

Dynamical Diffraction Theory for Distorted Crystals

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Dedicated to Prof. G. Borrmann on the occasion of his 65th birthday

A set of linear equations for the Fourier components of the field vectors $D_0(\mathbf{p})$ (direct waves) and $D_g(\mathbf{p})$ (Bragg-reflected waves) is formulated by the Fourier transform of the Maxwell equations. Starting from these equations, the scattering matrix theory and the equation equivalent to the Takagi-Taupin equation are derived systematically. The equivalence of these formulations is concluded. The formal similarity of the Takagi-Taupin equation to the Dirac equation for a relativistic charged particle is pointed out.

§ 1. Introduction

The dynamical diffraction theory for distorted crystals can be formulated in terms of a scattering matrix¹. The theory itself is very general so that it can be applied to both X-rays and electrons, whatever are the distortions and the magnitude of the Bragg angle Θ_B . This theory in its approximation for small Θ_B has brought about fruitful results in studies of lattice defects by means of high-voltage electron microscopy². Unfortunately, however, the theory has not been applied to X-ray problems except for one special topic¹, because Θ_B is not small in X-ray studies, in general.

Another approach having a quite different aspect was developed by Takagi³ and Taupin⁴. The fundamental equation, which will be called the T equation in this paper, is more easily handled than the original master equations, namely the Maxwell (X-ray case) and Schrödinger (electron case) equations. This situation is particularly true for numerical calculations, and some practical applications have been reported^{4, 5}.

The aim of this paper is to elucidate the relations between these two methods. For this purpose, first, a set of basic equations of the Bethe-Laue type are formulated for distorted crystals (§ 2). Starting from these equations, one can derive the T equation by a three-dimensional Fourier transform, with reasonable approximations commonly used in the dynamical theory. The scattering matrix theory, whose basic equation is called the S equation hereafter, can also be derived by the same principle but using

a one-dimensional Fourier transform (§ 4). Through this systematic approach of formulation, one can understand the physical meanings of the approximations adopted in each theory.

Another aim is to point out the similarity of the T and the S equations or their equivalents to the Dirac equation including electromagnetic potentials⁶. This fact suggests the use of field theory techniques for solving the problems of dynamical diffraction in distorted crystals.

§ 2. The Basic Equation of Bethe-Laue Type

In this paper, the theory for X-rays is developed and for simplicity, the two-beam approximation is employed. The transformation to the electron theory and the generalization to many beam cases, however, are a matter of formalism.

The polarizability of a perfect crystal for X-rays must have the form

$$\chi_D(\mathbf{r}) = \chi_0 + \chi_g \exp\{2\pi i(\bar{\mathbf{g}} \cdot \mathbf{r})\} + \chi_{-g} \exp\{-2\pi i(\bar{\mathbf{g}} \cdot \mathbf{r})\}, \quad (1)$$

where $(\chi_0, \chi_g, \chi_{-g})$ are the Fourier coefficients of the zeroth and $\pm \mathbf{g}$ -th orders. When the crystal is distorted by a displacement vector $\mathbf{u}(\mathbf{r})$ at the position \mathbf{r} , the polarizability is modified to

$$\chi(\mathbf{r}) = \chi_0 + \chi_g \exp\{2\pi i(\bar{\mathbf{g}} \cdot (\mathbf{r} - \mathbf{u}))\} + \chi_{-g} \exp\{-2\pi i(\bar{\mathbf{g}} \cdot (\mathbf{r} - \mathbf{u}))\}. \quad (2)$$

In this approximation the changes in $(\chi_0, \chi_{\pm g})$ are neglected.

Since the expression

$$G(\mathbf{r}) = -(\bar{\mathbf{g}} \cdot \mathbf{u}) \quad (3)$$

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is a function of position, one can write

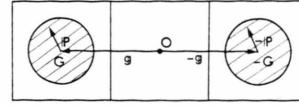
$$\exp\{2\pi i G(\mathbf{r})\} = \sum_p \alpha(\mathbf{p}) \exp\{2\pi i(\mathbf{p} \cdot \mathbf{r})\}, \quad (4a)^*$$

$$\exp\{-2\pi i G(\mathbf{r})\} = \sum_p \beta(\mathbf{p}) \exp\{2\pi i(\mathbf{p} \cdot \mathbf{r})\}, \quad (4b)^*$$

where \mathbf{p} can be assumed to be a vector lying within a single reciprocal cell (Figure 1). Obviously, the relation

$$\alpha(\mathbf{p}) = \beta^*(-\mathbf{p}) \quad (5)$$

must be satisfied.



