicists. A condensed representation of the theory appears in 'Reports on progress in physics' (Born,1943). The present paper will follow the methods of this Report and in Sections 1 and 2 a summary of the principal definitions and formulae is included.

The main point is that the scattering power of a crystal is not expressed in terms of the frequencies, as in all the other papers quoted, but directly in terms of the "dynamical matrix" of the lattice, which is defined as a system of the coefficients of the potential energy for small displacements. H. A. Jahn (1941/2) has shown that for observations fairly close to Laue-Bragg reflections only the limiting case of this matrix is needed, which corresponds to the ordinary theory of elasticity. Here we shall treat the general case numerically for one example (the face-centred cubic lattice) and outline it in another (the hexagonal close-packed lattice), but in the latter case numerical calculations are only made for the Jahn approximation.

It is the intention of this paper to avoid arbitrary assumptions about atomic forces, particularly the

assumption of central forces between the atoms. Now the dependence of the elastic constants on the atomic forces has been developed by Professor Born in his first book, "Dynamik der Krystallgitter", for this general case, but the formulae are not quite in order. In his second book,"Atomtheorie des festen Zustandes", he has restricted himself to the use of central forces. Hence it was necessary to reconsider these formulae and this is done in Section 3 for a general lattice. The two following Sections contain a specialisation to the face-centred cubic and the hexagonal close-packed lattices.

Section 6 discusses the method of representing the scattering power in reciprocal space. In Sections 7 and 8 this is applied to the two particular lattices under consideration.

Notation

Throughout this paper the components of the vectors and tensors which occur are expressed in a rectangular system of axes. Consequently the distinction between covariant and contravariant indices is a purely formal one and for simplicity all co-ordinate indices are written in the lower position.

Vectors will be distinguished by a bar underneath the symbols, and the signs . and $\wedge$ will be used to denote the scalar and the vector product respectively.

The asterisk * is used for the complex conjugate.

CHAPTER I

OUTLINE OF THE THERMAL THEORY

Section 1 Lattice dynamics

Let $\underline{a}^1$, $\underline{a}^2$, $\underline{a}^3$, be the three elementary vectors of the lattice cell, so that the position vectors of particles at the vertices of the cells are:-

$$\underline{r}\begin{pmatrix} l \\ \cdots \end{pmatrix} = l^1\underline{a}^1 + l^2\underline{a}^2 + l^3\underline{a}^3 \tag{1.1}$$

where l^1 , l^2 , l^3 , are integers.

If there are n particles in each cell with masses m_k ($k = 1,2,\ldots\ldots n$) and if the position with respect to a cell of an atom is indicated by the vector $\underline{r}\begin{pmatrix} \cdots \\ k \end{pmatrix}$, then

$$\underline{r}\begin{pmatrix} l \\ k \end{pmatrix} = \underline{r}\begin{pmatrix} l \\ \cdots \end{pmatrix} + \underline{r}\begin{pmatrix} \cdots \\ k \end{pmatrix} \tag{1.2}$$

defines the position of the particle in equilibrium. In a rectangular system of axes S, fixed in space, let $\underline{r}\begin{pmatrix} l \\ k \end{pmatrix}$ have the components $x_1\begin{pmatrix} l \\ k \end{pmatrix}$, $x_2\begin{pmatrix} l \\ k \end{pmatrix}$, $x_3\begin{pmatrix} l \\ k \end{pmatrix}$.

Cyclic boundary conditions.

In all the work that follows the postulate of the "cyclic lattice" (Born 1923) is assumed. That is to say, a finite portion of the infinite lattice is taken and boundary conditions of a cyclic type are applied to this portion. The effect of this on summations over points of the lattice will be stated here at once as it is very much used in later Sections. Consider the

summation $\sum_{\ell}\sum_{\ell'} f(\ell-\ell')$, where $f(\ell-\ell')$ is a function of the differences of the cell indices. Then the inner summation over ℓ' is taken to be infinite so that $\sum_{\ell'} f(\ell-\ell')$ is independent of ℓ'. The outer summation is taken over the finite portion of the lattice which contains, say, N cells. Thus :

$$(1.3) \qquad \sum_{\ell}\sum_{\ell'} f(\ell-\ell') = N\sum_{\ell'} f(\ell-\ell') = N\sum_{\ell} f(\ell)$$

After an arbitrary displacement of the particles they will take up, say, the positions $\underline{r}\binom{\ell}{k} + \underline{u}\binom{\ell}{k}$, where $\underline{u}\binom{\ell}{k}$ has components $u_1\binom{\ell}{k}$, $u_2\binom{\ell}{k}$, $u_3\binom{\ell}{k}$, in S. (Hereafter the lower indices 1, 2, 3, will always refer to this rectangular system S). Then the potential energy Φ, which is a function of all coordinates, can be expanded in powers of the displacements $\underline{u}\binom{\ell}{k}$, and the second order terms of this expansion give

$$(1.4) \qquad \Phi_2 = \frac{1}{2}\sum_{\ell,k}\sum_{\ell',k'}\sum_{\alpha,\beta}\Phi_{\alpha\beta}\binom{\ell\ell'}{kk'} u_\alpha\binom{\ell}{k} u_\beta\binom{\ell'}{k'}$$

where

$$(1.5) \qquad \Phi_{\alpha\beta}\binom{\ell\ell'}{kk'} = \left[\frac{\partial^2\Phi}{\partial x_\alpha\binom{\ell}{k}\,\partial x_\beta\binom{\ell'}{k'}}\right] \text{(in equilibrium)}$$

and α and β run through 1, 2, 3.

These symbols posses the following properties:-

(1) By their definition they satisfy the symmetry law:

$$\Phi_{\alpha\beta}\begin{pmatrix} \ell\ell' \\ kk' \end{pmatrix} = \Phi_{\beta\alpha}\begin{pmatrix} \ell'\ell \\ k'k \end{pmatrix} \tag{1.6}$$

(2) Owing to the periodicity of the lattice, the indices ℓ and ℓ' enter into the symbols only in the combination $\ell - \ell'$, and accordingly a modification is introduced and one writes

$$\Phi_{\alpha\beta}\begin{pmatrix} \ell\ell' \\ kk' \end{pmatrix} = \Phi_{\alpha\beta}\begin{pmatrix} \ell-\ell' \\ kk' \end{pmatrix} \tag{1.7}$$

(3) For the later work it is more convenient to deal with quantities $D_{\alpha\beta}\begin{pmatrix} \ell-\ell' \\ kk' \end{pmatrix}$ defined by

$$D_{\alpha\beta}\begin{pmatrix} \ell-\ell' \\ kk' \end{pmatrix} = \frac{1}{\sqrt{m_k m_{k'}}} \Phi_{\alpha\beta}\begin{pmatrix} \ell-\ell' \\ kk' \end{pmatrix} \tag{1.8}$$

Clearly they satisfy

$$D_{\alpha\beta}\begin{pmatrix} \ell-\ell' \\ kk' \end{pmatrix} = D_{\beta\alpha}\begin{pmatrix} \ell'-\ell \\ k'k \end{pmatrix} \tag{1.9}$$

(4) The $D_{\alpha\beta}\begin{pmatrix} \ell-\ell' \\ kk' \end{pmatrix}$ are the elements of the so-called "dynamical matrix" of the lattice. They may be collected together into sub-matrices which form a condensed representation suitable for manipulating. This may be done in the following way: Firstly matrices of order (3 x 3) can be formed :-

$$(1.10) \qquad \mathcal{D}\binom{\ell-\ell'}{kk'} = \begin{bmatrix} \mathcal{D}_{11}\binom{\ell-\ell'}{kk'} & \mathcal{D}_{12}\binom{\ell-\ell'}{kk'} & \mathcal{D}_{13}\binom{\ell-\ell'}{kk'} \\ \mathcal{D}_{21}\binom{\ell-\ell'}{kk'} & \mathcal{D}_{22}\binom{\ell-\ell'}{kk'} & \mathcal{D}_{23}\binom{\ell-\ell'}{kk'} \\ \mathcal{D}_{31}\binom{\ell-\ell'}{kk'} & \mathcal{D}_{32}\binom{\ell-\ell'}{kk'} & \mathcal{D}_{33}\binom{\ell-\ell'}{kk'} \end{bmatrix}.$$

and these in turn may be regarded as sub-matrices of larger matrices of order (3n x 3n) and having the form:

$$(1.11) \qquad \mathcal{D}(\ell-\ell') = \begin{bmatrix} \mathcal{D}\binom{\ell-\ell'}{11} & \mathcal{D}\binom{\ell-\ell'}{12} - - - \mathcal{D}\binom{\ell-\ell'}{1n} \\ \mathcal{D}\binom{\ell-\ell'}{21} & \mathcal{D}\binom{\ell-\ell'}{22} - - - \mathcal{D}\binom{\ell-\ell'}{2n} \\ - \; - \; - \; - \; - \; - \; - \\ \mathcal{D}\binom{\ell-\ell'}{n1} & \mathcal{D}\binom{\ell-\ell'}{n2} - - - \mathcal{D}\binom{\ell-\ell'}{nn} \end{bmatrix}$$

Equations of motion

Let a modified displacement vector $\upsilon\binom{\ell}{k} = \sqrt{m_k}\, u\binom{\ell}{k}$ be introduced; then (1.4) may be written as :-

$$(1.12) \qquad \overline{\Phi}_2 = \frac{1}{2} \sum_{\ell,k} \sum_{\ell',k'} \sum_{\alpha,\beta} \mathcal{D}_{\alpha\beta}\binom{\ell-\ell'}{kk'} \upsilon_\alpha\binom{\ell}{k} \upsilon_\beta\binom{\ell'}{k'}$$

The equations of motion:-

$$\ddot{\upsilon}_\alpha\binom{\ell}{k} = - \frac{\partial \overline{\Phi}_2}{\partial \upsilon_\alpha\binom{\ell}{k}}$$

become

$$\ddot{u}_\alpha\binom{l}{k} = -\sum_{l',k'} \sum_{\beta} D_{\alpha\beta}\binom{l\cdot l'}{k k'} u_\beta\binom{l'}{k'} \tag{1.13}$$

where a dot denotes differentiation with respect to time t.

If the cyclic boundary conditions (Born,1923, Ledermann, 1944) are taken into account, (1.13) may be solved by a plane wave with the frequency ω and wave-vector $\underline{q}$:-

$$\underline{u}\binom{l}{k} = \underline{U}(k)\, e^{-i\omega t}\, e^{i\left(\underline{q}\cdot \underline{r}\binom{l}{\cdots}\right)} \tag{1.14}$$

Substitute (1.14) in (1.13). Then, writing $\underline{r}\binom{l\cdot l'}{\cdots}$ for the difference $\underline{r}\binom{l}{\cdots} - \underline{r}\binom{l'}{\cdots}$, one has

$$\omega^2 U_\alpha(k) = \sum_{k',\beta} D_{\alpha\beta}\left(\frac{q}{k k'}\right) U_\beta(k') \tag{1.15}$$

where

$$D_{\alpha\beta}\left(\frac{q}{k k'}\right) = \sum_{l'} D_{\alpha\beta}\binom{l-l'}{k k'} e^{-i\left(\underline{q}\cdot \underline{r}\binom{l-l'}{\cdots}\right)} = \sum_{l} D_{\alpha\beta}\binom{l}{k k'} e^{-i\left(\underline{q}\cdot \underline{r}\binom{l}{\cdots}\right)} \tag{1.16}$$

This result can be obtained also (Born,1943) by the following considerations. Let

$$U(q,l) = (2\pi)^{-3/2}\, e^{-i\left(\underline{q}\cdot \underline{r}\binom{l}{\cdots}\right)}\, I \tag{1.17}$$

(where I is the unit matrix of order (3n x 3n))

be the matrix of a unitary transformation which is

applied to the dynamical matrix. The transformed dynamical matrix whose elements are

$$(1.18) \qquad \mathcal{D}_{\alpha\rho}\begin{pmatrix} \varrho\,\varrho' \\ k\,k' \end{pmatrix} = \sum_{\varrho,\varrho'} U(\varrho,\varrho)\, \mathcal{D}_{\alpha\rho}\begin{pmatrix} \varrho-\varrho' \\ k\,k' \end{pmatrix} U(\varrho',\varrho')$$

can be shown (op.cit.) to be diagonal in the sub-matrices $\mathcal{D}(\underline{\varrho})$ defined by (1.16). Hence this transformation when applied to the equations of motion leads to (1.15).

The quantities $\mathcal{D}_{\alpha\rho}\left(\frac{\varrho}{k\,k'}\right)$ are the elements of the new representation of the dynamical matrix in the Q-space. They may be gathered together in the same way as the $\mathcal{D}_{\alpha\rho}\left(\frac{\varrho-\varrho'}{k\,k'}\right)$ to give successively $\mathcal{D}\left(\frac{\varrho}{k\,k'}\right)$ of order (3 x 3), and $\mathcal{D}(\underline{\varrho})$ of order (3n x 3n).

Section 2 — X-ray scattering

Assume a beam of X-rays passing through the crystal and let $\underline{K}$ be the wave-vector of the incident beam, and let $\underline{K}'$ be the wave-vector of the scattered beam. Then if $\underline{K}-\underline{K}'=\underline{Q}$, it can be shown that the intensity power of the background (diffuse) scattering is

$$(2.1) \qquad \sigma_B = \sigma_0 N \sum_{\substack{k\lambda \\ k'\beta}} \mathcal{S}_{\lambda\beta}\left(\frac{Q}{kk'}\right) \mu_\lambda(k) \mu_\beta^*(k')$$

where $\mathcal{S}_{\lambda\beta}\left(\frac{Q}{kk'}\right)$ are the elements of the "scattering matrix":-

$$(2.2) \qquad \mathcal{S}(\underline{Q}) = k\,T\,[\mathcal{D}(\underline{Q})]^{-1} \quad (\text{approx.})$$

where k is Boltzmann's constant and T is the absolute temperature.

The other symbols have the following meanings:-

$$(2.3) \qquad \underline{\mu}(k) = (f_k/\sqrt{m_k})\, e^{i(\underline{Q}\cdot\underline{r}(k))}\,\underline{Q}$$

(2.4) f_k = modified scattering factor dependent on T.

(2.5) N = number of cells in the crystal.

(2.6) σ_0 = Thomson factor $= \left(\frac{e^2}{mc^2 r}\right)^2 \tfrac{1}{2}(1+\cos^2\chi)$.

(2.7)
- e = charge on electron.
- m = mass of electron.
- c = velocity of light.
- χ = angle of deflection of X-ray beam.
- r = distance of the small scattering volume from the point of observation.

CHAPTER II

CALCULATION OF THE DYNAMICAL MATRIX

Section 3 The calculation in general

There are two factors that enable relations to be established between the elements of the dynamical matrix: (1) The symmetry properties of the particular lattice considered, (Section 3a); (2) The fact that if the lattice is moved as a whole without distortion, the potential energy is independent of such motion, (Section 3b). If the assumption is added that only neighbouring atoms act on each other, the effect of these relations is that the dynamical matrix is expressible in terms of a (generally) small number of parameters.

There also exists a connection between the dynamical matrix and the elastic constants of the crystal. This may be obtained, either by assuming a homogeneous deformation, expressing Φ_1 in terms of the external and internal strain and eliminating the internal strain (Section 3c(A)), or by solving the equations of motion for long waves of the accoustical type (Section 3c(B)). The elastic constants may be considered as measurable quantities and their values are known in some cases.

For crystals of fairly simple symmetry, the above information is sufficient to determine the elements of the dynamical matrix completely.

Once the dynamical matrix is known in the ℓ representation, it can be transformed to the $\mathfrak{A}$ representation with the help of (1.16)

Section 3a Symmetry of the lattice

In order to find the relations that exist between the elements of the dynamical matrix, all those symmetry operations are applied to the lattice which will bring it into self-coincidence. The number and nature of these operations are found by a consideration of the space-group of the lattice. They comprise rotations, reflections, glide-planes and combinations of these. Translations which consist of multiples of the base vectors have already been taken into account by assuming that the dynamical matrix $\mathcal{D}\binom{l-l'}{k\,k'}$ only depends on the combination $l-l'$, and not on l and l' separately.

Consider the rectangular system of axes S in which a point of space has the co-ordinates x_α ($\alpha = 1, 2, 3$). Let a transformation T act on these axes so that they take up a new position, and in this transformed system let the point have the co-ordinates x_β ($\beta = 1, 2, 3$). Then relations will hold of the form:-

$$x_\alpha = \sum_\beta T_{\alpha\beta}\, x_\beta \tag{3.1}$$

The coefficients $T_{\alpha\beta}$ depend on the particular transformation chosen. If the point x_α is taken to be a lattice-point, then (3.1) becomes:-

$$x_\alpha\binom{l}{k} = \sum_\beta T_{\alpha\beta}\, x_\beta\binom{l}{k} \tag{3.2}$$

Let T now be a symmetry operation of the lattice, then it will be possible to find a point of the lattice $\binom{L}{K}$ say, such that :-

$$x_\alpha\binom{l}{k} = x_A\binom{L}{K} \qquad (3.3)$$

for $\alpha = A = 1$ or 2 or 3.

A combination of (3.2) and (3.3) gives

$$x_A\left(\tfrac{L}{K}\right) = \sum_A T_{\alpha A}\, x_A\binom{l}{k} \qquad (3.4)$$

If the symbol T stands for the matrix formed from the quantities $T_{\alpha A}$ ordered according to their suffices, so that $T \equiv [T_{\alpha A}]$, then (3.4) can be written in the matrix form:-

$$\underline{r}\left(\tfrac{L}{K}\right) = T\,\underline{r}\left(\tfrac{l}{k}\right) \qquad (3.5)$$

The elements $\Phi_{\alpha\beta}\binom{l-l'}{k\,k'}$ of the dynamical matrix behave, with respect to the suffices α and β, as a covariant tensor of rank two. Their transformation law will be

$$\Phi_{\alpha\beta}\binom{l-l'}{k-k'} = \sum_{A,B} T_{\alpha A}\, T_{\beta B}\, \Phi_{AB}\binom{l-l'}{k\,k'} \qquad \left.\begin{matrix} A \\ B \end{matrix}\right\} = 1,2,3. \qquad (3.6)$$

Now points $\left(\tfrac{L}{K}\right)$ and $\left(\tfrac{L'}{K'}\right)$ can be found such that :-

$$\Phi_{\alpha\beta}\binom{l-l'}{k\,k'} = \Phi_{AB}\binom{L-L'}{K\,K'} \qquad (3.7)$$

where $\begin{cases} \alpha = A = 1 \text{ or } 2 \text{ or } 3 \\ \beta = B = 1 \text{ or } 2 \text{ or } 3. \end{cases}$

Hence

$$\underline{\Phi}_{\alpha\beta}\begin{pmatrix} l-l' \\ k\,k' \end{pmatrix} = \sum_{A,B} T_{\alpha A}\, T_{\beta B}\, \underline{\Phi}_{AB}\begin{pmatrix} \rho-\rho' \\ k\,k' \end{pmatrix} \tag{3.8}$$

or, in matrix notation:-

$$\underline{\Phi}\begin{pmatrix} l-l' \\ k\,k' \end{pmatrix} = T\,\underline{\Phi}\begin{pmatrix} \rho-\rho' \\ k\,k' \end{pmatrix}\tilde{T} \tag{3.9}$$

where $\tilde{T}$ is the transpose of the matrix T, and the change from $\begin{pmatrix} \rho \\ k \end{pmatrix}$ to $\begin{pmatrix} l \\ k \end{pmatrix}$ and from $\begin{pmatrix} \rho' \\ k' \end{pmatrix}$ to $\begin{pmatrix} l' \\ k' \end{pmatrix}$ is to be obtained from (3.4) or (3.5).

Section 3b Rigid motion

If the crystal lattice is moved as a whole without distortion, the displacements $\underline{u}\binom{l}{k}$ of the particles will be a combination of translations and rotations. The latter may be taken as infinitesimal without loss of generality. Let them

$$u_\alpha\binom{l}{k} = t_\alpha + \sum_\lambda \omega_{\alpha\lambda} x_\lambda \binom{l}{k} \tag{3.10}$$

where

t_α = translational part of displacement. (3.11)

$\sum_\lambda \omega_{\alpha\lambda} x_\lambda \binom{l}{k}$ = rotational part of displacement. (3.12)

$\omega_{\alpha\lambda} = -\omega_{\lambda\alpha}$ (for an infinitesimal rotation). (3.13)

The condition that this displacement should have no effect on the potential energy Φ is given by the two equations:-

$$\frac{\partial}{\partial t_\alpha}\Phi = 0 \tag{3.14}$$

$$\frac{\partial}{\partial \omega_{\alpha\lambda}}\Phi = 0 \tag{3.15}$$

Or, writing these in terms of derivatives with respect to the co-ordinates:-

$$(3.16) \qquad \sum_{\ell,k} \frac{\partial}{\partial x_\alpha\left(\begin{smallmatrix}\ell\\k\end{smallmatrix}\right)} \Phi = 0$$

$$(3.17) \qquad \sum_{\ell,k} \left\{ x_\gamma\left(\begin{smallmatrix}\ell\\k\end{smallmatrix}\right) \frac{\partial}{\partial x_\alpha\left(\begin{smallmatrix}\ell\\k\end{smallmatrix}\right)} - x_\alpha\left(\begin{smallmatrix}\ell\\k\end{smallmatrix}\right) \frac{\partial}{\partial x_\gamma\left(\begin{smallmatrix}\ell\\k\end{smallmatrix}\right)} \right\} \Phi = 0$$

In order to find what these imply for the second order derivatives $\Phi_{\alpha\beta}\left(\begin{smallmatrix}\ell-\ell'\\k\,k'\end{smallmatrix}\right)$, the equations must be differentiated again and then taken at the equilibrium position.