The Maxwell equations are equivalent to the differential equation for an electric displacement vector $\mathbf{D}(\mathbf{r})$,

$$\Delta \mathbf{D} + K^2 \mathbf{D} = -\text{rot rot}[\chi(\mathbf{r}) \mathbf{D}(\mathbf{r})] \quad (6a)$$

$$\text{and} \quad \text{div } \mathbf{D} = 0, \quad (6b)$$

where K is 2π times the wave number in vacuum. Here, we shall seek the formal solution

$$\mathbf{D}(\mathbf{r}) = \sum_p [\mathbf{D}_0(\mathbf{p}) + \mathbf{D}_g(\mathbf{p}) \exp\{2\pi i(\mathbf{g} \cdot \mathbf{r})\}] \exp\{2\pi i((\bar{\mathbf{k}}_0 + \mathbf{p}) \cdot \mathbf{r})\}, \quad (7)$$

where $\{\mathbf{D}_0(\mathbf{p}), \mathbf{D}_g(\mathbf{p})\}$ must satisfy the conditions

$$\{(\bar{\mathbf{k}}_0 + \mathbf{p}) \cdot \mathbf{D}_0(\mathbf{p})\} = 0, \quad \{(\bar{\mathbf{k}}_g + \mathbf{p}) \cdot \mathbf{D}_g(\mathbf{p})\} = 0 \quad (8a, b)$$

owing to the relation (6b).

Inserting Eq. (2) for $\chi(\mathbf{r})$ and Eq. (7) into Eq. (6a), one obtains a set of linear equations

$$[k^2 - (\bar{\mathbf{k}}_0 + \mathbf{p})^2] \mathbf{D}_0(\mathbf{p}) + \chi_{-g} \sum_q \beta(\mathbf{p} - \mathbf{q}) [(\bar{\mathbf{k}}_0 + \mathbf{p}) \times (\bar{\mathbf{k}}_0 + \mathbf{p}) \times \mathbf{D}_g(\mathbf{q})] = 0 \quad (9a)$$

$$\chi_g \sum_q \alpha(\mathbf{p} - \mathbf{q}) [(\bar{\mathbf{k}}_g + \mathbf{p}) \times (\bar{\mathbf{k}}_g + \mathbf{p}) \times \mathbf{D}_0(\mathbf{q})] + [k^2 - (\bar{\mathbf{k}}_g + \mathbf{p})^2] \mathbf{D}_g(\mathbf{p}) = 0, \quad (9b)$$

where

$$\bar{\mathbf{k}}_g = \bar{\mathbf{k}}_0 + 2\pi \mathbf{g} \quad \text{and} \quad k^2 \equiv \bar{\mathbf{k}}_0^2 \equiv \bar{\mathbf{k}}_g^2 = K^2 + \chi_0. \quad (10, 11)$$

Since Eq. (8a) is satisfied, one can rewrite Eq. (9a) after a scalar multiplication of $\mathbf{D}_0(\mathbf{p})$ with Eq. (9a) as

$$[k^2 - (\bar{\mathbf{k}}_0 + \mathbf{p})^2] \mathbf{D}_0^{**}(\mathbf{p}) - \chi_{-g} \sum_q \beta(\mathbf{p} - \mathbf{q}) (\bar{\mathbf{k}}_0 + \mathbf{p})^2 C(\mathbf{p}, \mathbf{q}) \mathbf{D}_g(\mathbf{q}) = 0, \quad (12a)$$

where

$$\mathbf{D}_0(\mathbf{p}) = \{\mathbf{D}_0(\mathbf{p}) \cdot \mathbf{D}_0(\mathbf{p})\}^{1/2} \quad \text{and} \quad \mathbf{D}_g(\mathbf{p}) = \{\mathbf{D}_g(\mathbf{p}) \cdot \mathbf{D}_g(\mathbf{p})\}^{1/2} \quad (13a, b)$$

are the magnitudes of the vectors $\mathbf{D}_0(\mathbf{p})$ and $\mathbf{D}_g(\mathbf{p})$, respectively, and C is the polarization factor defined by

$$C(\mathbf{p}, \mathbf{q}) = \{\hat{\mathbf{D}}_0(\mathbf{p}) \cdot \hat{\mathbf{D}}_g(\mathbf{q})\}, \quad (14)$$

the sign $\hat{}$ indicating the unit vector. Similarly, by the multiplications of (8b) and $\mathbf{D}_g(\mathbf{p})$, one obtains

$$[k^2 - (\bar{\mathbf{k}}_g + \mathbf{p})^2] \mathbf{D}_g(\mathbf{p}) - \chi_g \sum_q \alpha(\mathbf{p} - \mathbf{q}) (\bar{\mathbf{k}}_g + \mathbf{p})^2 C(\mathbf{q}, \mathbf{p}) \mathbf{D}_0(\mathbf{q}) = 0. \quad (12b)$$