Firstly, differentiate (3.16) with respect to $x_\beta\left(\begin{smallmatrix}\ell'\\k'\end{smallmatrix}\right)$ and take the equilibrium value, then :-

$$(3.18) \qquad \sum_{\ell,k} \Phi_{\alpha\beta}\left(\begin{smallmatrix}\ell-\ell'\\k\,k'\end{smallmatrix}\right) = 0$$

It would have been equally possible to have taken (3.16) with ℓ', k', β, written instead of ℓ, k, α, and differentiated with respect to $x_\alpha\left(\begin{smallmatrix}\ell\\k\end{smallmatrix}\right)$, in which case the result would have been the corresponding equation;

$$(3.19) \qquad \sum_{\ell',k'} \Phi_{\alpha\beta}\left(\begin{smallmatrix}\ell-\ell'\\k\,k'\end{smallmatrix}\right) = 0$$

The last equation may also be obtained from (3.18) by the use of (1.6) and a change of indices.

Secondly, differentiation of (3.17) with respect to $x_\beta\left(\begin{smallmatrix}\ell'\\k'\end{smallmatrix}\right)$ gives:-

$$\sum_{\ell,k} \left\{ x_\gamma\left(\begin{smallmatrix}\ell\\k\end{smallmatrix}\right) \frac{\partial^2}{\partial x_\alpha\left(\begin{smallmatrix}\ell\\k\end{smallmatrix}\right) \partial x_\beta\left(\begin{smallmatrix}\ell'\\k'\end{smallmatrix}\right)} - x_\alpha\left(\begin{smallmatrix}\ell\\k\end{smallmatrix}\right) \frac{\partial^2}{\partial x_\gamma\left(\begin{smallmatrix}\ell\\k\end{smallmatrix}\right) \partial x_\beta\left(\begin{smallmatrix}\ell'\\k'\end{smallmatrix}\right)} \right\} \Phi + \sum_{\ell,k} \delta_{\ell\ell'} \delta_{kk'} \left\{ \delta_{\beta\gamma} \frac{\partial \Phi}{\partial x_\alpha\left(\begin{smallmatrix}\ell\\k\end{smallmatrix}\right)} - \delta_{\alpha\beta} \frac{\partial \Phi}{\partial x_\gamma\left(\begin{smallmatrix}\ell\\k\end{smallmatrix}\right)} \right\} = 0$$

where δ_{ij} is the usual Kronecker delta which vanishes unless i and j are equal in which case it has the value unity. But in the last equation the third and forth terms on the left-hand side vanish by (3.16). Hence in equilibrium:-

$$(3.20) \qquad \sum_{l,k} \Phi_{\alpha\beta}\begin{pmatrix} l-l' \\ k\,k' \end{pmatrix} x_\lambda\begin{pmatrix} l \\ k \end{pmatrix} = \sum_{l,k} \Phi_{\lambda\beta}\begin{pmatrix} l-l' \\ k\,k' \end{pmatrix} x_\alpha\begin{pmatrix} l \\ k \end{pmatrix}$$

Again it would have been possible to have written (3.17) with l', k', β, μ, instead of l, k, α, λ, and differentiated with respect to $x_\alpha\begin{pmatrix} l \\ k \end{pmatrix}$ instead of $x_\beta\begin{pmatrix} l' \\ k' \end{pmatrix}$. This would have given, as the equation corresponding to (3.20),

$$(3.21) \qquad \sum_{l',k'} \Phi_{\alpha\beta}\begin{pmatrix} l-l' \\ k\,k' \end{pmatrix} x_\mu\begin{pmatrix} l' \\ k' \end{pmatrix} = \sum_{l',k'} \Phi_{\alpha\mu}\begin{pmatrix} l-l' \\ k\,k' \end{pmatrix} x_\beta\begin{pmatrix} l' \\ k' \end{pmatrix}$$

The equation (3.21) may also be obtained immediately from (3.20) by a change of indices and the application of (1.6).

The equations (3.18),(3.19),(3.20),(3.21), expressing the fact that the potential energy is independent of rigid motion of the lattice, are not however complete since the summations involved are infinite and no mention has yet been made of end-conditions. The form in which these relations are actually used will be developed in the course of the next Section.

Section 3c(A) Homogeneous deformations and the elastic constants

Expansion of Φ_2 for a homogeneous deformation

Such a deformation will give rise to a displacement of the form:-

$$u_\alpha\left(\begin{matrix}\ell\\k\end{matrix}\right) = u_\alpha(k) + \sum_\lambda u_{\alpha\lambda} x_\lambda\left(\begin{matrix}\ell\\k\end{matrix}\right) \tag{3.22}$$

where the $u_\alpha(k)$ are the internal strain components.
and the $u_{\alpha\lambda}$ are the external strain components.

Substitute (3.22) and a similar expression for $u_\beta\left(\begin{matrix}\ell'\\k'\end{matrix}\right)$, with μ as summation index, in (1.4). Then

$$\Phi_2 = \Phi_2^A + \Phi_2^B + \Phi_2^C \tag{3.23}$$

where

$$\Phi_2^A = \tfrac{1}{2}\sum_{\ell,k}\sum_{\ell',k'}\sum_{\alpha,\beta}\Phi_{\alpha\beta}\left(\begin{matrix}\ell-\ell'\\k\,k'\end{matrix}\right) u_\alpha(k)\, u_\beta(k') \tag{3.24}$$

$$\Phi_2^B = \tfrac{1}{2}\sum_{\ell,k}\sum_{\ell',k'}\sum_{\alpha,\beta}\sum_{\lambda,\mu}\Phi_{\alpha\beta}\left(\begin{matrix}\ell-\ell'\\k\,k'\end{matrix}\right) x_\lambda\left(\begin{matrix}\ell\\k\end{matrix}\right) x_\mu\left(\begin{matrix}\ell'\\k'\end{matrix}\right) u_{\alpha\lambda}\, u_{\beta\mu} \tag{3.25}$$

$$\Phi_2^C = \tfrac{1}{2}\sum_{\ell,k}\sum_{\ell',k'}\sum_{\alpha,\beta}\Phi_{\alpha\beta}\left(\begin{matrix}\ell-\ell'\\k\,k'\end{matrix}\right)\Big[\sum_\mu u_{\beta\mu}\, x_\mu\left(\begin{matrix}\ell'\\k'\end{matrix}\right) u_\alpha(k) + \sum_\lambda u_{\alpha\lambda}\, x_\lambda\left(\begin{matrix}\ell\\k\end{matrix}\right) u_\beta(k')\Big] \tag{3.26}$$

$$= \sum_{l,k} \sum_{l',k'} \sum_{\alpha,\beta,\mu} \Phi_{\alpha\beta}\begin{pmatrix} l\,l' \\ k\,k' \end{pmatrix} x_\mu\begin{pmatrix} l' \\ k' \end{pmatrix} u_{\beta\mu}\, u_\alpha(k)$$

by changing indices in the second term.

As a consequence of the results established in Section 3b it can now be shown that the expressions (3.24), (3.25), (3.26) depend only on the differences of the internal strain components and on the symmetric part of the external strain components and not on these quantities themselves. In order to do this, put

(3.27) $$u_{\alpha\lambda} = e_{\alpha\lambda} + \omega_{\alpha\lambda}$$

where

(3.28) $$e_{\alpha\lambda} = \tfrac{1}{2}(u_{\alpha\lambda} + u_{\lambda\alpha}) = e_{\lambda\alpha}$$

(3.29) $$\omega_{\alpha\lambda} = \tfrac{1}{2}(u_{\alpha\lambda} - u_{\lambda\alpha}) = -\omega_{\lambda\alpha}$$

and let, say

(3.30) $$e_\alpha(k) = u_\alpha(k) - u_\alpha(1)$$

with similar expressions for $u_{\beta\mu}$ and $u_\beta(k')$.

$\underline{\Phi_2^A}$

Then

$$\Phi_2^A = \tfrac{1}{2} \sum_{l,k} \sum_{l',k'} \sum_{\alpha,\beta} \Phi_{\alpha\beta}\begin{pmatrix} l\,l' \\ k\,k' \end{pmatrix} \left[e_\alpha(k) + u_\alpha(1)\right] \left[e_\beta(k') + u_\beta(1)\right]$$

$$= \tfrac{1}{2} \sum_{l,k} \sum_{l',k'} \sum_{\alpha,\beta} \Phi_{\alpha\beta}\binom{l-l'}{kk'} e_\alpha(k)\, e_\beta(k')$$

by (3.18) and (3.19)

i.e.

(3.31) $$\underline{\Phi}_2^{\alpha} = \frac{N}{2} \sum_{k,k'} \sum_{\alpha,\beta} \begin{bmatrix} kk' \\ \alpha\beta \end{bmatrix} e_\alpha(k)\, e_\beta(k')$$

where

(3.32) $$\begin{bmatrix} kk' \\ \alpha\beta \end{bmatrix} = \frac{1}{N} \sum_{l,l'} \Phi_{\alpha\beta}\binom{l-l'}{kk'} = \sum_{l} \Phi_{\alpha\beta}\binom{l}{kk'}$$

by the cyclic boundary conditions (1.3)

These symbols satisfy the relations:-

(3.33) $$\begin{bmatrix} kk' \\ \alpha\beta \end{bmatrix} = \begin{bmatrix} k'k \\ \beta\alpha \end{bmatrix}$$ by (1.6)

(3.34) $$\sum_{k} \begin{bmatrix} kk' \\ \alpha\beta \end{bmatrix} = \sum_{k'} \begin{bmatrix} kk' \\ \alpha\beta \end{bmatrix} = 0$$ by (3.18) and (3.19)

The relations (3.34) embody the results of (3.18) and (3.19) and in practice replace them.

$\underline{\Phi}_2^{\beta}$

If α and λ are interchanged in $\underline{\Phi}_2^{\beta}$ and the result added to the original expression, one has

$$\Phi_2^{\beta} = \tfrac{1}{4}\sum_{\ell,k}\sum_{\ell',k'}\sum_{\beta,\mu} x_\mu\binom{\ell'}{k'} u_{\beta\mu} \sum_{\alpha,\lambda}\left[u_{\alpha\lambda}\Phi_{\alpha\beta}\binom{\ell-\ell'}{k\,k'} x_\lambda\binom{\ell}{k} + u_{\lambda\alpha}\Phi_{\lambda\beta}\binom{\ell-\ell'}{k\,k'} x_\alpha\binom{\ell}{k}\right]$$

$$= \tfrac{1}{2}\sum_{\ell,k}\sum_{\ell',k'}\sum_{\beta,\mu} x_\mu\binom{\ell'}{k'} u_{\beta\mu} \sum_{\alpha,\lambda} e_{\alpha\lambda}\Phi_{\alpha\beta}\binom{\ell-\ell'}{k\,k'} x_\lambda\binom{\ell}{k}$$

by (3.20) and (3.28)

If, in this, β and μ are interchanged and the result added to the original expression, one has

$$\Phi_2^{\beta} = \tfrac{1}{4}\sum_{\ell,k}\sum_{\ell',k'}\sum_{\alpha,\lambda} x_\lambda\binom{\ell}{k} e_{\alpha\lambda} \sum_{\beta,\mu}\left[u_{\beta\mu}\Phi_{\alpha\beta}\binom{\ell-\ell'}{k\,k'} x_\mu\binom{\ell'}{k'} + u_{\mu\beta}\Phi_{\alpha\mu}\binom{\ell-\ell'}{k\,k'} x_\beta\binom{\ell'}{k'}\right]$$

(3.35) i.e.
$$\Phi_2^{\beta} = \frac{N}{2}\sum_{\alpha,\lambda}\sum_{\beta,\mu}[\alpha\lambda,\beta\mu]\, e_{\alpha\lambda}\, e_{\beta\mu}$$

by (3.21) and (3.28)

where

(3.36)
$$[\alpha\lambda,\beta\mu] = \frac{1}{N}\sum_{\ell,k}\sum_{\ell',k'}\Phi_{\alpha\beta}\binom{\ell-\ell'}{k\,k'} x_\lambda\binom{\ell}{k} x_\mu\binom{\ell'}{k'}$$

Now
$$\sum_{\ell,k}\sum_{\ell',k'}\Phi_{\alpha\beta}\binom{\ell-\ell'}{k\,k'} x_\lambda\binom{\ell}{k} x_\mu\binom{\ell'}{k'} = \sum_{\ell,k}\sum_{\ell',k'}\Phi_{\lambda\beta}\binom{\ell-\ell'}{k\,k'} x_\alpha\binom{\ell}{k} x_\mu\binom{\ell'}{k'}$$

by (3.20)

Hence the symbols $[\alpha\lambda,\beta\mu]$ are symmetric in α and λ. Similarly they can be shown to be symmetric in β and μ, by means of (3.21).

So

(3.37a) $$[\alpha\lambda,\beta\mu] = [\lambda\alpha,\beta\mu] = [\alpha\lambda,\mu\beta]$$

This equation embodies the two conditions (3.20) and (3.21) and in practice replaces them.

Also by interchanging ℓ and ℓ', k and k', in (3.36) and using (1.6), the symbols $[\alpha\lambda,\beta\mu]$ can be seen to be symmetric in the pairs $(\alpha\lambda)$ and $(\beta\mu)$, i.e.

(3.37b) $$[\alpha\lambda,\beta\mu] = [\beta\mu,\alpha\lambda]$$

It can be shown that the symbols are independent of N, just as were the $\begin{bmatrix} hk' \\ \alpha\beta \end{bmatrix}$, in the following way:-

Write

$$\Upsilon\binom{\ell}{k} - \Upsilon\binom{\ell'}{k'} = \Upsilon\binom{\ell-\ell'}{k k'}$$

Then $$[\alpha\lambda,\beta\mu] + [\alpha\mu,\beta\lambda] = -\frac{1}{N}\sum_{\ell,h}\sum_{\ell',k'}\Phi_{\alpha\beta}\binom{\ell-\ell'}{hk'}x_\lambda\binom{\ell-\ell'}{hk'}x_\mu\binom{\ell-\ell'}{hk'}$$

by (3.18) and (3.19)

Similarly

$$[\alpha\beta,\lambda\mu] + [\alpha\mu,\lambda\beta] = -\frac{1}{N}\sum_{\ell,h}\sum_{\ell',k'}\Phi_{\alpha\lambda}\binom{\ell-\ell'}{hk'}x_\beta\binom{\ell-\ell'}{hk'}x_\mu\binom{\ell-\ell'}{hk'}$$

and $$[\alpha\beta,\mu\lambda] + [\alpha\lambda,\mu\beta] = -\frac{1}{N}\sum_{\ell,h}\sum_{\ell',k'}\Phi_{\alpha\mu}\binom{\ell-\ell'}{hk'}x_\beta\binom{\ell-\ell'}{hk'}x_\lambda\binom{\ell-\ell'}{hk'}$$

Hence

(3.38) $$[\alpha\lambda,\beta\mu] = \frac{1}{2N}\sum_{\ell,h}\sum_{\ell',k'}\left[\Phi_{\alpha\lambda}\binom{\ell-\ell'}{hk'}x_\beta\binom{\ell-\ell'}{hk'}x_\mu\binom{\ell-\ell'}{hk'} - \Phi_{\alpha\beta}\binom{\ell-\ell'}{hk'}x_\lambda\binom{\ell-\ell'}{hk'}x_\mu\binom{\ell-\ell'}{hk'}\right.$$
$$\left. - \Phi_{\lambda\beta}\binom{\ell-\ell'}{hk'}x_\alpha\binom{\ell-\ell'}{hk'}x_\mu\binom{\ell-\ell'}{hk'}\right]$$

$$= \frac{1}{2}\sum_{e}\sum_{k,k'}\left[\Phi_{\alpha\lambda}\binom{e}{kk'}x_\beta\binom{e}{kk'}x_\mu\binom{e}{kk'} - \Phi_{\alpha\beta}\binom{e}{kk'}x_\lambda\binom{e}{kk'}x_\mu\binom{e}{kk'} - \Phi_{\alpha\mu}\binom{e}{kk'}x_\beta\binom{e}{kk'}x_\lambda\binom{e}{kk'}\right]$$

by the cyclic boundary conditions (1.3)

$\underline{\Phi_2^c}$.

If β and μ are interchanged in Φ_2^c and the result added to the original expression for Φ_2^c, one obtains :-

$$\Phi_2^c = \frac{1}{2}\sum_{e,k}\sum_{e',k'}\sum_{\alpha,\beta,\mu} u_\alpha(k)\left[u_{\beta\mu}\Phi_{\alpha\beta}\binom{e-e'}{kk'}x_\mu\binom{e'}{k'} + u_{\mu\beta}\Phi_{\alpha\mu}\binom{e-e'}{kk'}x_\beta\binom{e'}{k'}\right]$$

$$= \sum_{e,k}\sum_{e',k'}\sum_{\alpha,\beta,\mu} u_\alpha(k)\, e_{\beta\mu}\Phi_{\alpha\beta}\binom{e-e'}{kk'}x_\mu\binom{e'}{k'}$$

by (3.21) and (3.28)

$$= \sum_{e,k}\sum_{e',k'}\sum_{\alpha,\beta,\mu}\left[e_\alpha(k) + u_\alpha(1)\right]e_{\beta\mu}\Phi_{\alpha\beta}\binom{e-e'}{kk'}x_\mu\binom{e'}{k'}$$

by (3.30)

i.e.

$$(3.39)\quad \Phi_2^c = N\sum_{k}\sum_{\alpha,\beta,\mu}\left[\alpha,\beta\mu\right]^k e_{\beta\mu}e_\alpha(k) \quad \text{by (3. 18)}$$

where

$$(3.40)\quad \begin{bmatrix} k \\ \lambda,\rho\mu \end{bmatrix} = \frac{1}{N}\sum_{l,l'}\sum_{k'} \Phi_{\lambda\rho}\begin{pmatrix} l-l' \\ k\,k' \end{pmatrix} x_\mu\begin{pmatrix} l' \\ k' \end{pmatrix}$$

$$= -\frac{1}{N}\sum_{ll'}\sum_{k'} \Phi_{\lambda\rho}\begin{pmatrix} l-l' \\ k\,k' \end{pmatrix} x_\mu\begin{pmatrix} l-l' \\ k\,k' \end{pmatrix} \quad \text{by (3.19)}$$

$$= -\sum_{l}\sum_{k'} \Phi_{\lambda\rho}\begin{pmatrix} l \\ k\,k' \end{pmatrix} x_\mu\begin{pmatrix} l \\ k\,k' \end{pmatrix} \quad \text{by the cyclic boundary condition (1.3).}$$

These symbols satisfy the relations:-

$$(3.41)\quad \begin{bmatrix} k \\ \lambda,\rho\mu \end{bmatrix} = \begin{bmatrix} k \\ \lambda,\mu\rho \end{bmatrix} \quad \text{by (3.21)}$$

$$(3.42)\quad \sum_{k}\begin{bmatrix} k \\ \lambda,\rho\mu \end{bmatrix} = 0 \quad \text{by (3.16)}$$

If Δ is the volume of a cell, then the energy density $\mathcal{U}_2 = \frac{1}{N\Delta}\Phi_2$ can be written as :-

$$(3.43)\quad \mathcal{U}_2 = \frac{1}{\Delta}\Big\{\frac{1}{2}\sum_{k,k'}\sum_{\lambda\rho}\begin{bmatrix} k\,k' \\ \lambda\rho \end{bmatrix} e_\lambda(k)\,e_\rho(k') + \frac{1}{2}\sum_{\lambda,\lambda}\sum_{\rho,\mu}[\lambda\lambda,\rho\mu]\,e_{\lambda\lambda}\,e_{\rho\mu}$$

$$+ \sum_{k}\sum_{\lambda,\rho,\mu}\begin{bmatrix} k \\ \lambda,\rho\mu \end{bmatrix} e_{\rho\mu}\,e_\lambda(k)\Big\}$$

E l a s t i c c o n s t a n t s

The components of the stress-tensor S are

$$(3.44)\qquad S_{\rho\mu} \equiv \frac{\partial \mathcal{U}_2}{\partial e_{\rho\mu}} = \frac{1}{\Delta}\left\{ \sum_{\alpha,\lambda} [\alpha\lambda,\rho\mu] e_{\alpha\lambda} + \sum_{k,\alpha} \left[\alpha, {}^{k}_{\rho\mu}\right] e_\alpha(k) \right\}$$

in accordance with the usual definition of this quantity. In this, the internal strain components can be eliminated by using the fact that Φ_2 is essentially independent of them, i.e.

$$(3.45)\qquad \frac{1}{N}\frac{\partial \Phi_2}{\partial e_\alpha(k)} \equiv \sum_{k'} \sum_{\beta} \left[{}^{kk'}_{\alpha\beta}\right] e_\beta(k') + \sum_{\beta,\rho} \left[{}^{k}_{\alpha,\rho\mu}\right] e_{\rho\mu} = 0$$

The solution of this is of the form:-

$$(3.46)\qquad e_\delta(k') = \sum_{\beta,\rho} \left\{ \delta, {}^{k'}_{\beta\rho} \right\} e_{\rho\mu}$$

$$(3.47)\qquad \text{where} \quad \left\{ \delta, {}^{k'}_{\rho\mu} \right\} = \left\{ \delta, {}^{k'}_{\mu\rho} \right\} \qquad \text{since } e_{\rho\mu} = e_{\mu\rho}$$

This gives after altering the summation index β in the first term of (3.45) to δ, and writing γ for α throughout the equation, -

$$\sum_{\rho,\mu} \left[\sum_{k'} \sum_{\delta} \left[{}^{kk'}_{\gamma\delta}\right] \left\{ \delta, {}^{k'}_{\rho\mu} \right\} + \left[{}^{k}_{\gamma,\rho\mu} \right] \right] e_{\rho\mu} = 0$$

or, since both $e_{\rho\mu}$ and its coefficient are symmetric in ρ and μ,

$$(3.48)\qquad \sum_{k'} \sum_{\delta} \left[{}^{kk'}_{\gamma\delta}\right] \left\{ \delta, {}^{k'}_{\rho\mu} \right\} + \left[{}^{k}_{\gamma,\rho\mu} \right] = 0$$

After changing the summation index α to γ in the second term of $S_{\rho\mu}$ given by (3.44), and then inserting a suitable form of (3,47) viz. $e_\gamma(k) = \sum_{\alpha,\lambda} \{\gamma,\alpha\lambda\}^k e_{\alpha\lambda}$, one has, with the help of (3.48) :-

$$(3.49) \qquad S_{\rho\mu} = \frac{1}{\Delta} \sum_{\alpha,\lambda} \left[[\alpha\lambda,\rho\mu] - \sum_{k,k'} \sum_{\gamma,\delta} \begin{bmatrix} kk' \\ \gamma\delta \end{bmatrix} \{\gamma,\alpha\lambda\}^k \{\delta,\rho\mu\}^{k'} \right] e_{\alpha\lambda}$$

The expression $\sum_{k,k'} \sum_{\gamma,\delta} \begin{bmatrix} kk' \\ \gamma\delta \end{bmatrix} \{\gamma,\alpha\lambda\}^k \{\delta,\rho\mu\}^{k'}$ is symmetric in α and λ and in ρ and μ by (3.47). Also if one interchanges k and k', γ and δ and uses (3.33) it is seen that it is also symmetric in the pairs $(\alpha\lambda)$ and $(\rho\mu)$. It therefore possesses the same symmetry as $[\alpha\lambda,\rho\mu]$, and this makes it permissible to write (3.49) as :-

$$(3.50) \qquad S_{\rho\mu} = \sum_{\alpha,\lambda} \{\alpha\lambda,\rho\mu\} e_{\alpha\lambda}$$

where

$$(3.51) \qquad \{\alpha\lambda,\rho\mu\} = \frac{1}{\Delta} \left[[\alpha\lambda,\rho\mu] - \sum_{k,k'} \sum_{\gamma,\delta} \begin{bmatrix} kk' \\ \gamma\delta \end{bmatrix} \{\gamma,\alpha\lambda\}^k \{\delta,\rho\mu\}^{k'} \right]$$

and

$$(3.52) \qquad \{\alpha\lambda,\rho\mu\} = \{\lambda\alpha,\rho\mu\} = \{\alpha\lambda,\mu\rho\} = \{\rho\mu,\alpha\lambda\}$$

The equation (3.50) is the formulation for crystals of Hookes' Law, that stress is proportional to strain

and the quantities $\{\alpha\lambda, \beta\mu\}$ are the usual elastic constants. They are generally written in the notation of Voigt (1910), which makes use of the symmetry properties (3.52). Each pair of indices $(\alpha\lambda)$ or $(\beta\mu)$ is replaced by a single index according to the scheme:

The pairs	11	22	33	$\{^{23}_{32}$	$\{^{31}_{13}$	$\{^{12}_{21}$
replaced by	1	2	3	4	5.	6

These numbers are then attached to the letter **c** thus $\{33, 12\} = c_{36}$ etc. The only symmetry relation that remains is $c_{\nu\sigma} = c_{\sigma\nu}$ $(\nu, \sigma = 1,2,3,4,5,6)$.

Section 3c(B) Accoustical vibrations and the elastic constants

The elastic constants are here introduced in an alternative way to that adopted in Section 3c(A). The method is the same as that used by Born (1923) but a matrix notation is employed and no assumptions are made about the nature of the forces.

Equations of motion

The equations of motion are solved for long-wave accoustical vibrations. In order to throw into prominence the vectors $\underline{r}(k)$ which are of importance for accoustical vibrations, write

$$\underline{U}(k) = \underline{W}(k)\, e^{i(\underline{q}\cdot\underline{r}(k))} \tag{3.53}$$

Hence

$$\underline{v}(l_k) = \underline{W}(k)\, e^{-i\omega t}\, e^{i(\underline{q}\cdot\underline{r}(l_k))} \tag{3.54}$$

and (1.15) becomes

$$\omega^2 W_\alpha(k) = \sum_{k'}\sum_{\beta} C_{\alpha\beta}\left(\frac{q}{kk'}\right) W_\beta(k') \tag{3.55}$$

where

$$(3.56)\qquad C_{\alpha\beta}\left(\frac{q}{kk'}\right) = \sum_{\ell'} D_{\alpha\beta}\left(\frac{\ell-\ell'}{kk'}\right) e^{-i\left(\underline{q}\cdot\underline{r}\left(\frac{\ell-\ell'}{kk'}\right)\right)}$$

$$= \sum_{\ell} D_{\alpha\beta}\left(\frac{\ell}{kk'}\right) e^{-i\left(\underline{q}\cdot\underline{r}\left(\frac{\ell}{kk'}\right)\right)}$$

$$= D_{\alpha\beta}\left(\frac{q}{kk'}\right) e^{-i\left(\underline{q}\cdot\underline{r}\left(\frac{\cdots}{kk'}\right)\right)}$$

where $\underline{r}\left(\frac{\cdots}{kk'}\right) = \underline{r}\left(\frac{\cdots}{k}\right) - \underline{r}\left(\frac{\cdots}{k'}\right)$

The $C_{\alpha\beta}\left(\frac{q}{kk'}\right)$ can be collected in the same way as the $D_{\alpha\beta}\left(\frac{q}{kk'}\right)$ into matrices and will finally form a matrix of order (3n x 3n), $C(\underline{q})$.

Let the $W_\alpha(k)$ of (3.53) be ordered according to the indices k and then according to the suffices α and let

$$(3.57)\qquad \underline{W} = \{W_1(1)\, W_2(1)\, W_3(1)\, W_1(2) \cdots\cdots W_2(n)\, W_3(n)\}$$

be a column vector.

Then writing the scalar ω^2 as Ω , equation (3.55) takes the matrix form:-

$$(3.58)\qquad \Omega\underline{W} = C(\underline{q})\underline{W}$$

In this, Ω , $\underline{W}$, and $C(\underline{q})$ are all functions of the wave-vector $\underline{q}$ and can be expanded in powers of $q = |\underline{q}|$

$$(3.59)\qquad \Omega = \overset{(0)}{\Omega} + \overset{(1)}{\Omega} + \overset{(2)}{\Omega} + \cdots$$

$$(3.60)\qquad \underline{W} = \overset{(0)}{\underline{W}} + \overset{(1)}{\underline{W}} + \overset{(2)}{\underline{W}} + \cdots\cdots$$

and

$$C(\underline{Q}) = \overset{(0)}{C}(\underline{Q}) + \overset{(1)}{C}(\underline{Q}) + \overset{(2)}{C}(\underline{Q}) + \cdots\cdots \tag{3.61}$$

where $\overset{(r)}{\Omega}$, $\overset{(r)}{\underline{W}}$, and $\overset{(r)}{C}(\underline{Q})$ are the terms in the respective expansions which contain the $r^{th.}$ power of Q . The elements of $\overset{(0)}{C}(\underline{Q}), \overset{(1)}{C}(\underline{Q}), \overset{(2)}{C}(\underline{Q}), \ldots$ are given by

$$\overset{(0)}{C}_{\alpha\beta}\left(\frac{Q}{kk'}\right) = \frac{1}{\sqrt{m_k m_{k'}}} \sum_{l} \Phi_{\alpha\beta}\left(\frac{l}{kk'}\right) \tag{3.62}$$

$$\overset{(1)}{C}_{\alpha\beta}\left(\frac{Q}{kk'}\right) = \frac{-i}{\sqrt{m_k m_{k'}}} \sum_{l} \sum_{\gamma} \Phi_{\alpha\beta\gamma}\left(\frac{l}{kk'}\right) x_\gamma\left(\frac{l}{kk'}\right) Q_\gamma \tag{3.63}$$

$$\overset{(2)}{C}_{\alpha\beta}\left(\frac{Q}{kk'}\right) = \frac{-1/2}{\sqrt{m_k m_{k'}}} \sum_{l} \sum_{\lambda,\mu} \Phi_{\alpha\beta\lambda\mu}\left(\frac{l}{kk'}\right) x_\lambda\left(\frac{l}{kk'}\right) x_\mu\left(\frac{l}{kk'}\right) Q_\lambda Q_\mu \tag{3.64}$$

etc.

By equating the terms which contain like powers of Q on either side of (3.58), the following set of equations is obtained:-

$$\overset{(0)}{\Omega}\,\overset{(0)}{\underline{W}} = \overset{(0)}{C}(\underline{Q})\,\overset{(0)}{\underline{W}} \tag{3.65}$$

$$\overset{(0)}{\Omega}\,\overset{(1)}{\underline{W}} + \overset{(1)}{\Omega}\,\overset{(0)}{\underline{W}} = \overset{(0)}{C}(\underline{Q})\,\overset{(1)}{\underline{W}} + \overset{(1)}{C}(\underline{Q})\,\overset{(0)}{\underline{W}} \tag{3.66}$$

$$\overset{(0)}{\Omega}\,\overset{(2)}{\underline{W}} + \overset{(1)}{\Omega}\,\overset{(1)}{\underline{W}} + \overset{(2)}{\Omega}\,\overset{(0)}{\underline{W}} = \overset{(0)}{C}(\underline{Q})\,\overset{(2)}{\underline{W}} + \overset{(1)}{C}(\underline{Q})\,\overset{(1)}{\underline{W}} + \overset{(2)}{C}(\underline{Q})\,\overset{(0)}{\underline{W}} \tag{3.67}$$

etc.

L e m m a o n s o l v a b i l i t y

Introduce a matrix :-

(3.68) $$M = \begin{bmatrix} \sqrt{m_1} & 0 & 0 \\ 0 & \sqrt{m_1} & 0 \\ 0 & 0 & \sqrt{m_1} \\ \sqrt{m_2} & 0 & 0 \\ 0 & \sqrt{m_2} & 0 \\ 0 & 0 & \sqrt{m_2} \\ - & - & - \\ - & - & - \\ 0 & 0 & \sqrt{m_n} \end{bmatrix}$$

The matrix $\overset{(0)}{C}(\underline{\varphi})$ is singular of rank (3n - 3). Since

(3.69) $$\begin{bmatrix} k & k' \\ \alpha & \beta \end{bmatrix} = \sqrt{m_k m_{k'}}\, \overset{(0)}{C}_{\alpha\beta}\left(\frac{\varphi}{k\,k'}\right) \quad \text{by (3.62)}$$

we may write (3.34) in matrix notation to give the three relations between the rows or columns of $\overset{(0)}{C}(\underline{\varphi})$ viz.

(3.70) $$\tilde{M}\,\overset{(0)}{C}(\underline{\varphi}) = \overset{(0)}{C}(\underline{\varphi})\,M = 0$$

Consequently one has the following result:-
An equation of the type

(3.71) $$\overset{(0)}{C}(\underline{\varphi})\,\underline{w} = \underline{L}$$

can only be solved if

(3.72) $$\tilde{M}\,\underline{L} = 0$$

Since the rank of $\overset{(0)}{C}(\underline{\varphi})$ is (3n - 3), the general solution of such an equation will admit of three arbitrary constants.

E q u a t i o n (3.65)

For accoustical vibrations the frequency approaches zero with α , and consequently $\underset{(0)}{\Omega}$ is zero. Hence (3.65) becomes

$$\underset{(0)}{C}(\underline{\alpha})\underset{(0)}{\underline{W}} = 0 \tag{3.73}$$

But from (3.70)

$$\underset{(0)}{C}(\underline{\alpha})M = 0$$

Hence

$$\underset{(0)}{\underline{W}} = M\underline{W} \tag{3.74}$$

where

$$\underline{W} = \begin{bmatrix} W_1 \\ W_2 \\ W_3 \end{bmatrix} \tag{3.75}$$

and W_1 , W_2 , W_3 , are the three arbitrary constants mentioned at the end of the preceding paragraph.

E q u a t i o n (3.66)

If one puts $\underset{(0)}{\Omega} = 0$ and $\underset{(0)}{\underline{W}} = M\underline{W}$ in (3.66) one has

$$\overset{(0)}{C}(\underline{Q})\,\underline{\overset{(1)}{W}} = \overset{(1)}{\Omega}\, M\,\underline{W} - \overset{(1)}{C}(\underline{Q})\, M\,\underline{W} \tag{3.76}$$

The condition for this to be solvable is, by (3.72),

$$\overset{(1)}{\Omega}(\tilde{M} M)\underline{W} - (\tilde{M}\,\overset{(1)}{C}(\underline{Q}) M)\,\underline{W} = 0 \tag{3.77}$$

But $$\tilde{M}\,\overset{(1)}{C}(\underline{Q}) M = -i \sum_{\ell} \sum_{k,k'} \Phi_{\alpha\beta}\left(\begin{smallmatrix}\ell\\ k k'\end{smallmatrix}\right) \sum_{\gamma} x_{\gamma}\left(\begin{smallmatrix}\ell\\ k k'\end{smallmatrix}\right) Q_{\gamma}$$

by (3.63)

$$= 0 \qquad \text{by (3.42)}$$

Hence (3.77) becomes:-

$$\overset{(1)}{\Omega}(\tilde{M} M)\underline{W} = 0$$

i.e.

$$\overset{(1)}{\Omega} = 0 \tag{3.78}$$

Therefore (3.76) is now

$$\overset{(0)}{C}(\underline{Q})\,\underline{\overset{(1)}{W}} = -\overset{(1)}{C}(\underline{Q})\, M\,\underline{W} \tag{3.79}$$

E q u a t i o n (3.67)

If one puts $\overset{(0)}{\Omega} = 0$ and uses (3.74) and (3.78), (3.67) is

$$(3.80)\qquad \overset{(0)}{C}(\underline{q})\,\underline{\overset{(2)}{w}} = \overset{(2)}{\Omega}\, m\,\underline{w} - \overset{(1)}{C}(\underline{q})\,\underline{\overset{(1)}{w}} - \overset{(2)}{C}(\underline{q})\, m\,\underline{w}$$

The condition for this to be solvable is, by (3.72),

$$(3.81)\qquad \overset{(2)}{\Omega}(\tilde{m} m)\,\underline{w} = \tilde{m}\,\overset{(1)}{C}(\underline{q})\,\underline{\overset{(1)}{w}} + \tilde{m}\,\overset{(2)}{C}(\underline{q})\, m\,\underline{w}$$

Equations (3.79) and (3.81) which are, taken together, an approximation of the second order in the wave-vector to the equations of motion, may be written in terms of the matrix elements as :-

$$(3.82)\qquad \sum_{k'}\sum_{\beta} \overset{(0)}{C}_{\alpha\beta}\left(\frac{q}{k k'}\right) \overset{(1)}{w}_{\beta}(k') + \sum_{k'}\sum_{\beta} \sqrt{m_{k'}}\,\overset{(1)}{C}_{\alpha\beta}\left(\frac{q}{k k'}\right) w_{\beta} = 0$$

$$(3.83)\qquad \left(\sum_{k} m_k\right) \overset{(2)}{\Omega}\, w_{\alpha} = \sum_{k,k'}\sum_{\beta} \sqrt{m_k}\,\overset{(1)}{C}_{\alpha\beta}\left(\frac{q}{k k'}\right) \overset{(0)}{w}_{\beta}(k') + \sum_{k,k'}\sum_{\beta} \sqrt{m_k m_{k'}}\,\overset{(2)}{C}_{\alpha\beta}\left(\frac{q}{k k'}\right) w_{\beta}$$

Connection with Section 3c(B)

In order to link up equations (3.82) and (3.83) with the work of the previous Section, it is necessary to compare the two expressions for the displacement:-

$$(3.84)\qquad v_{\alpha}\left(\frac{l}{k}\right) = \sqrt{m_k}\; u_{\alpha}\left(\frac{l}{k}\right) = \sqrt{m_k}\left[u_{\alpha}(k) + \sum_{\lambda} u_{\alpha\lambda}\, x_{\lambda}\left(\frac{l}{k}\right)\right]$$

and

(3.85) $$v_\alpha(l_k) = [\overset{(0)}{w}_\alpha(k) + \overset{(1)}{w}_\alpha(k) + \cdots][1 + i\sum_\lambda x_\lambda(l_k)q_\lambda - \cdots]$$

If, in these two expressions, the terms independent of the co-ordinates $x_\lambda(l_k)$ are equated without going beyond linear powers of q , one has

$$\sqrt{m_k}\, u_\alpha(k) = \overset{(0)}{w}_\alpha(k) + \overset{(1)}{w}_\alpha(k)$$

$$= \sqrt{m_k}\, w_\alpha + \overset{(1)}{w}_\alpha(k)$$

(3.86) i.e. $$e_\alpha(k) = \frac{1}{\sqrt{m_k}}\, \overset{(1)}{w}_\alpha(k)$$

Again if the terms linear in the co-ordinates are equated without going beyond linear powers of q , one has

$$\sqrt{m_k}\, u_{\alpha\lambda} = i\, \overset{(0)}{w}_\alpha(k)\, q_\lambda$$

(3.87) i.e. $$e_{\alpha\lambda} = \tfrac{i}{2}\left[w_\alpha q_\lambda + w_\lambda q_\alpha\right]$$

Now in (3.82) the first term is

(3.88) $$\sum_{k'}\sum_\beta \overset{(0)}{\zeta}_{\alpha\beta}\left(\begin{matrix} l \\ k\,k' \end{matrix}\right) \overset{(0)}{w}_\beta(k') = \sum_{k'}\sum_\beta \frac{1}{\sqrt{m_k m_{k'}}} \begin{bmatrix} k\,k' \\ \alpha\,\beta \end{bmatrix} \overset{(0)}{w}_\beta(k')$$

by (3.32) and (3.62)

$$= \frac{1}{\sqrt{m_k}} \sum_{k'} \sum_{\beta} \begin{bmatrix} k k' \\ \alpha \beta \end{bmatrix} e_\beta(k')$$

by (3.86)

and the second term of (3.82) is

$$(3.89) \quad \sum_{k'} \sum_{\beta} \sqrt{m_{k'}}\, C''_{\alpha\beta}\begin{pmatrix} \alpha \\ k k' \end{pmatrix} W_\beta = -i \sum_{\ell} \sum_{k'} \sum_{\beta,\mu} \frac{1}{\sqrt{m_k}} \Phi_{\alpha\mu}\begin{pmatrix} \ell \\ k k' \end{pmatrix} x_\mu\begin{pmatrix} \ell \\ k k' \end{pmatrix} W_\beta\, a_\mu$$

by (3.63)

$$= \frac{i}{\sqrt{m_k}} \sum_{\beta,\mu} \begin{bmatrix} k \\ \alpha, \beta\mu \end{bmatrix} W_\beta\, a_\mu$$

by (3.40)

$$= \frac{1}{\sqrt{m_k}} \sum_{\beta,\mu} \begin{bmatrix} k \\ \alpha, \beta\mu \end{bmatrix} e_{\beta\mu}$$

by (3.87)

Hence (3.82) becomes, after removing a factor $\frac{1}{\sqrt{m_k}}$,

$$(3.90) \quad \sum_{k'} \sum_{\beta} \begin{bmatrix} k k' \\ \alpha \beta \end{bmatrix} e_\beta(k') + \sum_{\beta,\mu} \begin{bmatrix} k \\ \alpha, \beta\mu \end{bmatrix} e_{\beta\mu} = 0$$

which is precisely (3.45). The same solution (3.46) will be taken, and this is written in the present notation as :-

$$(3.91) \quad W''_\delta(k') = i\sqrt{m_{k'}} \sum_{\beta,\mu} \left\{ \delta^{k'}_{,\beta\mu} \right\} W_\beta\, a_\mu$$

Now in equation (3.83) the first term on the right-hand side is

$$(3.92)\quad \sum_{k,k'}\sum_{\beta}\sqrt{m_k}\,\overset{(1)}{C}_{\alpha\beta}\left(\begin{smallmatrix}\ell\\ kk'\end{smallmatrix}\right)\overset{(1)}{W}_{\beta}(k') = -i\sum_{\ell}\sum_{k,k'}\sum_{\delta,\lambda}\frac{1}{\sqrt{m_{k'}}}\,\Phi_{\alpha\delta}\left(\begin{smallmatrix}\ell\\ kk'\end{smallmatrix}\right)x_{\lambda}\left(\begin{smallmatrix}\ell\\ kk'\end{smallmatrix}\right)\overset{(1)}{W}_{\delta}(k')\,Q_{\lambda}$$

by (3.63), after changing the summation index β to δ.

$$= \sum_{k'}\sum_{\delta,\lambda}\sum_{\beta,\mu}\left[\begin{smallmatrix}k'\\ \alpha\lambda\end{smallmatrix}\right]\left\{\begin{smallmatrix}k'\\ \beta\mu\end{smallmatrix}\right\}W_{\beta}\,Q_{\lambda}\,Q_{\mu}$$

by (3.40) and (3.91)

$$= -\sum_{k,k'}\sum_{\gamma,\delta}\sum_{\rho,\lambda,\mu}\left[\begin{smallmatrix}kk'\\ \gamma\delta\end{smallmatrix}\right]\left\{\begin{smallmatrix}k\\ \gamma\alpha\lambda\end{smallmatrix}\right\}\left\{\begin{smallmatrix}k'\\ \delta\beta\mu\end{smallmatrix}\right\}W_{\rho}\,Q_{\lambda}\,Q_{\mu}$$

by (3.48)