Since the field vectors $\mathbf{D}_0(\mathbf{p})$ and $\mathbf{D}_g(\mathbf{p})$ are orthogonal to the wave vectors $(\bar{\mathbf{k}}_0 + \mathbf{p})$ and $(\bar{\mathbf{k}}_g + \mathbf{p})$ respectively, it is sufficient to specify two components of the field vector. In the present problem, it is convenient to take one component within the plane determined by $\bar{\mathbf{k}}_0$ and $\bar{\mathbf{k}}_g$ and another perpendicular to it. For convenience, we call them the

“parallel” and “perpendicular” components, respectively. Then, it is obvious that the polarization factors (14) among the wave fields of these two different components are zero. Thus, the parallel and perpendicular components can be independently determined. For this reason, Eqs. (12a and b) will be used as a set of equations for determining the wave fields of either parallel or perpendicular components.

The treatment is similar to that of the many-beam theories for a perfect crystal developed by Bethe and Laue, if one imagines a set of infinitesimal lat-

* Here, the integral $\int d\mathbf{p}$ is deliberately written in the form of a summation \sum_p . See the statement above Eq. (15).

** Anm. d. Red.: For technical reasons here and in the following a bold face \mathbf{D} is used instead of a italic D .

tice cells in \mathbf{p} -space. For this reason, the set of Eqs. (12 a and b) is called the basic equation of the Bethe-Lauve type. With this fact in mind, one can write Eqs. (12 a and b) in a kind of matrix form:

$$\begin{pmatrix} \mathbf{L}_{0,0} & \mathbf{L}_{0,g} \\ \mathbf{L}_{g,0} & \mathbf{L}_{g,g} \end{pmatrix} \begin{pmatrix} \tilde{\mathbf{D}}_0 \\ \tilde{\mathbf{D}}_g \end{pmatrix} = 0, \quad (15)$$

where $\mathbf{L}_{0,0}$ and $\mathbf{L}_{g,g}$ are diagonal matrices, whose matrix elements are given respectively as

$$\mathbf{L}_{0,0}(\mathbf{p}) \equiv \langle \mathbf{p} | \mathbf{L}_{0,0} | \mathbf{p} \rangle = k^2 - (\bar{\mathbf{k}}_0 + \mathbf{p})^2, \quad (16 a)$$

$$\mathbf{L}_{g,g}(\mathbf{p}) \equiv \langle \mathbf{p} | \mathbf{L}_{g,g} | \mathbf{p} \rangle = k^2 - (\bar{\mathbf{k}}_g + \mathbf{p})^2. \quad (16 b)$$

The elements of the skew matrices $\mathbf{L}_{0,g}$ and $\mathbf{L}_{g,0}$ are given by

$$\begin{aligned} \mathbf{L}_{0,g}(\mathbf{p}, \mathbf{q}) &\equiv \langle \mathbf{p} | \mathbf{L}_{0,g} | \mathbf{q} \rangle \\ &= \chi_{-g} \beta(\mathbf{p} - \mathbf{q}) C(\mathbf{p}, \mathbf{q}) (\bar{\mathbf{k}}_0 + \mathbf{p})^2, \end{aligned} \quad (16 c)$$

$$\begin{aligned} \mathbf{L}_{g,0}(\mathbf{p}, \mathbf{q}) &\equiv \langle \mathbf{p} | \mathbf{L}_{g,0} | \mathbf{q} \rangle \\ &= \chi_g \alpha(\mathbf{p} - \mathbf{q}) C(\mathbf{q}, \mathbf{p}) (\bar{\mathbf{k}}_g + \mathbf{p})^2. \end{aligned} \quad (16 d)$$

In addition, $\tilde{\mathbf{D}}_0(\mathbf{q})$ and $\tilde{\mathbf{D}}_g(\mathbf{q})$ are column matrices (vectors), the elements being given by $\mathbf{D}_0(\mathbf{q})$ and $\mathbf{D}_g(\mathbf{q})$, respectively. Since the running indices specifying the elements are three-dimensional vectors, the expression (15) is rather formal. Nevertheless, the relations between the Fourier amplitudes $\mathbf{D}_0(\mathbf{q})$ and $\mathbf{D}_g(\mathbf{q})$ can conveniently be understood from Equation (15).

§ 3. The Derivation of the T Equation

In this section, an alternative method to derive the T equation will be presented. First of all, the diagonal elements (16 a and b) are approximated as follows;

$$\mathbf{L}_{00}(\mathbf{p}) \cong -2(\bar{\mathbf{k}}_0 \cdot \mathbf{p}), \quad (17 a)$$

$$\mathbf{L}_{gg}(\mathbf{p}) \cong -2(\bar{\mathbf{k}}_g \cdot \mathbf{p}). \quad (17 b)$$

The approximation is valid provided that $|\mathbf{p}|$ is sufficiently small compared to k . Optically speaking, it is equivalent to replacing the Ewald sphere

in the vicinity of $\bar{\mathbf{O}}$ and $\bar{\mathbf{G}}$ by the tangential planes at $\bar{\mathbf{O}}$ and $\bar{\mathbf{G}}$, respectively, or to replace the hyperbolic dispersion surfaces by plane asymptotic surfaces, which are commonly used in the ordinary dynamical theory.