The second term on the right-hand side of (3.83) is

$$(3.93)\quad \sum_{k,k'}\sum_{\beta}\sqrt{m_k m_{k'}}\,\overset{(2)}{C}_{\alpha\beta}\left(\begin{smallmatrix}\ell\\ kk'\end{smallmatrix}\right)W_{\beta} = -\tfrac{1}{2}\sum_{\ell}\sum_{k,k'}\sum_{\beta}\sum_{\lambda,\mu}\Phi_{\alpha\beta}\left(\begin{smallmatrix}\ell\\ kk'\end{smallmatrix}\right)x_{\lambda}\left(\begin{smallmatrix}\ell\\ kk'\end{smallmatrix}\right)x_{\mu}\left(\begin{smallmatrix}\ell\\ kk'\end{smallmatrix}\right)W_{\beta}\,Q_{\lambda}\,Q_{\mu}$$

by (3.64)

$$= -\frac{1}{2N}\sum_{\ell,\ell'}\sum_{k,k'}\sum_{\beta}\sum_{\lambda,\mu}\Phi_{\alpha\beta}\left(\begin{smallmatrix}\ell-\ell'\\ kk'\end{smallmatrix}\right)x_{\lambda}\left(\begin{smallmatrix}\ell-\ell'\\ kk'\end{smallmatrix}\right)x_{\mu}\left(\begin{smallmatrix}\ell-\ell'\\ kk'\end{smallmatrix}\right)W_{\beta}\,Q_{\lambda}\,Q_{\mu}$$

by the cyclic boundary conditions (1.3).

$$= \frac{1}{2N}\sum_{\ell,\ell'}\sum_{k,k'}\sum_{\beta}\sum_{\lambda,\mu}\left[\Phi_{\alpha\beta}\left(\begin{smallmatrix}\ell-\ell'\\ kk'\end{smallmatrix}\right)x_{\lambda}\left(\begin{smallmatrix}\ell\\ k\end{smallmatrix}\right)x_{\mu}\left(\begin{smallmatrix}\ell'\\ k'\end{smallmatrix}\right) + \Phi_{\alpha\beta}\left(\begin{smallmatrix}\ell-\ell'\\ kk'\end{smallmatrix}\right)x_{\lambda}\left(\begin{smallmatrix}\ell'\\ k'\end{smallmatrix}\right)x_{\mu}\left(\begin{smallmatrix}\ell\\ k\end{smallmatrix}\right)\right]W_{\beta}\,Q_{\lambda}\,Q_{\mu}$$

by (3.18) and (3.19).

$$= \sum_{\beta}\sum_{\lambda,\mu}\left[\begin{smallmatrix}\alpha\lambda,\beta\mu\end{smallmatrix}\right]W_{\beta}\,Q_{\lambda}\,Q_{\mu}$$

by (3.36)

$$= \sum_{\beta} \sum_{\lambda,\mu} [\alpha\lambda,\beta\mu] W_\beta \omega_\lambda \omega_\mu$$

by (3.36)

Hence putting $\omega^2 \equiv \Omega = \Omega^{(2)}$ for this approximation, (3.83) becomes

$$\omega^2 W_\alpha = \left(\sum_k m_k\right)^{-1} \sum_{\beta,\lambda,\mu} \left[[\alpha\lambda,\beta\mu] - \sum_{k,k'} \sum_{\gamma,\delta} \left[\begin{matrix} k & k' \\ \gamma & \delta \end{matrix} \right] \{\gamma, k\alpha\} \{\delta, k'\beta\mu\} \right] W_\beta \omega_\lambda \omega_\mu \qquad (3.94)$$

$$= \frac{1}{\rho} \sum_{\beta,\lambda,\mu} \{\alpha\lambda,\beta\mu\} W_\beta \omega_\lambda \omega_\mu$$

by (3.51)

where ρ (density) $= \left(\sum_k m_k\right)/\Delta$.

The result of this Section may then be summarised briefly thus:-

The equations of motion -

$$\omega^2 W_\alpha(k) = \sum_{k',\beta} C_{\alpha\beta}\left(\frac{q}{k,k'}\right) W_\beta(k') \qquad (3.95)$$

have been reduced, for the case of accoustical vibrations, to an approximation of the second order in the wave-vector, and having the form:-

$$\omega^2 W_\alpha = \sum_\beta \mathcal{D}'_{\alpha\beta}(\underline{q}) W_\beta \qquad (3.96)$$

where now

$$(3.97)\quad \begin{bmatrix} \mathcal{D}'_{11}(\underline{Q}) \\ \mathcal{D}'_{22}(\underline{Q}) \\ \mathcal{D}'_{33}(\underline{Q}) \\ \mathcal{D}'_{23}(\underline{Q}) \\ \mathcal{D}'_{31}(\underline{Q}) \\ \mathcal{D}'_{12}(\underline{Q}) \end{bmatrix} = \frac{1}{\rho} \begin{bmatrix} c_{11} & c_{66} & c_{55} & c_{65} & c_{51} & c_{16} \\ c_{66} & c_{22} & c_{44} & c_{24} & c_{46} & c_{62} \\ c_{55} & c_{44} & c_{33} & c_{43} & c_{35} & c_{54} \\ c_{65} & c_{24} & c_{43} & \frac{1}{2}(c_{23}+c_{44}) & \frac{1}{2}(c_{45}+c_{36}) & \frac{1}{2}(c_{64}+c_{25}) \\ c_{51} & c_{46} & c_{35} & \frac{1}{2}(c_{45}+c_{36}) & \frac{1}{2}(c_{31}+c_{55}) & \frac{1}{2}(c_{56}+c_{14}) \\ c_{16} & c_{62} & c_{54} & \frac{1}{2}(c_{64}+c_{25}) & \frac{1}{2}(c_{56}+c_{14}) & \frac{1}{2}(c_{12}+c_{66}) \end{bmatrix} \begin{bmatrix} Q_1^2 \\ Q_2^2 \\ Q_3^2 \\ 2Q_2Q_3 \\ 2Q_3Q_1 \\ 2Q_1Q_2 \end{bmatrix}$$

where Voigt's notation for the elastic constants has been used.

Note on the effect of rigid motion.

The equations (3.34) and (3.37a) have been shown to represent the condition that the potential energy is invariant under rigid motions of the lattice. They may be restated thus:-

(1) (3.34) can be used to define $\Phi\binom{\ell}{kk'}$ when $\ell = 0$ and $k = k'$, i.e.

$$\Phi\binom{0}{kk} = -\sum_{\ell,k}{}' \Phi\binom{\ell}{kk'} \tag{3.98}$$

where the dash on the summation sign denotes that the term in which $\ell = 0$ is to be omitted from the summation.

(2) Since the quantity $\sum_{k,k'} \sum_{\gamma,\delta} \left[\begin{smallmatrix} kk' \\ \gamma\delta \end{smallmatrix}\right] \{\gamma, \alpha\lambda\}^{k} \{\delta, \beta\rho\}^{k'}$ is symmetric in α and λ, and in β and ρ, by the definition of the symbols $\{-,-\}$, it follows that (3.37a) is equivalent to a part of (3.52), viz.

$$\{\alpha\lambda, \beta\rho\} = \{\lambda\alpha, \beta\rho\} = \{\alpha\lambda, \rho\beta\}$$

This can at once be recognised as the condition that the large matrix in (3.97) should be symmetric.

Section 4 Monatomic face-centred cubic lattice

In the face-centred cubic lattice it is possible to choose a unit cell which contains only one particle, and so the indices k can be dropped from all the symbols in which they occur. This property is used extensively later, but for the investigation of the symmetry of the lattice it is more convenient to deal with the cubic cell containing four particles (see Fig. 1) and the length of whose side is $2a$, where a is the lattice constant. The cell-vectors $\underline{a}^1$, $\underline{a}^2$, $\underline{a}^3$ are taken to be parallel to the sides of this cubic cell and of length a.

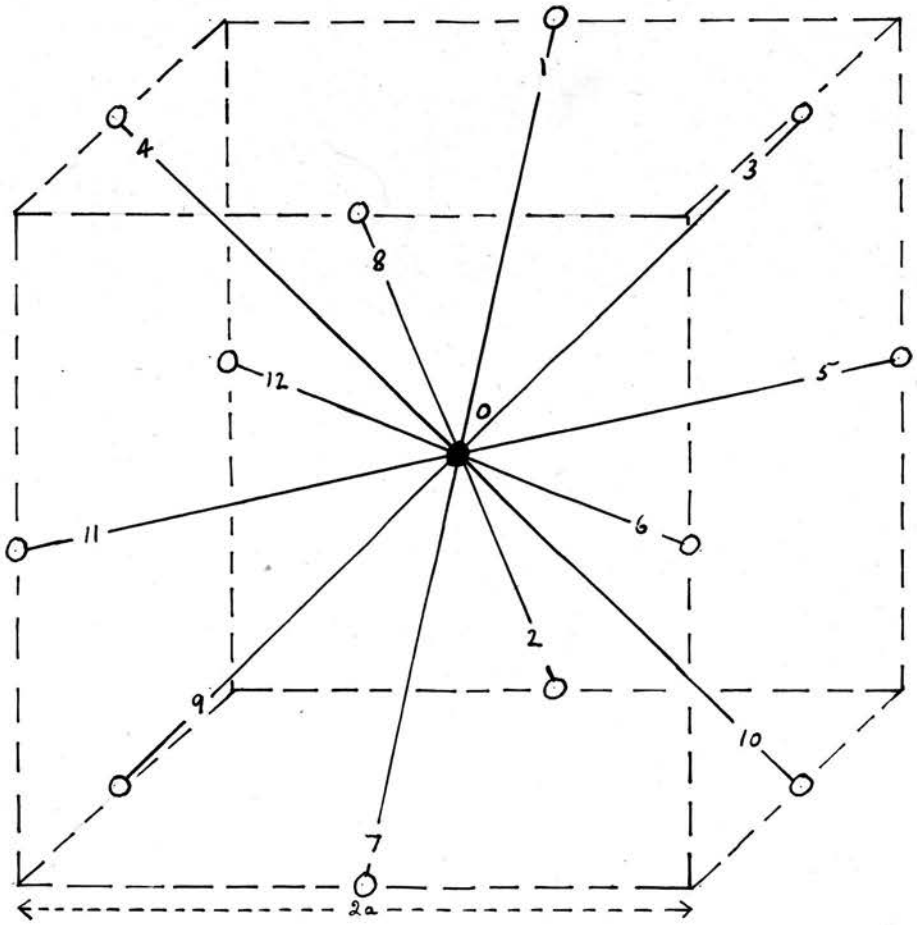
Since in the calculations which follow only the first neighbours of one point, labelled 0 in Fig. 1, will be taken into account, the number of matrices $\Phi\binom{l-l'}{\cdots}$ is twelve. In these l' can be taken to be the triad $(0,0,0)$. Then a label l may conveniently be affixed to the line joining 0 to the point whose cell-indices are given by l. The connection between the numbers l of the Figure and the integers (1.1) is given in the following Table:-

Table 1

l	1	2	3	4	5	6	7	8	9	10	11	12
l^1	0	0	1	-1	1	1	0	0	-1	1	-1	-1
l^2	1	1	0	0	1	-1	-1	-1	0	0	-1	1
l^3	1	-1	1	1	0	0	-1	1	-1	-1	0	0

FIGURE I

First neighbours of a point
in the face-centred cubic lattice.



Section 4a Symmetry of the face-centred cubic lattice

The rectangular system of axes S, introduced in Section 1, is so oriented that its three vectors (x_1, x_2, x_3) co-incide with ($\underline{a}^1, \underline{a}^2, \underline{a}^3$) respectively.

The complete set of symmetry operations that this lattice allows form a group (the space-group) which may be generated by the following three primitive operations:-

A,

A three-fold axis of rotation in the position $x_1 = x_2 = x_3$. This operation can be represented, in accordance with Section 3a, by the matrix:-

$$T_t = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$$

In order to use the formula (3.9) the change of the indices l must also be specified. This is given by (3.5) but is more concisely put in the notation of substitution groups, thus :-

$$(1\,3\,5)(7\,9\,11)(2\,4\,6)(8\,10\,12)$$

which means that a matrix with a certain number in a cycle is to be derived from the matrix with the number following it in the cycle by the operation $T \ldots \tilde{T}$

e.g. $$\Phi^3 = T_t \Phi^5 \tilde{T}_t$$

A_2

A plane of reflection in the position $x_3 = 0$. For this the matrix is

$$T_m = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

while the indices change according to the substitutions:-

$$(1\ 2)(3\ 10)(4\ 9)(7\ 8)(5)(6)(11)(12)$$

A_3

A plane of reflection in the position $x_1 = x_2$. Here the matrix is

$$T_d = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

with the indices changing according to

$$(1\ 3)(2\ 10)(4\ 8)(6\ 12)(7\ 9)(5)(11)$$

C a l c u l a t i o n

Since Φ^5 is invariant under A_2 one has

$$\begin{bmatrix} \Phi^5_{11} & \Phi^5_{12} & \Phi^5_{13} \\ \Phi^5_{21} & \Phi^5_{22} & \Phi^5_{23} \\ \Phi^5_{31} & \Phi^5_{32} & \Phi^5_{33} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} \Phi^5_{11} & \Phi^5_{12} & \Phi^5_{13} \\ \Phi^5_{21} & \Phi^5_{22} & \Phi^5_{23} \\ \Phi^5_{31} & \Phi^5_{32} & \Phi^5_{33} \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

$$= \begin{bmatrix} \overline{\Phi}^5_{11} & \overline{\Phi}^5_{12} & -\overline{\Phi}^5_{13} \\ \overline{\Phi}^5_{21} & \overline{\Phi}^5_{22} & -\overline{\Phi}^5_{23} \\ -\overline{\Phi}^5_{31} & -\overline{\Phi}^5_{32} & \overline{\Phi}^5_{33} \end{bmatrix}$$

Hence $\overline{\Phi}^5_{23} = \overline{\Phi}^5_{32} = \overline{\Phi}^5_{31} = \overline{\Phi}^5_{13} = 0$

Also, since $\overline{\Phi}^5$ is invariant under A_3 ,

$$\begin{bmatrix} \overline{\Phi}^5_{11} & \overline{\Phi}^5_{12} & 0 \\ \overline{\Phi}^5_{21} & \overline{\Phi}^5_{22} & 0 \\ 0 & 0 & \overline{\Phi}^5_{33} \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \overline{\Phi}^5_{11} & \overline{\Phi}^5_{12} & 0 \\ \overline{\Phi}^5_{21} & \overline{\Phi}^5_{22} & 0 \\ 0 & 0 & \overline{\Phi}^5_{33} \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$= \begin{bmatrix} \overline{\Phi}^5_{22} & \overline{\Phi}^5_{21} & 0 \\ \overline{\Phi}^5_{12} & \overline{\Phi}^5_{11} & 0 \\ 0 & 0 & \overline{\Phi}^5_{33} \end{bmatrix}$$

Hence $\overline{\Phi}^5_{12} = \overline{\Phi}^5_{21}$

and $\overline{\Phi}^5_{11} = \overline{\Phi}^5_{22}$

Let now $\overline{\Phi}^5 = -\begin{bmatrix} \beta & \gamma & 0 \\ \gamma & \beta & 0 \\ 0 & 0 & \alpha \end{bmatrix}$

Then from A_1 $\overline{\Phi}^1 = -\begin{bmatrix} \alpha & 0 & 0 \\ 0 & \beta & \gamma \\ 0 & \gamma & \beta \end{bmatrix}$

and

$$\underline{\Phi}^{3} = -\begin{bmatrix} \beta & 0 & \gamma \\ 0 & \alpha & 0 \\ \gamma & 0 & \beta \end{bmatrix}$$

The rest of the $\underline{\Phi}$ matrices follow very simply by continued application of the symmetry operations and the final result is:-

Table 2

$$\underline{\Phi}^{1} = -\begin{bmatrix} \alpha & 0 & 0 \\ 0 & \beta & \gamma \\ 0 & \gamma & \beta \end{bmatrix} = \underline{\Phi}^{7} \qquad \underline{\Phi}^{2} = -\begin{bmatrix} \alpha & 0 & 0 \\ 0 & \beta & -\gamma \\ 0 & -\gamma & \beta \end{bmatrix} = \underline{\Phi}^{8}$$

$$\underline{\Phi}^{3} = -\begin{bmatrix} \beta & 0 & \gamma \\ 0 & \alpha & 0 \\ \gamma & 0 & \beta \end{bmatrix} = \underline{\Phi}^{9} \qquad \underline{\Phi}^{4} = -\begin{bmatrix} \beta & 0 & -\gamma \\ 0 & \alpha & 0 \\ -\gamma & 0 & \beta \end{bmatrix} = \underline{\Phi}^{10}$$

$$\underline{\Phi}^{5} = -\begin{bmatrix} \beta & \gamma & 0 \\ \gamma & \beta & 0 \\ 0 & 0 & \alpha \end{bmatrix} = \underline{\Phi}^{11} \qquad \underline{\Phi}^{6} = -\begin{bmatrix} \beta & -\gamma & 0 \\ -\gamma & \beta & 0 \\ 0 & 0 & \alpha \end{bmatrix} = \underline{\Phi}^{12}$$

In accordance with (3.98), we take the value of $\underline{\Phi}^{\ell}$ when ℓ stands for the triad (0,0,0), to be

$$\underline{\Phi}^{0} = -\sum_{\ell=1}^{12} \underline{\Phi}^{\ell} = 4(\alpha+2\beta) \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Section 4b Elastic constants of the face-centred cubic lattice

The procedure of Section 3c(B) will be followed here since it offers some practical advantages over that of Section 3c(A).

The mass of the elementary particle will be denoted by m , Since the indices k are to be omitted for this lattice, the matrix $C(\underline{q})$ is now of order (3 x 3). Its elements, which are given by (3.56), are now

$$C_{\alpha\beta}(\underline{q}) = \sum_{l} \mathcal{D}_{\alpha\beta}\begin{pmatrix} l \\ \cdots \end{pmatrix} e^{-i(\underline{q}\cdot\underline{r}(\frac{l}{\cdots}))} = \mathcal{D}_{\alpha\beta}(\underline{q}) \tag{4.1}$$

If each term in Table 1 is multiplied by a , the lattice constant, the values of the components of $\underline{r}\begin{pmatrix} l \\ \cdots \end{pmatrix}$ can be read off immediately. Since $\mathcal{D}_{\alpha\beta}\begin{pmatrix} l \\ \cdots \end{pmatrix} = \frac{1}{m}\Phi^{l}_{\alpha\beta}$ by (1.8), Table 2 will give, after dividing each matrix by m , the values of $\mathcal{D}_{\alpha\beta}\begin{pmatrix} l \\ \cdots \end{pmatrix}$. With the help then of these two tables, (4.1) gives

$$\overset{(0)}{C}(\underline{q}) = 0 \tag{4.2}$$

$$\overset{(1)}{C}(\underline{q}) = 0 \tag{4.3}$$

$$(4.4)\quad \overset{(2)}{C}(\underline{Q}) = \frac{2a^2}{m}\begin{bmatrix} 2\beta Q_1^2 + (\alpha+\beta)(Q_2^2+Q_3^2) & 2\gamma Q_1 Q_2 & 2\gamma Q_1 Q_3 \\ 2\gamma Q_2 Q_1 & 2\beta Q_2^2 + (\alpha+\beta)(Q_3^2+Q_1^2) & 2\gamma Q_2 Q_3 \\ 2\gamma Q_3 Q_1 & 2\gamma Q_3 Q_2 & 2\beta Q_3^2 + (\alpha+\beta)(Q_1^2+Q_2^2) \end{bmatrix}$$

Since $\overset{(0)}{C}(\underline{Q})$ and $\overset{(1)}{C}(\underline{Q})$ both vanish, equation (3.82) does not exist and (3.83) becomes

$$(4.5)\quad \omega^2 W_\alpha = \sum_\beta \overset{(2)}{C}_{\alpha\beta}(\underline{Q})\, W_\beta$$

and the equation corresponding to (3.97) is

$$(4.6)\quad \begin{bmatrix} \mathcal{D}_{11}'(\underline{Q}) \\ \mathcal{D}_{22}'(\underline{Q}) \\ \mathcal{D}_{33}'(\underline{Q}) \\ \mathcal{D}_{23}'(\underline{Q}) \\ \mathcal{D}_{31}'(\underline{Q}) \\ \mathcal{D}_{12}'(\underline{Q}) \end{bmatrix} = \frac{2a^2}{m}\begin{bmatrix} 2\beta & \alpha+\beta & \alpha+\beta & 0 & 0 & 0 \\ \alpha+\beta & 2\beta & \alpha+\beta & 0 & 0 & 0 \\ \alpha+\beta & \alpha+\beta & 2\beta & 0 & 0 & 0 \\ 0 & 0 & 0 & \gamma & 0 & 0 \\ 0 & 0 & 0 & 0 & \gamma & 0 \\ 0 & 0 & 0 & 0 & 0 & \gamma \end{bmatrix} \begin{bmatrix} Q_1^2 \\ Q_2^2 \\ Q_3^2 \\ 2Q_2Q_3 \\ 2Q_3Q_1 \\ 2Q_1Q_2 \end{bmatrix}$$

When this is compared with (3.97) and it is noted that for this lattice the density $\rho = m/2a^3$, the following relations are seen to hold:-

$$
\left.\begin{aligned}
c_{11} &= c_{22} = c_{33} = \tfrac{1}{a} 2\beta \\
c_{44} &= c_{55} = c_{66} = \tfrac{1}{a}(\alpha+\beta) \\
c_{23}+c_{44} &= c_{31}+c_{55} = c_{12}+c_{66} = \tfrac{1}{a} 2\gamma
\end{aligned}\right\} \quad \text{whence} \quad \left\{\begin{aligned}
\alpha &= a/2\,(2c_{44}-c_{11}) \\
\beta &= a/2\; c_{11} \\
\gamma &= a/2\,(c_{44}+c_{12})
\end{aligned}\right. \tag{4.7}
$$

The remaining elastic constants vanish.

The first of the relations mentioned in the Note at the end of Section 3c(B) has already been used in the formation of $\underline{\Phi}^{\circ}$. The second is automatically satisfied since the large matrix in (4.6) is always symmetric whatever the values of α , β , γ .

Section 4c **Dynamical matrix in the Q-space**

From (1.16) one has

$$\mathcal{D}(\underline{Q}) = \frac{1}{m} \sum_{\ell} \underline{\Phi}^{\ell} e^{-i(\underline{Q}\cdot \underline{r}(\ell))} \tag{4.8}$$

Using Tables 1 and 2 the elements of $\mathcal{D}(\underline{Q})$ are:-

$$\left.\begin{aligned}
\mathcal{D}_{11}(\underline{Q}) &= \tfrac{4}{m}\{\alpha[1-\cos(aQ_2)\cos(aQ_3)]+\beta[2-\cos(aQ_3)\cos(aQ_1)-\cos(aQ_1)\cos(aQ_2)]\}\\
\mathcal{D}_{22}(\underline{Q}) &= \tfrac{4}{m}\{\alpha[1-\cos(aQ_3)\cos(aQ_1)]+\beta[2-\cos(aQ_1)\cos(aQ_2)-\cos(aQ_2)\cos(aQ_3)]\}\\
\mathcal{D}_{33}(\underline{Q}) &= \tfrac{4}{m}\{\alpha[1-\cos(aQ_1)\cos(aQ_2)]+\beta[2-\cos(aQ_2)\cos(aQ_3)-\cos(aQ_3)\cos(aQ_1)]\}\\
\mathcal{D}_{23}(\underline{Q}) &= \tfrac{4}{m}\gamma\sin(aQ_2)\sin(aQ_3) = \mathcal{D}_{32}(\underline{Q})\\
\mathcal{D}_{31}(\underline{Q}) &= \tfrac{4}{m}\gamma\sin(aQ_3)\sin(aQ_1) = \mathcal{D}_{13}(\underline{Q})\\
\mathcal{D}_{12}(\underline{Q}) &= \tfrac{4}{m}\gamma\sin(aQ_1)\sin(aQ_2) = \mathcal{D}_{21}(\underline{Q})
\end{aligned}\right\} \tag{4.9}$$

Write

$$\cos(aQ_\alpha) = c_\alpha \qquad \sin(aQ_\alpha) = s_\alpha \qquad (\alpha = 1,2,3) \tag{4.10}$$

and put

$$F_1 = \frac{4}{m}\left[\alpha\left[1-c_2c_3\right]+\beta\left[2-c_3c_1-c_1c_2\right]-\gamma s_1^2\right]$$

(4.11)

$$F_2 = \frac{4}{m}\left[\alpha\left[1-c_3c_1\right]+\beta\left[2-c_1c_2-c_2c_3\right]-\gamma s_2^2\right]$$

$$F_3 = \frac{4}{m}\left[\alpha\left[1-c_1c_2\right]+\beta\left[2-c_2c_3-c_3c_1\right]-\gamma s_3^2\right]$$

Then the dynamical matrix may be written as :-

(4.12)

$$\mathcal{D}(\underline{q}) = \begin{bmatrix} F_1+\frac{4\gamma}{m}s_1^2 & \frac{4\gamma}{m}s_1s_2 & \frac{4\gamma}{m}s_1s_3 \\ \frac{4\gamma}{m}s_2s_1 & F_2+\frac{4\gamma}{m}s_2^2 & \frac{4\gamma}{m}s_2s_3 \\ \frac{4\gamma}{m}s_3s_1 & \frac{4\gamma}{m}s_3s_2 & F_3+\frac{4\gamma}{m}s_3^2 \end{bmatrix}$$

The matrix $\mathcal{D}(\underline{q})$ is clearly periodic in the components of $\underline{q}$ with period $\frac{2\pi}{a}$, and it will be sufficient to consider its value in a cube of the Q-space defined by $-\pi/a \leq q \leq \pi/a$. By the symmetry of the face-centred cubic lattice, only one-eighth of this cube is actually needed. In order to give results which could be compared with those obtained by Iona (1941) in his calculation of $\mathcal{D}(\underline{q})$ ($A(\varphi)$ in his notation) by means of a numerical formula due to Waller, the values of the elastic constants were taken to be those of the substance which Iona considered, namely potassium chloride (Försterling, 1920), although its lattice is neither monatomic nor face-centred. With this assumption, the values of $\mathcal{D}(\underline{q})$ were calculated for representative set of points and are given in Table 3.

Table 3 — The dynamical matrix

The values of $m\,\mathcal{D}(\mathbf{q})$ are given in dynes cm.$^{-1}$

The units of q_1 , q_2 , q_3 , are π/a where $a = 3.12 \times 10^{-8}$ cm.

q_1	q_2	q_3	$m\mathcal{D}_{11}(\mathbf{q})\times10^{-3}$	$m\mathcal{D}_{22}(\mathbf{q})\times10^{-3}$	$m\mathcal{D}_{33}(\mathbf{q})\times10^{-3}$	$m\mathcal{D}_{12}(\mathbf{q})\times10^{-3}$	$m\mathcal{D}_{31}(\mathbf{q})\times10^{-3}$	$m\mathcal{D}_{23}(\mathbf{q})\times10^{-3}$
0	0	1/4	1.13	1.13	6.97	0.00	0.00	0.00
0	0	1/2	4.06	4.06	24.00	0.00	0.00	0.00
0	0	3/4	6.94	6.94	41.02	0.00	0.00	0.00
0	0	1	8.12	8.12	47.98	0.00	0.00	0.00
0	1/4	1/4	2.99	7.18	7.18	2.03	0.00	1.00
0	1/4	1/2	7.53	7.53	21.68	2.88	0.00	0.00
0	1/4	3/4	12.09	7.90	36.20	2.03	0.00	0.00
0	1/4	1	13.90	8.12	42.20	0.00	0.00	0.00
0	1/2	1/2	16.06	16.06	16.06	4.06	0.00	0.00
0	1/2	3/4	24.59	10.43	24.59	2.88	0.00	0.00
0	1/2	1	28.05	8.12	28.05	0.00	0.00	0.00
0	3/4	3/4	37.05	12.93	12.93	2.03	0.00	0.00
0	3/4	1	42.20	13.90	13.90	0.00	0.00	0.00
0	1	1	47.98	8.12	8.12	0.00	0.00	0.00
1/4	1/4	1/4	8.03	8.03	8.03	2.03	2.03	2.03
1/4	1/4	1/2	10.06	10.06	20.03	2.88	2.88	2.03
1/4	1/4	3/4	12.09	12.09	32.02	2.03	2.03	2.03
1/4	1/4	1	12.93	12.93	37.05	0.00	0.00	2.03
1/4	1/2	1/2	16.06	16.06	16.06	4.06	2.88	2.88
1/4	1/2	3/4	22.06	12.09	22.06	2.88	2.03	2.88
1/4	1/2	1	24.59	10.43	24.59	0.00	0.00	2.88
1/4	3/4	3/4	32.02	12.09	12.09	2.03	2.03	2.03
1/4	3/4	1	36.20	7.90	12.09	0.00	0.00	2.03
1/4	1	1	41.02	6.94	6.94	0.00	0.00	0.00
1/2	1/2	1/2	16.06	16.06	16.06	4.06	4.06	4.06
1/2	1/2	3/4	16.06	16.06	16.06	2.88	2.88	4.06
1/2	1/2	1	16.06	16.06	16.06	0.00	0.00	4.06
1/2	3/4	3/4	20.03	10.06	10.06	2.03	2.88	2.88
1/2	3/4	1	21.68	7.53	7.53	0.00	0.00	2.88
1/2	1	1	24.00	4.06	4.06	0.00	0.00	0.00
3/4	3/4	3/4	8.03	8.03	8.03	2.03	2.03	2.03
3/4	3/4	1	7.18	7.18	2.99	0.00	0.00	2.03
3/4	1	1	6.94	1.19	1.19	0.00	0.00	0.00

Section 5 Monatomic hexagonal close-packed lattice

In this lattice there are two particles in the unit cell, $k = 1$ and $k = 2$. The cell vectors $\underline{a}^1$, $\underline{a}^2$, $\underline{a}^3$, are such that the angle between $\underline{a}^1$ and $\underline{a}^2$ is $\frac{2\pi}{3}$, and $\underline{a}^3$ is at right angles to the plane of $\underline{a}^1$ and $\underline{a}^2$, in the direction that makes the system of axes right-handed; $|\underline{a}^1| = |\underline{a}^2| = a$, $|a^3| = c$; $c^2 = 8/3 a^2$.

Only those matrices $\Phi\left(\begin{smallmatrix} \ell-\ell' \\ k k' \end{smallmatrix}\right)$ will be considered which arise from the first neighbours of the two particles in a chosen unit cell. These two particles are labelled O and O' in Figs. II and III. Each point has twelve first neighbours, six in a plane containing the point, and three above and three below this plane. ℓ' which stands for the indices of the basic cell containing O and O', will be taken to represent the triad (0,0,0). For convenience in writing the symmetry relations later, a single symbol P is introduced in place of the composite symbol $\left(\begin{smallmatrix} \ell \\ k k' \end{smallmatrix}\right)$, i.e. Φ^P is written for $\Phi\left(\begin{smallmatrix} \ell \\ k k' \end{smallmatrix}\right)$. This suggests that the <u>line</u> joining O or O' to a point be labelled by the letter P. The lines radiating from O' are distinguished by a dash in their symbol, while those from O are unaccented. Each of these sets is further sub-divided into two sets of six, related to each other by a certain symmetry operation described in the next Section. This is made clear by a bar over half of

the symbols. The complete tabulation may be represented schematically thus:-

$$P \text{ includes } \begin{cases} p \text{ includes } 1,2,3,4,5,6 \\ \bar{p} \text{ includes } \bar{1},\bar{2},\bar{3},\bar{4},\bar{5},\bar{6} \end{cases} \text{Neighbours of } O.$$

$$\begin{cases} p' \text{ includes } 1',2',3',4',5',6' \\ \bar{p}' \text{ includes } \bar{1}',\bar{2}',\bar{3}',\bar{4}',\bar{5}',\bar{6}' \end{cases} \text{Neighbours of } O'.$$

The six particles that lie in a plane containing the point O are taken to be of the type $k = 1$, the six that lie in the plane containing O' are of the type $k = 2$, and so on alternately, so that the particles of one type lie on a set of planes that interleave the set of planes which contain the other type of particles.

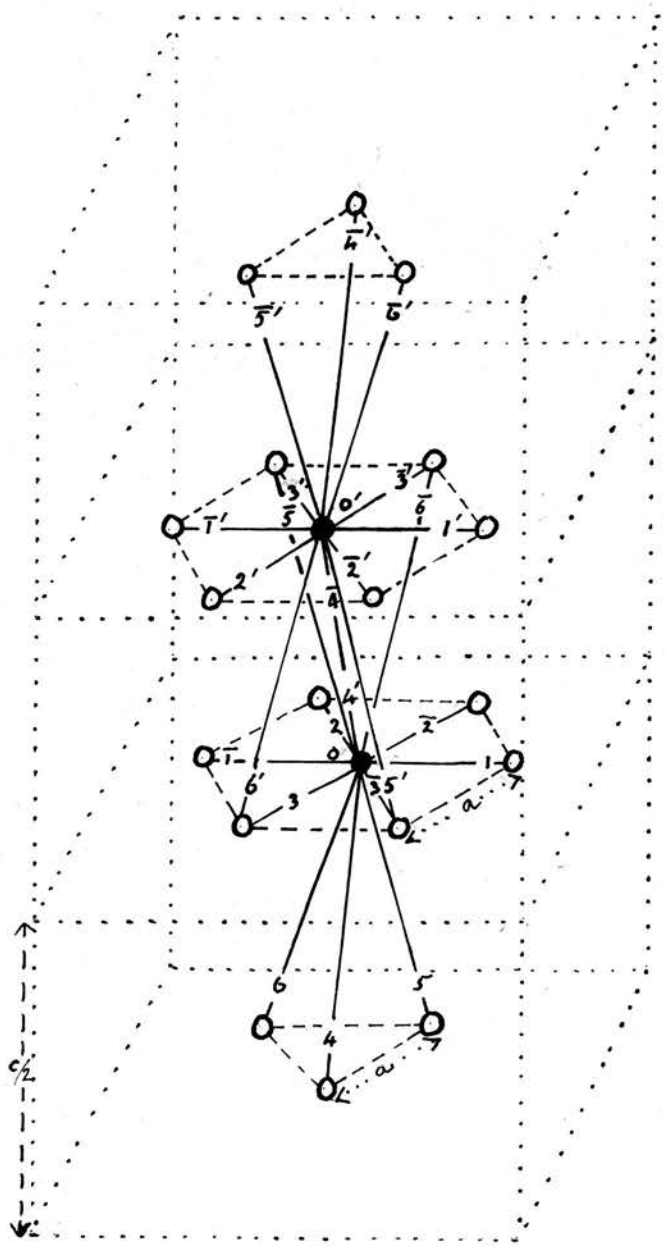
The connection between the symbols P and $\binom{l}{kk'}$ is given in the Table below:

Table 4

l \ P	1	2	3	4	5	6	$\bar{1}$	$\bar{2}$	$\bar{3}$	$\bar{4}$	$\bar{5}$	$\bar{6}$
l^1	0	-1	1	0	-1	-1	0	-1	1	0	-1	-1
l^2	1	-1	0	0	0	-1	-1	0	1	0	-1	0
l^3	0	0	0	-1	-1	-1	0	0	0	0	0	0
(kk')	(11)	(11)	(11)	(21)	(21)	(21)	(11)	(11)	(11)	(21)	(21)	(21)
l \ P	$1'$	$2'$	$3'$	$4'$	$5'$	$6'$	$\bar{1}'$	$\bar{2}'$	$\bar{3}'$	$\bar{4}'$	$\bar{5}'$	$\bar{6}'$
l^1	0	1	-1	0	1	1	0	1	-1	0	1	1
l^2	1	0	-1	0	1	0	-1	1	0	0	0	1
l^3	0	0	0	0	0	0	0	0	0	1	1	1
(kk')	(22)	(22)	(22)	(12)	(12)	(12)	(22)	(22)	(22)	(12)	(12)	(12)

Figure II

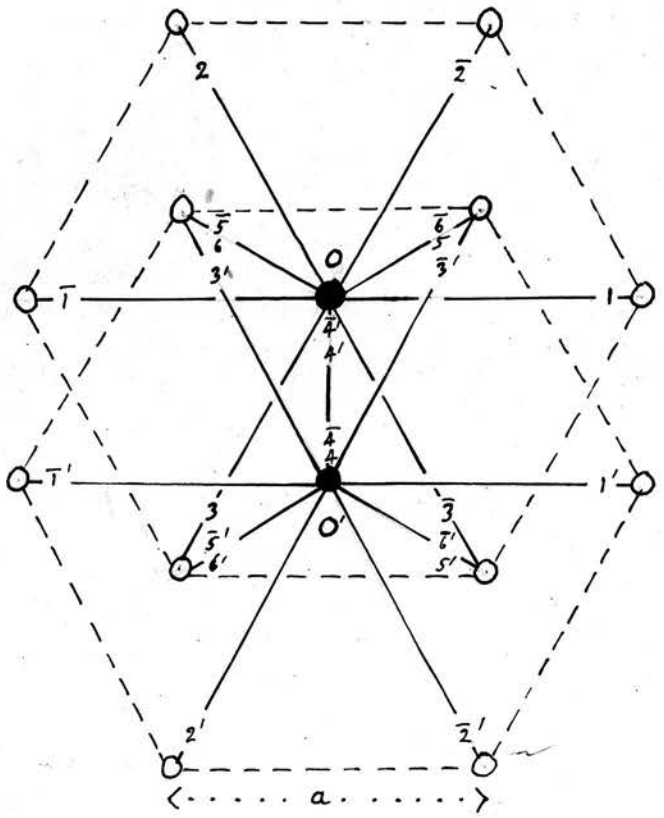
First neighbours of the two points in the unit cell of the close-packed hexagonal lattice

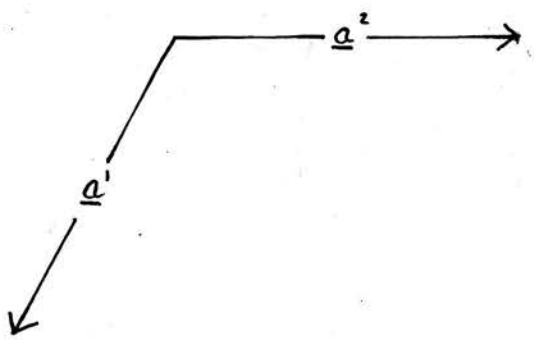


The vertical scale has been exaggerated for clarity.

Figure III

Projection of the structure in Fig. II
on to a plane perpendicular to the lattice vector $\underline{a}^3$.





Section 5a — Symmetry of the hexagonal close-packed lattice.

The right-angled system S with axes (x_1 , x_2 , x_3) is so oriented that x_1 lies along the positive direction of $\underline{a}^2$ and x_3 along the positive direction of $\underline{a}^3$.

The symmetry operations form a group (the space-group) which may be generated by the following three primitive operations:-

A_1

A six-fold axis of rotatory inversion in the direction of the x_3 -axis, that is to say, a rotation of amount $\pi/3$ or a multiple of $\pi/3$ about the x_3 - axis together with an inversion in the origin. This operation can be represented by the matrix :-

$$T_r = \begin{bmatrix} -1/2 & -\sqrt{3}/2 & 0 \\ \sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

The change of the label P is specified in the same way as that used for the face-centred cubic lattice, by the notation of substitution groups. In this case, the change is denoted by:-

$$(3\ 2\ 1)(\bar{1}\ \bar{2}\ \bar{3})(5\ \bar{4}\ 6\ \bar{5}\ 4\ \bar{5})$$

A_2

A two-fold axis of rotation namely the x_2 -axis.

This has the matrix:-

$$T_u = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

and for the change of label one has, briefly,

$$(p\,\bar{p})$$

A_3

A glide-plane. This involves a reflection in the plane $x_2 = -a/\sqrt{3}$ followed by a translation of amount $x_1 = 0$, $x_2 = 0$, $x_3 = c/2$, parallel to this plane. This is equivalent to a reflection in $x_2 = 0$ together with a translation of amount $x_1 = 0$, $x_2 = -\frac{2a}{\sqrt{3}}$, $x_3 = c/2$. The latter only affects the change of label and the T -matrix is therefore that due to the reflection in $x_2 = 0$ i.e.

$$T_g = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

along with

$$(p\,p')\,(\bar{p}\,\bar{p}')$$

In addition use will also be made of the following three combinations of these three primitive operations.

A_4

A reflection in the plane $x_3 = 0$. This is repres-

ented by the matrix:-

$$(T_r)^3 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

with

$$(1)\,(2)\,(3)\,(\bar{1})\,(\bar{2})\,(\bar{3})\,(5\bar{6})\,(6\bar{5})\,(4\bar{4})$$

A_5

A reflection in the plane $x_1 = 0$. For this one has

$$T_u\,(T_r)^3 = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

with

$$(1\bar{1})\,(2\bar{2})\,(3\bar{3})\,(56)\,(\bar{5}\,\bar{6})\,(4)\,(\bar{4})$$

A_6

From A_2 it follows that

$$\Phi^{\mu} = T_u\,\Phi^{\bar{\mu}}\,\tilde{T}_u$$

$$= \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \Phi^{\bar{\mu}} \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

$$= \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \Phi^{\bar{\mu}} \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$= T_g\,\Phi^{\bar{\mu}}\,\tilde{T}_g \quad = \Phi^{\mu'} \text{ by } A_3$$

Similarly $\Phi^{\bar{\mu}} = \Phi^{\mu'}$

A_7

Lastly the symmetry properties (1.6) are needed. They are expressed by :-

$$\underline{\Phi}^{1} = \underline{\tilde{\Phi}}^{7} \qquad \underline{\Phi}^{4} = \underline{\tilde{\Phi}}^{\bar{4}'} \qquad \underline{\Phi}^{1'} = \underline{\tilde{\Phi}}^{7'} \qquad \underline{\Phi}^{4'} = \underline{\tilde{\Phi}}^{\bar{4}}$$

$$\underline{\Phi}^{2} = \underline{\tilde{\Phi}}^{\bar{3}} \qquad \underline{\Phi}^{5} = \underline{\tilde{\Phi}}^{\bar{6}'} \qquad \underline{\Phi}^{2'} = \underline{\tilde{\Phi}}^{\bar{3}'} \qquad \underline{\Phi}^{5'} = \underline{\tilde{\Phi}}^{\bar{6}}$$

$$\underline{\Phi}^{3} = \underline{\tilde{\Phi}}^{\bar{2}} \qquad \underline{\Phi}^{6} = \underline{\tilde{\Phi}}^{\bar{5}'} \qquad \underline{\Phi}^{3'} = \underline{\tilde{\Phi}}^{\bar{2}'} \qquad \underline{\Phi}^{6'} = \underline{\tilde{\Phi}}^{\bar{5}}$$

C a l c u l a t i o n

Only the twelve matrices $\underline{\Phi}^{p}$ and $\underline{\Phi}^{\bar{p}}$ need be calculated since A_6 gives $\underline{\Phi}^{p'}$ and $\underline{\Phi}^{\bar{p}'}$ immediately.

From A_4 ,

$$\begin{bmatrix} \Phi'_{11} & \Phi'_{12} & \Phi'_{13} \\ \Phi'_{21} & \Phi'_{22} & \Phi'_{23} \\ \Phi'_{31} & \Phi'_{32} & \Phi'_{33} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} \Phi'_{11} & \Phi'_{12} & \Phi'_{13} \\ \Phi'_{21} & \Phi'_{22} & \Phi'_{23} \\ \Phi'_{31} & \Phi'_{32} & \Phi'_{33} \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

Hence $\Phi'_{13} = \Phi'_{31} = \Phi'_{23} = \Phi'_{32} = 0$

Let $\underline{\Phi}^{1} = -\begin{bmatrix} \alpha+2\beta & \delta & 0 \\ \epsilon & \alpha-2\beta & 0 \\ 0 & 0 & \gamma \end{bmatrix}$ The notation is chosen to avoid fractions

Now $\underline{\Phi}^{7} = -\begin{bmatrix} \alpha+2\beta & -\delta & 0 \\ -\epsilon & \alpha-2\beta & 0 \\ 0 & 0 & \gamma \end{bmatrix}$ by A_2

But $\underline{\Phi}^{\bar{1}} = -\begin{bmatrix} \lambda+2\mu & \epsilon & 0 \\ \delta & \lambda-2\mu & 0 \\ 0 & 0 & \gamma \end{bmatrix}$ by A_7

Hence $\epsilon = -\delta$

Now $\underline{\Phi}^{\bar{2}}$, $\underline{\Phi}^{\bar{3}}$, $\underline{\Phi}^{\bar{\bar{1}}}$, $\underline{\Phi}^{\bar{\bar{3}}}$, may be calculated directly from A_1. Thus $\underline{\Phi}^{\bar{2}} = T_r \underline{\Phi}^{\bar{1}} \tilde{T}_r$ and $\underline{\Phi}^{\bar{3}} = T_r \underline{\Phi}^{\bar{2}} \tilde{T}_r$, where for a general $\underline{\Phi}$-matrix:-

$$T_r \underline{\Phi} \tilde{T}_r = \begin{bmatrix} \frac{1}{4}\Phi_{11} + \frac{\sqrt{3}}{4}\Phi_{21} + \frac{\sqrt{3}}{4}\Phi_{12} + \frac{3}{4}\Phi_{22} & -\frac{\sqrt{3}}{4}\Phi_{11} - \frac{3}{4}\Phi_{21} + \frac{1}{4}\Phi_{12} + \frac{\sqrt{3}}{4}\Phi_{22} & \frac{1}{2}\Phi_{13} + \frac{\sqrt{3}}{2}\Phi_{23} \\ -\frac{\sqrt{3}}{4}\Phi_{11} + \frac{1}{4}\Phi_{21} - \frac{3}{4}\Phi_{12} + \frac{\sqrt{3}}{4}\Phi_{22} & \frac{3}{4}\Phi_{11} - \frac{\sqrt{3}}{4}\Phi_{21} - \frac{\sqrt{3}}{4}\Phi_{12} + \frac{1}{4}\Phi_{22} & -\frac{\sqrt{3}}{2}\Phi_{13} + \frac{1}{2}\Phi_{23} \\ \frac{1}{2}\Phi_{31} + \frac{\sqrt{3}}{2}\Phi_{32} & -\frac{\sqrt{3}}{2}\Phi_{31} + \frac{1}{2}\Phi_{32} & \Phi_{33} \end{bmatrix}$$

Again $\underline{\Phi}^{4} = \underline{\Phi}^{\bar{4}'}$ by A_6. But $\underline{\Phi}^{4} = \tilde{\underline{\Phi}}^{\bar{4}'}$ by A_7. Hence $\underline{\Phi}^{4} = \tilde{\underline{\Phi}}^{4}$. Moreover from A_5, one has

$$\begin{bmatrix} \Phi^4_{11} & \Phi^4_{12} & \Phi^4_{31} \\ \Phi^4_{12} & \Phi^4_{22} & \Phi^4_{23} \\ \Phi^4_{31} & \Phi^4_{23} & \Phi^4_{33} \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \Phi^4_{11} & \Phi^4_{12} & \Phi^4_{31} \\ \Phi^4_{12} & \Phi^4_{22} & \Phi^4_{23} \\ \Phi^4_{31} & \Phi^4_{23} & \Phi^4_{33} \end{bmatrix} \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

From which it follows that $\underline{\Phi}^{4}_{12} = \underline{\Phi}^{4}_{31} = 0$

Let $\underline{\Phi}^{4} = -\begin{bmatrix} \lambda+2\mu & 0 & 0 \\ 0 & \lambda-2\mu & 2\sigma \\ 0 & 2\sigma & \nu \end{bmatrix}$ the notation is again chosen to avoid fractions

Then $\overline{\Phi}^{\bar{1}}$, $\overline{\Phi}^{6}$, $\overline{\Phi}^{\bar{2}}$, $\overline{\Phi}^{5}$, $\overline{\Phi}^{\bar{5}}$, can be calculated from A_1 with the help of the formula for $T_r \overline{\Phi} \tilde{T}_r$ om the preceding page.

The complete results are

Table 5

$$\overline{\Phi}^{1} = -\begin{bmatrix} \alpha+2\beta & \delta & 0 \\ -\delta & \alpha-2\beta & 0 \\ 0 & 0 & \gamma \end{bmatrix} = \overline{\Phi}^{\bar{1}\prime} \qquad \overline{\Phi}^{\bar{1}} = -\begin{bmatrix} \alpha+2\beta & -\delta & 0 \\ \delta & \alpha-2\beta & 0 \\ 0 & 0 & \gamma \end{bmatrix} = \overline{\Phi}^{1\prime}$$

$$\overline{\Phi}^{2} = -\begin{bmatrix} \alpha-\beta & \delta-\sqrt{3}\beta & 0 \\ -\delta-\sqrt{3}\beta & \alpha+\beta & 0 \\ 0 & 0 & \gamma \end{bmatrix} = \overline{\Phi}^{\bar{2}\prime} \qquad \overline{\Phi}^{\bar{2}} = -\begin{bmatrix} \alpha-\beta & -\delta+\sqrt{3}\beta & 0 \\ \delta+\sqrt{3}\beta & \alpha+\beta & 0 \\ 0 & 0 & \gamma \end{bmatrix} = \overline{\Phi}^{2\prime}$$

$$\overline{\Phi}^{3} = -\begin{bmatrix} \alpha-\beta & \delta+\sqrt{3}\beta & 0 \\ -\delta+\sqrt{3}\beta & \alpha+\beta & 0 \\ 0 & 0 & \gamma \end{bmatrix} = \overline{\Phi}^{\bar{3}\prime} \qquad \overline{\Phi}^{\bar{3}} = -\begin{bmatrix} \alpha-\beta & -\delta-\sqrt{3}\beta & 0 \\ \delta-\sqrt{3}\beta & \alpha+\beta & 0 \\ 0 & 0 & \gamma \end{bmatrix} = \overline{\Phi}^{3\prime}$$

$$\overline{\Phi}^{4} = -\begin{bmatrix} \lambda+2\mu & 0 & 0 \\ 0 & \lambda-2\mu & 2\sigma \\ 0 & 2\sigma & \nu \end{bmatrix} = \overline{\Phi}^{\bar{4}\prime} \qquad \overline{\Phi}^{\bar{4}} = -\begin{bmatrix} \lambda+2\mu & 0 & 0 \\ 0 & \lambda-2\mu & -2\sigma \\ 0 & -2\sigma & \nu \end{bmatrix} = \overline{\Phi}^{4\prime}$$

$$\overline{\Phi}^{5} = -\begin{bmatrix} \lambda-\mu & -\sqrt{3}\mu & -\sqrt{3}\sigma \\ -\sqrt{3}\mu & \lambda+\mu & -\sigma \\ -\sqrt{3}\sigma & -\sigma & \nu \end{bmatrix} = \overline{\Phi}^{\bar{5}\prime} \qquad \overline{\Phi}^{\bar{5}} = -\begin{bmatrix} \lambda-\mu & \sqrt{3}\mu & -\sqrt{3}\sigma \\ \sqrt{3}\mu & \lambda+\mu & \sigma \\ -\sqrt{3}\sigma & \sigma & \nu \end{bmatrix} = \overline{\Phi}^{5\prime}$$

$$\overline{\Phi}^{6} = -\begin{bmatrix} \lambda-\mu & \sqrt{3}\mu & \sqrt{3}\sigma \\ \sqrt{3}\mu & \lambda+\mu & -\sigma \\ \sqrt{3}\sigma & -\sigma & \nu \end{bmatrix} = \overline{\Phi}^{\bar{6}\prime} \qquad \overline{\Phi}^{\bar{6}} = -\begin{bmatrix} \lambda-\mu & -\sqrt{3}\mu & \sqrt{3}\sigma \\ -\sqrt{3}\mu & \lambda+\mu & \sigma \\ \sqrt{3}\sigma & \sigma & \nu \end{bmatrix} = \overline{\Phi}^{6\prime}$$

The first of the conditions mentioned in the Note at the end of Section 3c(B) will define $\overline{\Phi}\binom{0}{11}$ and $\overline{\Phi}\binom{0}{22}$, or $\overline{\Phi}^{0}$ and $\overline{\Phi}^{0'}$, as they may be called ; thus —

$$\overline{\Phi}^{0} = \overline{\Phi}^{0'} = \begin{bmatrix} 6\alpha+6\lambda & 0 & 0 \\ 0 & 6\alpha+6\lambda & 0 \\ 0 & 0 & 6\gamma+6\nu \end{bmatrix}$$

Section 5b — Elastic constants of the hexagonal close-packed lattice

As in the case of the face-centred cubic lattice, the methods used here will be those of Section 3c(B).

The two particles in the unit cell of this lattice have equal masses m, say. As has been shown in Section 5a, the following relations hold between the $\underline{\Phi}$-matrices.

$$\underline{\Phi}^{b} = \underline{\Phi}^{\bar{b}'}$$

$$\underline{\Phi}^{\bar{b}} = \underline{\Phi}^{b'}$$

with corresponding relations for the $\mathcal{D}$-matrices. But, as is easily seen from the figure,

$$\underline{r}^{b} = -\underline{r}^{\bar{b}'}$$

$$\underline{r}^{\bar{b}} = -\underline{r}^{b'}$$

Hence

$$C\left(\frac{\underline{q}}{11}\right) = C\left(\frac{-\underline{q}}{22}\right) \qquad (5.1)$$

$$C\left(\frac{\underline{q}}{21}\right) = C\left(\frac{-\underline{q}}{12}\right) \qquad (5.2)$$

} by (3.56)

By expanding these matrices in terms of q and equating like powers of q, there arises the following set of equations:-

(5.3) $$C^{(0)}\left(\frac{Q}{11}\right) = C^{(0)}\left(\frac{Q}{22}\right) \qquad C^{(0)}\left(\frac{Q}{21}\right) = C^{(0)}\left(\frac{Q}{12}\right)$$

(5.4) $$C^{(1)}\left(\frac{Q}{11}\right) = -C^{(1)}\left(\frac{Q}{22}\right) \qquad C^{(1)}\left(\frac{Q}{21}\right) = -C^{(1)}\left(\frac{Q}{12}\right)$$

(5.5) $$C^{(2)}\left(\frac{Q}{11}\right) = C^{(2)}\left(\frac{Q}{22}\right) \qquad C^{(2)}\left(\frac{Q}{21}\right) = C^{(2)}\left(\frac{Q}{12}\right)$$

It is therefore only necessary to consider the terms in the expansion of $C\left(\frac{Q}{11}\right)$ and $C\left(\frac{Q}{21}\right)$. The values of $\Upsilon\left(\frac{l}{k\,l'}\right)$ are given in the following Table:-

Table 6

Υ \ p	1	2	3	$\overline{1}$	$\overline{2}$	$\overline{3}$	Υ \ p	4	5	6	$\overline{4}$	$\overline{5}$	$\overline{6}$
$\chi_1\left(\frac{l}{11}\right)$	a	$-a/2$	$-a/2$	$-a$	$a/2$	$a/2$	$\chi_1\left(\frac{l}{21}\right)$	0	$a/2$	$-a/2$	0	$-a/2$	$a/2$
$\chi_2\left(\frac{l}{11}\right)$	0	$a\sqrt{3}/2$	$-a\sqrt{3}/2$	0	$a\sqrt{3}/2$	$-a\sqrt{3}/2$	$\chi_2\left(\frac{l}{21}\right)$	$-a/\sqrt{3}$	$a/2\sqrt{3}$	$a/2\sqrt{3}$	$-a/\sqrt{3}$	$a/2\sqrt{3}$	$a/2\sqrt{3}$
$\chi_3\left(\frac{l}{11}\right)$	0	0	0	0	0	0	$\chi_3\left(\frac{l}{21}\right)$	$-c/2$	$-c/2$	$-c/2$	$c/2$	$c/2$	$c/2$

where $a = |\underline{a}^1| = |\underline{a}^2|$ and $c = |\underline{a}^3|$, and $c^2 = 8/3\, a^2$.

Since $C\left(\frac{Q}{11}\right) = \frac{1}{m} \sum_{p=1,2,3,\overline{1},\overline{2},\overline{3}} \overline{\Phi}^{p}\, e^{-i\,(Q\,.\,\underline{r}^{p})}$ by (3.56), one has for the successive terms in the expansion of $C\left(\frac{Q}{11}\right)$, with the aid of Tables 5 and 6 :-

(5.6) $$C^{(0)}\left(\frac{Q}{11}\right) = \frac{1}{m} \begin{bmatrix} 6\lambda & 0 & 0 \\ 0 & 6\lambda & 0 \\ 0 & 0 & 6\nu \end{bmatrix}$$

$$(5.7)\quad C^{(11)}\left(\frac{Q}{11}\right) = 0$$

$$(5.8)\quad C^{(2)}\left(\frac{Q}{11}\right) = \frac{3a^2}{2m}\begin{bmatrix} (\alpha+\beta)Q_1^2 + (\alpha-\beta)Q_2^2 & 2\beta Q_1 Q_2 & 0 \\ 2\beta Q_2 Q_1 & (\alpha-\beta)Q_1^2 + (\alpha+\beta)Q_2^2 & 0 \\ 0 & 0 & \gamma^*(Q_1^2+Q_2^2) \end{bmatrix}$$

Again from the fact that $C\left(\frac{Q}{21}\right) = \sum_{p=4,5,6,\bar{4},\bar{5},\bar{6}} \Phi^p e^{-i(Q\cdot x^p)}$ it follows that :-

$$(5.9)\quad C^{(0)}\left(\frac{Q}{21}\right) = \frac{1}{m}\begin{bmatrix} -G\lambda & 0 & 0 \\ 0 & -G\lambda & 0 \\ 0 & 0 & -G\nu \end{bmatrix}$$

$$(5.10)\quad C^{(11)}\left(\frac{Q}{21}\right) = -\frac{ia^2\beta\mu}{m}\begin{bmatrix} Q_2 & Q_1 & 0 \\ Q_1 & -Q_2 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$(5.11)\quad C^{(2)}\left(\frac{Q}{21}\right) = \frac{1}{2m}\begin{bmatrix} a^2\left[(\lambda-\mu)Q_1^2+(\lambda+\mu)Q_2^2\right] + \tfrac{3}{2}c^2Q_3^2 & -2a^2\mu\, Q_1Q_2 & 2\sqrt{3}ac\sigma Q_1Q_3 \\ -2a^2\mu\, Q_1Q_2 & a^2\left[(\lambda+\mu)Q_1^2+(\lambda-\mu)Q_2^2\right] + \tfrac{3}{2}c^2Q_3^2 & 2\sqrt{3}ac\sigma Q_2Q_3 \\ 2\sqrt{3}ac\sigma Q_3Q_1 & 2\sqrt{3}ac\sigma Q_3Q_2 & \nu\left[a^2(Q_1^2+Q_2^2)+\tfrac{3}{2}c^2Q_3^2\right] \end{bmatrix}$$

Now if use is made of these values, (3.82) splits up into two identical equations each of which has the form:

$$\frac{1}{m}\begin{bmatrix} 6\lambda & 0 & 0 \\ 0 & 6\lambda & 0 \\ 0 & 0 & 6\nu \end{bmatrix}\left[\underline{\ddot{w}}(2)-\underline{\ddot{w}}(1)\right] = -\frac{ia\,2\sqrt{3}\mu}{\sqrt{m}}\begin{bmatrix} q_2 & q_1 & 0 \\ q_1 & -q_2 & 0 \\ 0 & 0 & 0 \end{bmatrix}\underline{W}$$

i.e.

$$\underline{\ddot{w}}(1)-\underline{\ddot{w}}(2) = \frac{ia\,2\sqrt{3}\mu\sqrt{m}}{\lambda}\begin{bmatrix} q_2 & q_1 & 0 \\ q_1 & -q_2 & 0 \\ 0 & 0 & 0 \end{bmatrix}\underline{W} \qquad (5.12)$$

Equation 3.83) may be written as :-

$$\omega^2\underline{W} = \left[C^{(1)}\left(\frac{q}{11}\right)+C^{(2)}\left(\frac{q}{21}\right)+C^{(2)}\left(\frac{q}{12}\right)+C^{(2)}\left(\frac{q}{22}\right)\right]\underline{W} + \frac{1}{\sqrt{m}}C^{(1)}\left(\frac{q}{21}\right)\left[\underline{\ddot{w}}(1)-\underline{\ddot{w}}(2)\right] \qquad (5.13)$$

Now

$$\frac{1}{\sqrt{m}}C^{(1)}\left(\frac{q}{21}\right)\left[\underline{\ddot{w}}(1)-\underline{\ddot{w}}(2)\right] = \frac{2a^2\mu^2}{\lambda m}\begin{bmatrix} q_2 & q_1 & 0 \\ q_1 & -q_2 & 0 \\ 0 & 0 & 0 \end{bmatrix}\begin{bmatrix} q_2 & q_1 & 0 \\ q_1 & -q_2 & 0 \\ 0 & 0 & 0 \end{bmatrix}\underline{W}$$

$$= \frac{2a^2\mu^2}{\lambda m}\begin{bmatrix} q_1^2+q_2^2 & 0 & 0 \\ 0 & q_1^2+q_2^2 & 0 \\ 0 & 0 & 0 \end{bmatrix}\underline{W}$$

Hence (5.13) becomes

$$\omega^2 W_\alpha = \sum_\beta D'_{\alpha\beta}\left(\underline{q}\right)W_\beta \qquad (5.14)$$

where

$$
(5.15)\qquad
\begin{bmatrix} \mathcal{D}'_{11}(\underline{Q}) \\ \mathcal{D}'_{22}(\underline{Q}) \\ \mathcal{D}'_{33}(\underline{Q}) \\ \mathcal{D}'_{23}(\underline{Q}) \\ \mathcal{D}'_{31}(\underline{Q}) \\ \mathcal{D}'_{12}(\underline{Q}) \end{bmatrix} =
$$

$$
\frac{1}{m}
\begin{bmatrix}
-\frac{2\mu^2}{\lambda}a^2 + (3\alpha+3\beta+\lambda-\mu)a^2 & -\frac{2\mu^2}{\lambda}a^2 + (3\alpha-3\beta+\lambda+\mu)a^2 & \frac{3}{2}c^2\lambda & 0 & 0 & 0 \\
-\frac{2\mu^2}{\lambda}a^2 + (3\alpha-3\beta+\lambda+\mu)a^2 & -\frac{2\mu^2}{\lambda}a^2 + (3\alpha+3\beta+\lambda-\mu)a^2 & \frac{3}{2}c^2\lambda & 0 & 0 & 0 \\
(3\gamma+\nu)a^2 & (3\gamma+\nu)a^2 & \frac{3}{2}c^2\lambda & 0 & 0 & 0 \\
0 & 0 & 0 & \sqrt{3}ac\sigma & 0 & 0 \\
0 & 0 & 0 & 0 & \sqrt{3}ac\sigma & 0 \\
0 & 0 & 0 & 0 & 0 & a^2(3\beta-\mu)
\end{bmatrix}
\times
\begin{bmatrix} Q_1^2 \\ Q_2^2 \\ Q_3^2 \\ 2Q_2Q_3 \\ 2Q_3Q_1 \\ 2Q_1Q_2 \end{bmatrix}
$$

On comparing this with (3.97) and noting that for this lattice $\rho = \frac{4m}{\sqrt{3}a^2c}$, one has

$$
\left\{
\begin{aligned}
C_{11} = C_{22} &= \frac{4}{\sqrt{3}a^2c}\left[-\frac{2\mu^2}{\lambda}a^2 + (3\lambda+3\beta+\lambda-\mu)a^2\right] \\
C_{33} &= \frac{4}{\sqrt{3}a^2c}\left[\tfrac{3}{2}c^2\nu\right] \\
C_{44} = C_{55} &= \frac{4}{\sqrt{3}a^2c}\left[\tfrac{3}{2}c^2\lambda\right] \\
C_{66} &= \frac{4}{\sqrt{3}a^2c}\left[-\frac{2\mu^2}{\lambda}a^2 + (3\lambda-3\beta+\lambda+\mu)a^2\right] \\
C_{23} = C_{31} &= \frac{4}{\sqrt{3}a^2c}\left[2\sqrt{3}ac\sigma - \tfrac{3}{2}c^2\lambda\right] \\
C_{12} &= \frac{4}{\sqrt{3}a^2c}\left[\frac{2\mu^2}{\lambda}a^2 - (3\lambda-9\beta+\lambda+3\mu)a^2\right]
\end{aligned}
\right. \qquad (5.16)
$$

The remaining elastic constants vanish. From the expressions above, the well-known hexagonal symmetry relations† (see e.g. Voigt 1910) are seen to be satisfied. The first condition of the Note at the end of Section 3c(B) has been used in the definition of Φ^0 and $\Phi^{0\prime}$. The second, namely that the large matrix in (5.15) should be symmetric, gives

$$
\tfrac{3}{2}c^2\lambda = (3\gamma+\nu)a^2 \quad \text{or} \quad 4\lambda = 3\gamma+\nu \qquad (5.17)
$$

† e.g. $c_{66} = \tfrac{1}{2}(c_{11}-c_{12})$

Section 5c **Dynamical matrix in the Q-space**

The relations (5.1) and (5.2) apply mutatis mutandis to the matrices $\mathcal{D}\left(\frac{Q}{\alpha\beta}\right)$, so that :-

$$\mathcal{D}\left(\frac{Q}{11}\right) = \mathcal{D}\left(\frac{-Q}{22}\right) \tag{5.18}$$

$$\mathcal{D}\left(\frac{Q}{21}\right) = \mathcal{D}\left(\frac{-Q}{12}\right) \tag{5.19}$$

It is therefore only necessary to calculate $\mathcal{D}\left(\frac{Q}{11}\right)$ and $\mathcal{D}\left(\frac{Q}{21}\right)$. Hence from (1.16):-

$$\left.\begin{aligned}
\mathcal{D}_{11}\left(\tfrac{Q}{11}\right) &= 6\lambda + 4(\lambda+2\beta)\left[1-\cos^2\left(\tfrac{aQ_1}{2}\right)\right] + 4(\lambda-\beta)\left[1-\cos\left(\tfrac{aQ_1}{2}\right)\cos\left(\tfrac{a\sqrt{3}Q_2}{2}\right)\right] \\
\mathcal{D}_{22}\left(\tfrac{Q}{11}\right) &= 6\lambda + 4(\lambda-2\beta)\left[1-\cos^2\left(\tfrac{aQ_1}{2}\right)\right] + 4(\lambda+\beta)\left[1-\cos\left(\tfrac{aQ_1}{2}\right)\cos\left(\tfrac{a\sqrt{3}Q_2}{2}\right)\right] \\
\mathcal{D}_{33}\left(\tfrac{Q}{11}\right) &= 6\nu + 4\gamma\left[2-\cos^2\left(\tfrac{aQ_1}{2}\right) - \cos\left(\tfrac{aQ_1}{2}\right)\cos\left(\tfrac{a\sqrt{3}Q_2}{2}\right)\right] \\
\mathcal{D}_{23}\left(\tfrac{Q}{11}\right) &= \mathcal{D}_{32}\left(\tfrac{Q}{11}\right) = \mathcal{D}_{31}\left(\tfrac{Q}{11}\right) = \mathcal{D}_{13}\left(\tfrac{Q}{11}\right) = 0 \\
\mathcal{D}_{12}\left(\tfrac{Q}{11}\right) &= 4\sqrt{3}\beta\sin\left(\tfrac{aQ_1}{2}\right)\sin\left(\tfrac{a\sqrt{3}Q_2}{2}\right) + 4i\delta\sin\left(\tfrac{aQ_1}{2}\right)\left[\cos\left(\tfrac{aQ_1}{2}\right) - \cos\left(\tfrac{a\sqrt{3}Q_2}{2}\right)\right] \\
\mathcal{D}_{21}\left(\tfrac{Q}{11}\right) &= 4\sqrt{3}\beta\sin\left(\tfrac{aQ_1}{2}\right)\sin\left(\tfrac{a\sqrt{3}Q_2}{2}\right) - 4i\delta\sin\left(\tfrac{aQ_1}{2}\right)\left[\cos\left(\tfrac{aQ_1}{2}\right) - \cos\left(\tfrac{a\sqrt{3}Q_2}{2}\right)\right]
\end{aligned}\right\} \tag{5.20}$$

$$
\begin{cases}
D_{11}\left(\frac{q}{2\nu}\right) = -2(\lambda+2\mu)\cos\left(\frac{cq_3}{2}\right)e^{i\frac{aq_2}{\sqrt{3}}} - 4(\lambda-\mu)\cos\left(\frac{cq_3}{2}\right)\cos\left(\frac{aq_1}{2}\right)e^{-i\frac{aq_2}{2\sqrt{3}}} \\
D_{22}\left(\frac{q}{2\nu}\right) = -2(\lambda+2\mu)\cos\left(\frac{cq_3}{2}\right)e^{i\frac{aq_2}{\sqrt{3}}} - 4(\lambda+\mu)\cos\left(\frac{cq_3}{2}\right)\cos\left(\frac{aq_1}{2}\right)e^{-i\frac{aq_2}{2\sqrt{3}}} \\
D_{33}\left(\frac{q}{2\nu}\right) = -2\nu\cos\left(\frac{cq_3}{2}\right)\left[e^{i\frac{aq_2}{\sqrt{3}}} + 2\cos\left(\frac{aq_1}{2}\right)e^{-i\frac{aq_2}{2\sqrt{3}}}\right] \\
D_{23}\left(\frac{q}{2\nu}\right) = D_{32}\left(\frac{q}{2\nu}\right) = 4i\sigma\sin\left(\frac{cq_3}{2}\right)\left[\cos\left(\frac{aq_1}{2}\right)e^{-i\frac{aq_2}{2\sqrt{3}}} - e^{i\frac{aq_2}{\sqrt{3}}}\right] \\
D_{31}\left(\frac{q}{2\nu}\right) = D_{13}\left(\frac{q}{2\nu}\right) = 4\sqrt{3}\sigma\sin\left(\frac{cq_3}{2}\right)\sin\left(\frac{aq_1}{2}\right)e^{-i\frac{aq_2}{2\sqrt{3}}} \\
D_{12}\left(\frac{q}{2\nu}\right) = D_{21}\left(\frac{q}{2\nu}\right) = -4\sqrt{3}i\mu\cos\left(\frac{cq_3}{2}\right)\sin\left(\frac{aq_1}{2}\right)e^{-i\frac{aq_2}{2\sqrt{3}}}
\end{cases}
\tag{5.21}
$$

In the method of calculating the scattering power which is applied to this lattice (Section 8), detailed numerical calculation of the dynamical matrix, such as was carried out for the face-centred lattice in Section 4c, is not needed.

CHAPTER III

INTENSITY OF THE BACKGROUND SCATTERING

Section 6 Representation of the scattering power

In order to give a graphical illustration of the results of this work it is necessary to introduce the notion of the reciprocal lattice. The latter is defined by its three base vectors:-

$$\underline{b}^1 = \frac{\underline{a}^2 \wedge \underline{a}^3}{[\underline{a}^1 \cdot \underline{a}^2 \wedge \underline{a}^3]} \qquad \underline{b}^2 = \cdot \cdot \cdot \tag{6.1}$$

$$\underline{a}^i \cdot \underline{b}^j = \delta^{ij} \qquad \delta^{ij} = \begin{cases} 1 \text{ if } i = j \\ 0 \text{ if } i \neq j \end{cases} \tag{6.2}$$

Now the well-known conditions for selective reflections (Bragg, Laue) have been shown to be equivalent to the statement that the intensity distribution of the Laue scattering has infinitely high and sharp maxima when

$$\underline{\varrho} = \underline{\varrho}^{(h)} \quad \text{where} \quad \underline{\varrho}^{(h)} \cdot \underline{a}^\alpha = 2\pi h^\alpha \tag{6.3}$$

(see e.g Born,1943) $\alpha = 1, 2, 3$; h^1, h^2, h^3 are integers.

The similarity of this with $r^{(\ell)} \cdot \underline{b}^\alpha = \ell^\alpha$ has suggested (Lonsdale and Smith,1941, Jahn.1941/2, Weigle,1941/2) that the vectors $\frac{1}{2\pi}\underline{\varrho}$ be interpreted as position vectors in the space of the reciprocal lattice ("reciprocal space"), so that the points whose position vectors are $\frac{1}{2\pi}\underline{\varrho}^{(h)}$ will be the lattice points of this lattice and will correspond to selective reflections.

Section 6a Interpretation of the general formula

The points $\underline{Q}^{(h)}$ of selective reflection in the Q-space will be surrounded by a distribution $\sigma_b(\underline{Q})$ of scattering power. If $\underline{Q}^{(h)}$ is that reciprocal lattice vector whose end-point lies nearest to that of $\underline{Q}$, then one writes $\underline{Q} - \underline{Q}^{(h)} = \underline{q}$. Now

$$(6.4) \quad \mathcal{D}_{\lambda\rho}\left(\frac{Q}{k k'}\right) = \mathcal{D}_{\lambda\rho}\left(\frac{\underline{Q}^{(h)}+\underline{q}}{k k'}\right)$$

$$= \sum_{l} \mathcal{D}_{\lambda\rho}\left(\frac{l}{k k'}\right) e^{-i\left(\underline{Q}^{(h)} \cdot \underline{r}\left(\frac{l}{\dots}\right)\right)} \; e^{-i\left(\underline{q} \cdot \underline{r}\left(\frac{l}{\dots}\right)\right)} \qquad \text{by (1.16)}$$

$$= \mathcal{D}_{\lambda\rho}\left(\frac{l}{k k'}\right) \qquad \text{by (6.3)}$$

Once the matrix $\mathcal{D}(\underline{q})$ has been found within a range corresponding to the cell of the reciprocal lattice, the formulae of Section 2 give $\sigma_b(\underline{Q})$ throughout the reciprocal space.

Special case

A particularly simple case arises when there is only one particle in the unit cell. When the indices k have been dropped from all the formulae in which they occur and the summations over k ignored, one has

(6.5) $$\sigma_B(\underline{Q}) = \sigma_o \, N k T \frac{|f|^2}{m} d(\underline{Q})$$

where

(6.6) $\begin{cases} m = \text{mass of the elementary particle} \\ f = \text{modified scattering factor} \end{cases}$

and

(6.7) $$d(\underline{Q}) = \sum_{\alpha,\beta} \mathcal{D}^{-1}_{\alpha\beta}(\underline{q}) Q_\alpha Q_\beta$$

The function $d(\underline{Q})$ will be called the "diffusion function". By plotting the values of $d(\underline{Q})$ for a sufficiently large number of values of $\underline{Q}$, and then using some form of interpolation, it is possible to construct in the Q-space the surfaces on which $d(\underline{Q})$ has a constant value, i.e. surfaces of isodiffusion.

Section 6b Approximation to the general formula

The general formulae of Section 2 are not always easy to apply if n , the number of particles in the unit cell, is large, for then the matrix $\mathfrak{D}(q)$, whose order is (3n x 3n), becomes unwieldy and its reciprocal is difficult to calculate. Accordingly an approximation is used which confines attention to the neighbourhood of the points of selective reflection. Jahn has made use of this method (Jahn,1942) to discuss the surfaces of isodiffusion for metallic sodium. It may be stated briefly thus:-

The scattering power in the neighbourhood of the points of selective reflection depends mainly on the accoustical vibrations (Born,1943), and for these it was shown in Section 3c(B) how the dynamical matrix could be expressed in terms only of the elastic constants and how it was thereby reduced effectively to a matrix of order (3 x 3), independent that is to say of the indices k . The same applies to the scattering matrix and the final result of this approximation (for full details see Born,1943) is that the Scattering power may be written as :-

$$\sigma_\beta = \sigma_0 \, N k T \, \frac{|F|^2}{\left(\sum_k m_k\right)} \, d(\underline{q}) \tag{6.8}$$

where

$$F = \sum_k f_k \, e^{-i(\underline{q} \cdot \underline{r}(k))} \tag{6.9}$$

and

(6.10) The diffusion function, $d(\underline{Q}) = \sum_{\alpha,\beta} \mathcal{D}'^{-1}_{\alpha\beta}(q)\, Q_\alpha Q_\beta$

$$= \sum_{\alpha,\beta} \mathcal{D}'^{-1}_{\alpha\beta}(q)\, Q^{(1)}_\alpha Q^{(1)}_\beta$$

for this approximation.

Let (l, m, n) be the direction cosines of q so that $q_1 = ql$, ... Since $\mathcal{D}'(q)$ is quadratic in the components of q (3.97), it will contain a factor q^2 and $\mathcal{D}'^{-1}(q)$ will contain a factor $1/q^2$. If $\mathcal{D}'^{-1}(l, m, n)$ is the same function of l, m, n, that $\mathcal{D}'^{-1}(q)$ is of q_1, q_2, q_3, then (6.10) becomes

(6.11) $$q^2 = \frac{1}{d(\underline{Q})} \sum_{\alpha,\beta} \mathcal{D}'^{-1}_{\alpha\beta}(l, m, n)\, Q^{(1)}_\alpha Q^{(1)}_\beta$$

By giving $d(\underline{Q})$ a constant value, this formula will give the intercepts which the surfaces of isodiffusion make on those radii vectors which have the direction cosines l, m, n. Hence an indication of the shape of the surfaces of isodiffusion in the neighbourhood of the lattice points of reciprocal space can be obtained.

The notation used here follows that of Jahn(1942) in some respects.

Section 7 — Surfaces of isodiffusion for the face-centred cubic lattice

Since there is only one particle in the unit cell the method of the special case in Section 6a can be applied.

R e c i p r o c a l m a t r i x

From (4.12) the elements of the reciprocal of the dynamical matrix are given by (writing $adj\,\mathcal{D}$ for the adjugate of the matrix $\mathcal{D}$)

$$(7.1)\qquad \mathcal{D}^{-1}_{\alpha\beta}(q) = \frac{adj_{\alpha\beta}\,\mathcal{D}(q)}{|\mathcal{D}(q)|}$$

where

$$(7.2)\qquad |\mathcal{D}(q)| = F_1 F_2 F_3 + \frac{4\chi}{m}\left[s_1^2 F_2 F_3 + s_2^2 F_3 F_1 + s_3^2 F_1 F_2\right]$$

$$(7.3)\qquad \left\{\begin{array}{l} adj_{11}\,\mathcal{D}(q) = F_2 F_3 + \frac{4\chi}{m}\left(s_2^2 F_3 + s_3^2 F_2\right) \\ \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \\ adj_{23}\,\mathcal{D}(q) = -\frac{4\chi}{m} s_2 s_3 F_1 \\ \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \end{array}\right.$$

and F_1 , F_2 , F_3 , are defined in (4.11), (putting q instead of $\underline{q}$)

In order to simplify the working, attention will be confined to the plane $q_3 = 0$. Then the elements $\mathcal{D}^{-1}_{23}(q)$, $\mathcal{D}^{-1}_{31}(q)$, $\mathcal{D}^{-1}_{33}(q)$ will not be needed since the terms of $\sigma_0(\underline{q})$, in which they occur, vanish. In any case $\mathcal{D}^{-1}_{23}(q)$ and $\mathcal{D}^{-1}_{31}(q)$ vanish identically for $q_3 = 0$. The remaining elements of the reciprocal matrix then become:

$$\mathcal{D}^{-1}_{11}(q) = \frac{F_2 + \frac{4\gamma}{m} s_2^2}{(F_1 + \frac{4\gamma}{m} s_1^2)(F_2 + \frac{4\gamma}{m} s_2^2) - \frac{16\gamma^2}{m^2} s_1^2 s_2^2} \tag{7.4}$$

$$\mathcal{D}^{-1}_{22}(q) = \frac{F_1 + \frac{4\gamma}{m} s_1^2}{(F_1 + \frac{4\gamma}{m} s_1^2)(F_2 + \frac{4\gamma}{m} s_2^2) - \frac{16\gamma^2}{m^2} s_1^2 s_2^2} \tag{7.5}$$

$$\mathcal{D}^{-1}_{12}(q) = \frac{-\frac{4\gamma}{m} s_1 s_2}{(F_1 + \frac{4\gamma}{m} s_1^2)(F_2 + \frac{4\gamma}{m} s_2^2) - \frac{16\gamma^2}{m^2} s_1^2 s_2^2} \tag{7.6}$$

The values of $\mathcal{D}^{-1}_{11}(q)$, $\mathcal{D}^{-1}_{22}(q)$, $\mathcal{D}^{-1}_{12}(q)$, have been calculated for points on a rectangular net in the plane $q_3 = 0$, having the spacing $\pi/8$, i.e twice as close as that used for the calculation of $\mathcal{D}(q)$ in Section 4, where however the points were not confined to one plane. As in the latter Section the elastic constants are taken to be those of potassium chloride (Försterling 1920). The results are given in Table 7.

Table 7

The reciprocal of the dynamical matrix

In this Table the values of $\frac{1}{m} D^{-1}(q)$ are given after the elastic constants have been made dimensionless by dividing them by e^2/a^4 where $e = 4.77 \times 10^{-10}$ e.s.u. and $a = 3.12 \times 10^{-8}$ cm. The components of q are in units of π/a .

q_1	q_2	q_3	$\frac{1}{m} \times D_{11}^{-1}(q)$	$\frac{1}{m} \times D_{22}^{-1}(q)$	$\frac{1}{m} \times D_{12}^{-1}(q)$	q_1	q_2	q_3	$\frac{1}{m} \times D_{11}^{-1}(q)$	$\frac{1}{m} \times D_{22}^{-1}(q)$	$\frac{1}{m} \times D_{12}^{-1}(q)$
0	1/8	0	23.36	3.95	0.00	1/4	1	0	0.92	0.18	0.00
0	1/4	0	6.35	1.07	0.00	3/8	3/8	0	0.63	0.63	0.14
0	3/8	0	2.99	0.52	0.00	3/8	1/2	0	0.70	0.41	0.14
0	1/2	0	1.85	0.30	0.00	3/8	5/8	0	0.77	0.30	0.08
0	5/8	0	1.33	0.22	0.00	3/8	3/4	0	0.85	0.26	0.08
0	3/4	0	1.07	0.18	0.00	3/8	7/8	0	0.89	0.22	0.00
0	7/8	0	0.96	0.15	0.00	3/8	1	0	0.92	0.22	0.00
0	1	0	0.92	0.15	0.00	1/2	1/2	0	0.52	0.52	0.14
1/8	1/8	0	3.84	3.84	1.10	1/2	5/8	0	0.59	0.37	0.08
1/8	1/4	0	2.77	1.14	0.44	1/2	3/4	0	0.74	0.30	0.08
1/8	3/8	0	2.03	0.52	0.22	1/2	7/8	0	0.85	0.30	0.08
1/8	1/2	0	1.51	0.33	0.08	1/2	1	0	0.92	0.26	0.00
1/8	5/8	0	1.22	0.22	0.08	5/8	5/8	0	0.48	0.48	0.08
1/8	3/4	0	1.03	0.18	0.00	5/8	3/4	0	0.66	0.41	0.08
1/8	7/8	0	0.96	0.18	0.00	5/8	7/8	0	0.81	0.37	0.08
1/8	1	0	0.92	0.15	0.00	5/8	1	0	0.92	0.37	0.00
1/4	1/4	0	1.14	1.14	0.30	3/4	3/4	0	0.59	0.59	0.08
1/4	3/8	0	1.14	0.59	0.22	3/4	7/8	0	0.81	0.55	0.08
1/4	1/2	0	1.05	0.37	0.14	3/4	1	0	0.92	0.55	0.00
1/4	5/8	0	1.00	0.26	0.08	7/8	7/8	0	0.77	0.77	0.08
1/4	3/4	0	0.96	0.22	0.08	7/8	1	0	0.92	0.77	0.00
1/4	7/8	0	0.92	0.18	0.00	1	1	0	0.92	0.92	0.00

D i f f u s i o n f u n c t i o n

The values of $\alpha(\underline{Q})$ were next calculated in a region of the plane bounded by $Q_1 = -\frac{\pi}{a}$, $Q_2 = -\frac{\pi}{a}$, $Q_1 = \frac{5\pi}{a}$, $Q_2 = \frac{5\pi}{a}$, so that the nine Laue points† (0, 0, 0) (1, 0, 0), (1, 1, 0), (0, 1, 0), (2, 0, 0), (2, 1, 0) (2, 2, 0), (1, 2, 0), (0, 2, 0), were included. The values are shown in Table 8.

It is now possible to plot $\alpha(\underline{Q})$ against $\underline{Q}$ along the lines $Q_1 = \frac{n\pi}{8a}$ and $Q_2 = \frac{n\pi}{8a}$. From these graphs a set of points on any assigned curve of isodiffusion could be found. Finally by combining these data the curves of isodiffusion were drawn for a suitable sequence of values of $\alpha(\underline{Q})$, and they are shown in Fig. IV.

In the neighbourhood of the Laue points, the contours approach closely to those found for potassium chloride by Weigle and Smith (1942), using a different method. A special study of these particular contours by themselves may be made, of course, by the methods of Section 6b, but the results have not been reproduced here since the form which the contours take is clearly seen from a study of Fig. IV.

† Here and elsewhere the co-ordinates of points of selective reflection are referred to the reciprocal lattice vectors $\underline{b}^1$, $\underline{b}^2$, $\underline{b}^3$, as axes.

Table 8 — The diffusion function

A portion of the plane $\alpha_3 = 0$ is set out below with the values of $d(\underline{\alpha})$ at those points on it whose co-ordinates are multiples of $\pi/4a$. The values of the diffusion function at the intermediate points (with co-ordinates which are multiples of $\pi/8a$) were only calculated in those regions where the contours of the subsequent graph (Fig. IV) demanded more precise detail.

3·75	4·56	6·73	14·27	23·92	15·19	8·57	7·32	7·43	9·16	12·25	20·71	31·28	23·47	17·77	17·44	18·47	21·12	25·13	34·51	46·00
4·06	4·83	6·57	13·01	21·31	15·78	9·57	9·23	8·34	8·11	9·49	15·68	25·71	22·01	18·49	21·31	21·18	19·07	18·38	23·01	34·51
6·08	7·24	10·03	14·61	18·89	16·25	13·59	12·91	13·48	9·97	10·63	15·27	20·97	20·78	21·31	24·77	35·58	21·10	15·39	18·38	25·13
19·32	20·02	18·46	16·95	16·86	18·53	21·58	28·54	44·72	20·57	18·30	17·13	18·24	21·87	27·66	46·18	120·92	30·34	21·10	19·07	21·12
0/2	101·60	29·56	17·32	14·87	17·40	30·18	104·87	1/2	107·01	31·38	18·48	16·07	19·02	33·18	116·64	2/2	120·92	35·58	21·18	18·47
15·04	16·66	15·38	14·07	13·12	13·09	14·02	15·58	40·40	26·86	19·09	16·81	14·56	13·76	18·25	23·62	116·64	46·18	24·77	21·31	17·44
3·68	4·84	8·32	9·65	11·53	8·73	6·07	6·03	11·08	12·05	12·06	12·87	13·61	10·41	11·76	18·25	33·18	27·66	21·31	18·49	17·77
1·90	2·51	3·61	6·95	10·27	6·50	4·05	4·35	6·18	8·35	9·09	12·12	14·67	10·77	10·41	13·76	19·02	21·87	20·78	22·01	23·47
1·35	1·68	2·57	5·47	9·20	6·39	4·41	4·44	5·03	6·28	8·09	11·91	16·56	14·67	13·61	14·56	16·07	18·24	20·97	25·71	31·28
1·36	1·61	2·23	4·46	7·51	5·93	4·59	5·37	5·64	5·53	6·23	7·70	11·91	12·12	12·87	16·81	18·48	17·13	15·27	15·68	20·71
1·88	2·20	3·03	4·49	6·01	5·59	5·47	6·75	9·28	6·16	4·75	6·23	8·09	9·09	12·06	19·09	31·38	18·30	10·63	9·49	12·25
5·41	5·50	5·09	4·71	4·84	5·20	7·09	11·62	30·81	8·50	6·16	5·53	6·28	8·35	12·05	26·86	107·01	20·57	9·97	8·11	9·16
0/1	25·46	7·48	4·38	3·83	4·56	8·08	28·67	1/1	30·81	9·28	5·64	5·03	6·18	11·08	40·40	2/1	44·72	13·48	8·34	7·43
3·27	3·82	3·55	3·27	3·00	2·93	3·31	5·14	28·67	11·62	6·75	5·37	4·44	4·35	6·03	15·58	104·87	28·54	12·91	9·23	7·32
0·68	1·00	1·51	2·01	2·33	1·73	1·73	3·31	8·08	7·09	5·47	4·59	4·41	4·05	6·07	14·02	30·18	21·58	13·59	9·57	8·57
0·28	0·45	0·75	1·40	1·99	1·54	1·73	2·93	4·56	5·20	5·59	5·93	6·39	6·50	8·73	13·09	17·40	18·53	16·25	15·78	15·19
0·15	0·24	0·59	1·07	1·84	1·99	2·33	3·00	3·83	4·84	6·01	7·51	9·20	10·27	11·53	13·12	14·87	16·80	18·89	21·31	23·92
0·10	0·15	0·29	0·57	1·07	1·40	2·01	3·27	4·38	4·71	4·49	4·46	5·47	6·95	9·65	14·07	17·32	16·95	14·61	13·01	14·27
0·08	0·12	0·19	0·29	0·59	0·75	1·51	3·55	7·48	5·09	3·03	2·23	2·57	3·61	8·32	15·38	29·56	18·46	10·03	6·57	6·73
0·06	0·10	0·12	0·15	0·24	0·45	1·00	3·82	25·46	5·50	2·20	1·61	1·68	2·51	4·84	16·66	101·60	20·02	7·24	4·83	4·56
0/0	0·06	0·08	0·10	0·15	0·28	0·68	3·27	1/0	5·41	1·88	1·36	1·35	1·90	3·68	15·04	2/0	19·32	6·08	4·06	3·75

Figure IV.

Curves of isodiffusion in the plane $Q_3 = 0$

for potassium chloride.

one half that of the face-centred unit cell of potassium chloride. They have determined the scattering power over the whole of the reciprocal lattice network which includes the origin and the first five $\{hk0\}$ reflexions (together with other reciprocal lattice points derived from these by symmetry operations), and their published diagram shows that contours of the Jahn type do indeed account for very much of the diffuse scattering.

Although it is scarcely fair to compare the isodiffusion curves calculated for a simple face-centred cubic model with the experimental results for potassium chloride crystals, which may more truly be regarded as simple cubic, yet Born and Begbie's diagram possesses features which are apparently typical of the observed data for both potassium and sodium chloride. For example, Laval's ionization spectrometer measurements[2], which showed that the 200 and 220 domains ((1,0) and (1,1) in the above diagram) were completely surrounded by regions of weak scattering, but that between 400 and 420 ((2,0) and (2,1)) and still more between 600 and 620, there were 'bridges' of strong scattering, are now seen to be consistent with the theoretical predictions. It may be of interest to mention that the observed value of the scattering power at the middle of the 600–620 bridge is about 3·4 times the minimum scattering power appropriate to this angle, Compton scattering being subtracted from both observed figures. Inclusive of Compton scattering, the ratio is about 2·2 : 1.

Born and Begbie have commented upon the appearance of isodiffusion lines forming squares the sides of which are parallel to [100] [010]. Almost equally striking are the presence of other lines parallel to the diagonals [110] [$1\bar{1}0$]. 'Bridges' of both these kinds are clearly to be seen on the beautiful monochromatic photograph of sodium chloride published by Gregg and Gingrich[3].

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Thermal Scattering of X-Rays by Crystals

THE influence of the thermal vibrations on the diffraction of X-rays by a crystal can be represented by a distribution of scattering power in the reciprocal lattice. The theoretical formula for this is the product of two parts : one, consisting of slowly varying factors which correspond to the atomic scattering factor, the polarization factor, Debye's temperature factor, the Lorentz factor, of Laue-Bragg scattering ; the other part consisting of a function characteristic of the dynamics of the crystal vibrations, the diffusion factor $d(Q)$. For a simple lattice the latter has the form

$$d(Q) = \sum_{\alpha,\beta=1}^{3} S_{\alpha\beta}(Q)\, Q_\alpha Q_\beta, \quad . \quad . \quad (1)$$

where Q_1, Q_2, Q_3 are the co-ordinates in the reciprocal lattice, and $S_{\alpha\beta}(Q)$ are the elements of the scattering matrix S, periodic functions of the Q. S can be expressed as a function of the dynamical matrix D, which is defined in terms of the coefficient matrix of the second order terms of the potential energy of the lattice. At normal temperatures one has, with a high degree of accuracy,

$$S = kTD^{-1}. \quad . \quad . \quad . \quad . \quad . \quad (2)$$

The elements of $D(Q)$ have zeros in the reciprocal lattice points, hence those of $S(Q)$ have sharp peaks there. In the neighbourhood of these, they can be expressed in terms of the elastic constants of the crystal. In this way Jahn has calculated[1] surfaces of isodiffusion for sodium, and Mrs. Lonsdale and Mr. Smith have shown[2] that the results are in good agreement with observations.

Since the experiments show, for many materials, a definite structure of scattering power ('streamers' or 'bridges') in the space between the lattice points, it seemed desirable to have a method of calculating the matrix $S(Q)$ for any point of the reciprocal space. This can be done in two ways : either by using numerical calculations of the matrix D as published by Iona[3] for potassium chloride, and by Kellermann[4] for sodium chloride, or by using a crystal model for which D can be theoretically constructed. We have applied both methods. But as Iona's tables are rather rough, containing only four points on each edge of the elementary cube in the Q-space, the resulting figure for $d(Q)$ does not show much interesting detail ; it is not worth while reproducing it here.

Values of the elastic constants (Försterling, 1920)

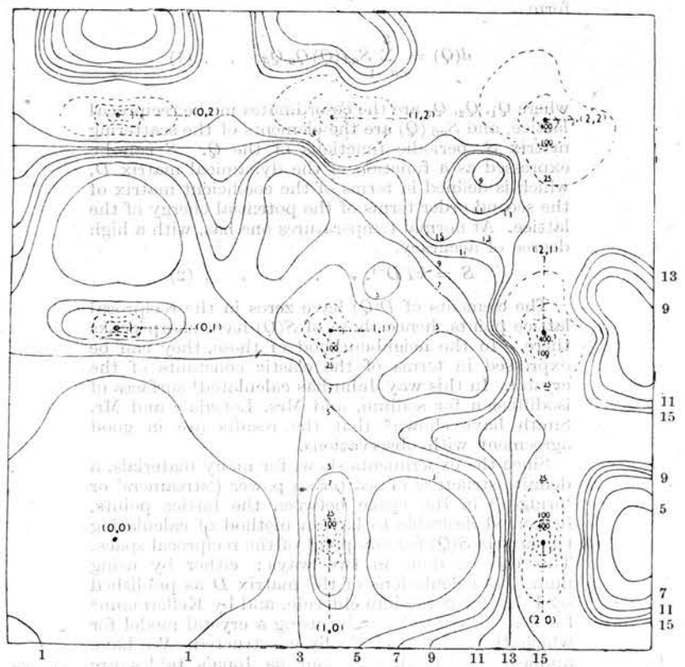
$C_{11} = 3.84$, $C_{12} = 0.65$, $C_{44} = 0.64 \times 10^{11}$ dynes/cm.^{2}

We have therefore developed the second method, taking as the model a face-centred cubic lattice in which only next neighbours act on one another, but with non-central forces. It can be shown that in this case there are exactly three force constants, which can be expressed in terms of the three elastic constants c_{11}, c_{12}, c_{44}. The typical elements of D are

$$D_{11} = (2c_{44} - c_{11})(1 - \cos Q_2 \cos Q_3) + c_{11}(2 - \cos Q_1 \cos Q_2 - \cos Q_1 \cos Q_3),$$

$$D_{22} = (c_{12} + c_{44}) \sin Q_2 \sin Q_3,$$

which for small Q go over, of course, into the expressions used by Jahn. We have in particular considered the plane $Q_3 = 0$, for which case it is not too tedious to form the reciprocal matrix D^{-1}.



Potassium chloride isodiffusion lines in the plane $Q_3 = 0$ of the reciprocal space (Q_1, Q_2, Q_3). The figures attached to the lines are the values of $d(Q)\ kT$ if the elastic constants are made dimensionless by dividing them by $e^2 a^4 = 2{\cdot}40 \times 10^{11}$ dyne cm.$^{-2}$ (e is charge of the electron, a is lattice constant, 3·14 A.). The bracketed figures are the indices of the reciprocal lattice points, referred to crystal axes the lengths of which are one half those of the face-centred unit cell.

In order to compare the results with the first method mentioned above, we took the constants c_{11}, c_{12}, c_{44} as those of potassium chloride, although this lattice is neither monatomic nor simple face-centred. Calculations for metallic crystals satisfying these conditions will be performed later.

We computed the elements of D^{-1} and from this the diffusion function (1) for a sufficiently fine network of points. With the help of graphical interpolation, curves of isodiffusion were constructed which are given in the accompanying figure. This comprises nine reciprocal lattice points including the origin (marked by dots). In the vicinity of each of these (except the origin) one recognizes contours of the type found by Jahn. But one sees that the background has a definite and complicated structure; for example, secondary maxima (labelled 15). A remarkable feature is the existence of isodiffusion lines (intensities of 3 and 15, in our scale), forming almost squares which separate the whole field into unconnected sections. We hope that figures of this kind will provide additional evidence for the thermal theory of X-ray scattering.

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In a recent lecture-survey given to the Physical Society[1] it was shown that calculations based on the Faxén-Waller theory gave good agreement with experiment, not only within the regions to which that theory could properly be applied, but also in the short wave-length range where its validity was open to question. Thus diagrams showing the observed scattering power of KCl and Na in reciprocal space and the scattering power calculated by means of Jahn's formula were in general agreement not only in the neighbourhood of the reciprocal lattice points (region of long waves) but also at a distance from those points.

Prof. Born and Mr. Begbie have now extended the calculation for the special case of a monatomic face-centred cubic model having the same elastic constants as potassium chloride, and a lattice constant equal to

Figure IV.

Curves of isodiffusion in the plane $Q_3 = 0$ for potassium chloride.

Values of the elastic constants (Försterling, 1920)

$c_{11} = 3.84$, $c_{12} = 0.65$, $c_{44} = 0.64 \times 10^{11}$ dynes/cm.^{2}

Section 8 Surfaces of isodiffusion for the hexagonal close-packed lattice

Since there are two particles in the unit cell, the reciprocal matrix is rather complicated to calculate and a full discussion of the general method of plotting the scattering power throughout reciprocal space is left for subsequent investigation. For the present the approximation of Section 6b will be used.

From (5.14) and (5.15) one has

(8.1)
$$\begin{bmatrix} \mathcal{D}'_{11}(q) \\ \mathcal{D}'_{22}(q) \\ \mathcal{D}'_{33}(q) \\ \mathcal{D}'_{23}(q) \\ \mathcal{D}'_{31}(q) \\ \mathcal{D}'_{12}(q) \end{bmatrix} = \begin{bmatrix} c_{11} & \frac{1}{2}(c_{11}-c_{12}) & c_{44} & 0 & 0 & 0 \\ \frac{1}{2}(c_{11}-c_{12}) & c_{11} & c_{44} & 0 & 0 & 0 \\ c_{44} & c_{44} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2}(c_{13}+c_{44}) & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2}(c_{13}+c_{44}) & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2}(c_{11}+c_{12}) \end{bmatrix} \begin{bmatrix} q_1^2 \\ q_2^2 \\ q_3^2 \\ 2q_2q_3 \\ 2q_3q_1 \\ 2q_1q_2 \end{bmatrix}$$

Write

(8.2)
$$a = \tfrac{1}{2}(c_{11}+c_{12}) \qquad c = c_{44}$$
$$f = c_{33}$$
$$b = \tfrac{1}{2}(c_{11}-c_{12}) \qquad d = c_{13}+c_{44}$$

and as in Section 6b put

$$q_1 = q\ell, \quad q_2 = qm, \quad q_3 = qn \qquad \ell^2 + m^2 + n^2 = 1 \tag{8.3}$$

and

$$A_1 = b(\ell^2 + m^2) + cn^2$$
$$A_2 = c(\ell^2 + m^2) + fn^2 \tag{8.4}$$

The elements of the reciprocal matrix are given by

$$\mathcal{D}^{-1}_{\alpha\beta}(q) = \frac{adj_{\alpha\beta}\,\mathcal{D}'(q)}{|\mathcal{D}'(q)|} \tag{8.5}$$

where

$$\frac{1}{\rho^3 q^6}\,|\mathcal{D}'(q)| = A_1\,[A_1 A_2 + (a A_2 - d^2 n^2)(\ell^2 + m^2)] \tag{8.6}$$

$$\left\{\begin{aligned}
\frac{1}{\rho^2 q^4}\,adj_{11}\,\mathcal{D}'(q) &= A_2\,(A_1 + a m^2) - d^2 m^2 n^2 \\
\frac{1}{\rho^2 q^4}\,adj_{22}\,\mathcal{D}'(q) &= A_2\,(A_1 + a\ell^2) - d^2 n^2 \ell^2 \\
\frac{1}{\rho^2 q^4}\,adj_{33}\,\mathcal{D}'(q) &= (A_1 + a\ell^2)(A_2 + a m^2) - a^2 \ell^2 m^2 \\
\frac{1}{\rho^2 q^4}\,adj_{23}\,\mathcal{D}'(q) &= -A_1\, d\, m n \\
\frac{1}{\rho^2 q^4}\,adj_{31}\,\mathcal{D}'(q) &= -A_1\, d\, n \ell \\
\frac{1}{\rho^2 q^4}\,adj_{12}\,\mathcal{D}'(q) &= -\ell m\,[a A_2 - d^2 n^2]
\end{aligned}\right. \tag{8.7}$$

For the purposes of calculation attention is confined to the plane $a_3 = 0$. For this the reciprocal matrix reduces to

$$(8.8)\qquad \mathfrak{D}^{-1}(q) = \rho/q^2 \begin{bmatrix} \frac{l^2}{a} + \frac{m^2}{b} & lm\left(\frac{1}{a} - \frac{1}{b}\right) & 0 \\ lm\left(\frac{1}{a} - \frac{1}{b}\right) & \frac{l^2}{b} + \frac{m^2}{a} & 0 \\ 0 & 0 & \frac{1}{c} \end{bmatrix}$$

Equation (6.11) now becomes, omitting a constant factor:

$$(8.9)\qquad q^2 = \left[\frac{l a_1^{(h)} + m a_2^{(h)}}{a}\right]^2 + \left[\frac{m a_1^{(h)} - l a_2^{(h)}}{b}\right]^2$$

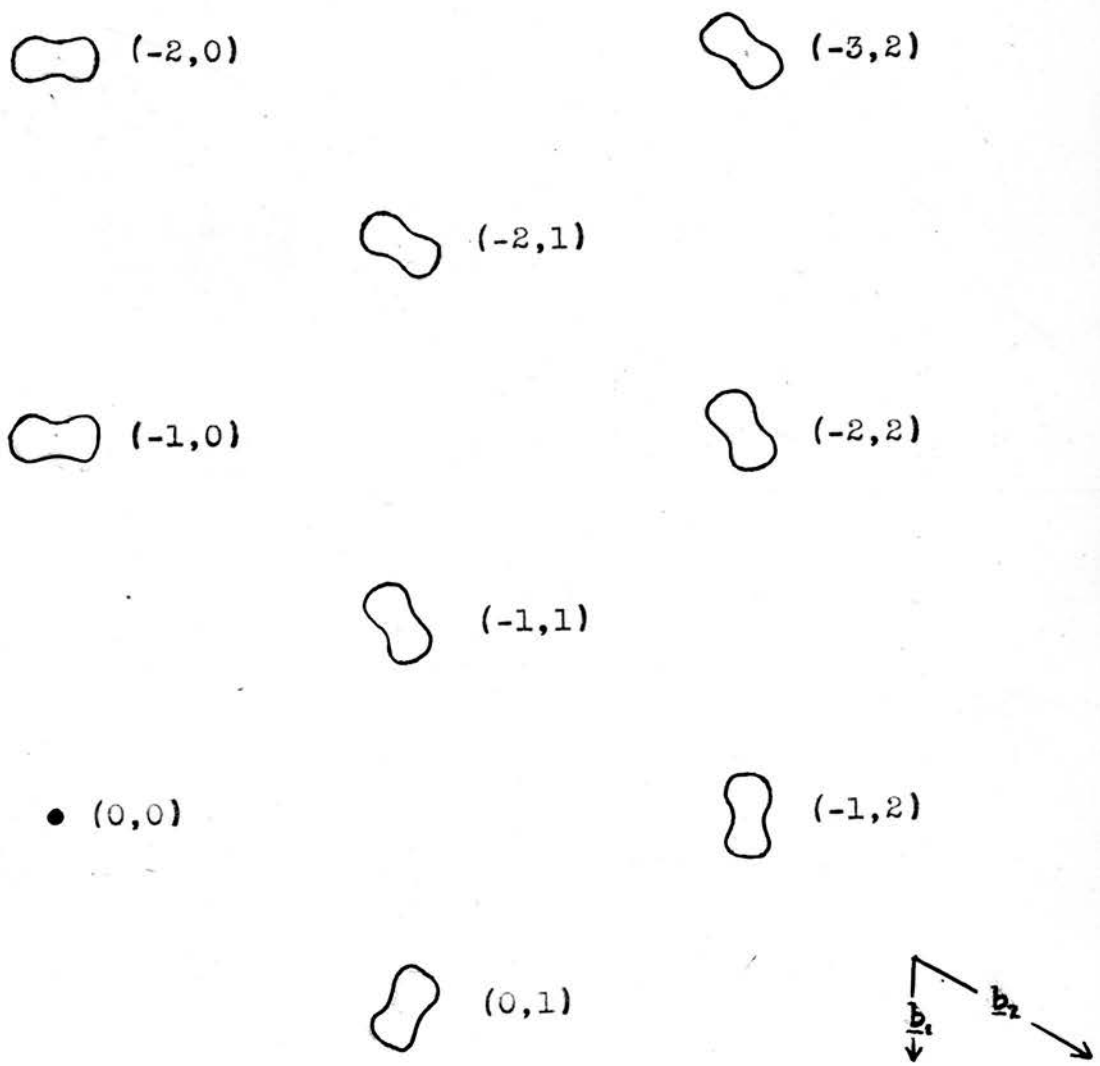
or, if Θ is the angle between q and $\underline{a}^{(h)}$,

$$(8.10)\qquad q^2 = \frac{1}{|\underline{a}^{(h)}|^2}\left\{\frac{\cos^2\Theta}{a^2} + \frac{\sin^2\Theta}{b^2}\right\}.$$

This is the equation in polar co-ordinates (q, Θ) of the curves of isodiffusion round the points $\underline{a}^{(h)}$. It follows from this formula that, neglecting considerations of scale, these curves have the same shape for all points $\underline{a}^{(h)}$ which lie in the plane $a_3 = 0$. A part of this plane is shown in Fig. V. and includes the reciprocal lattice points (0,0),(0,1),(-1,0),(-1,1),(-1,2),(-2,0) (-2,1),(-2,2),(-3,2), and the curves near each of them. The elastic constants are taken as those of Beryl(Voigt,1910)

Figure V.

Curves of isodiffusion in the plane $\varphi_3 = 0$ for beryl.



Values of the elastic constants (Voigt, 1910)

$c_{11} = 27.5$, $c_{33} = 24.1$, $c_{12} = 9.80$, $c_{13} = 6.74$, $c_{44} = 6.66 \times 10^{11}$ dynes/cm.^{2}

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