The second approximation is made on the polarization factor as

$$C(\mathbf{p}, \mathbf{q}) \cong 1 \quad \text{for perpendicular components} \quad (18 a)$$

$$\cong |\cos 2 \Theta_B| \quad \text{for parallel components.} \quad (18 b)$$

Thirdly, $(\bar{\mathbf{k}}_0 + \mathbf{p})^2$ and $(\bar{\mathbf{k}}_g + \mathbf{p})^2$ are replaced approximately by k^2 . These approximations are always justified when the approximations (17) can be allowed. It is worth noticing that, then, the multiplications $\mathbf{L}_{0,g} \cdot \tilde{\mathbf{D}}_g$ and $\mathbf{L}_{g,0} \cdot \tilde{\mathbf{D}}_0$ are nothing else but the convolution of the functions $\beta(\mathbf{p})$ with $\mathbf{D}_g(\mathbf{p})$, and $\alpha(\mathbf{p})$ with $\mathbf{D}_0(\mathbf{p})$, respectively.

With these approximations, Eq. (15) or Eqs. (12 a) and (12 b) are transformed into the relations in real space by the use of the three-dimensional Fourier transform. For doing this, we are employing the well-known properties of the Fourier transform;

$$\begin{aligned} \text{(A)} \quad \sum_{\mathbf{p}} (\bar{\mathbf{k}}_0 \cdot \mathbf{p}) f(\mathbf{p}) \exp\{i(\mathbf{p} \cdot \mathbf{r})\} &= (k/i) \partial F(\mathbf{r}) / \partial \mathbf{s}_g, \\ & \quad (19 a) \end{aligned}$$

$$\begin{aligned} \sum_{\mathbf{p}} (\bar{\mathbf{k}}_g \cdot \mathbf{p}) f(\mathbf{p}) \exp\{i(\mathbf{p} \cdot \mathbf{r})\} &= (k/i) \partial F(\mathbf{r}) / \partial \mathbf{s}_0, \\ & \quad (19 b) \end{aligned}$$

$$\begin{aligned} \text{(B)} \quad \sum_{\mathbf{q}} f(\mathbf{p} - \mathbf{q}) h(\mathbf{q}) \exp\{i(\mathbf{p} \cdot \mathbf{r})\} &= F(\mathbf{r}) H(\mathbf{r}), \\ & \quad (19 c) \end{aligned}$$

where $\partial/\partial_{\underline{0}}$ and $\partial/\partial_{\underline{g}}$ mean the positional derivatives along the directions $\bar{\mathbf{k}}_0$ and $\bar{\mathbf{k}}_g$, respectively, and $F(\mathbf{r})$ and $H(\mathbf{r})$ are the Fourier inverse transforms of $f(\mathbf{q})$ and $h(\mathbf{q})$, respectively.

As a result, one obtains a set of coupled equations in real space:

$$i k^{-1} \partial \mathbf{D}_0(\mathbf{r}) / \partial s_0 + [\tfrac{1}{2} C \chi_{-g} \exp\{-2\pi i G(\mathbf{r})\}] \mathbf{D}_g(\mathbf{r}) = 0, \quad (20 a)$$

$$i k^{-1} \partial \mathbf{D}_g(\mathbf{r}) / \partial s_g + [\tfrac{1}{2} C \chi_g \exp\{2\pi i G(\mathbf{r})\}] \mathbf{D}_0(\mathbf{r}) = 0. \quad (20 b)$$

They are equivalent to Takagi-Taupin's equation, although they present themselves in a different form. The equivalence will be shown in § 5, where the other forms will be presented in a systematic way.

The expressions (20) are most straightforward in understanding the dynamical interaction of waves in the displacement field $\mathbf{u}(\mathbf{r})$.

§ 4. Scattering Matrix Theory

Following a similar principle, the scattering matrix theory can be formulated from the Bethe-Laue type basic Eqs. (12 a and b). In conclusion, a theory of this type is a mixed representation of the fields in terms of a real space variable (t) and reciprocal space variables (τ or σ). The latter are two-dimensional vectors within a plane perpendicular to the direction of t .

In order to show the principle, we shall derive the matrix theory employing the same approximations (17) and (18) used in deriving the T equation. For convenience, although it is not necessary to do so, the depth below the crystal surface is taken as the variable (t). The vectors \mathbf{p} , \mathbf{k}_0 and \mathbf{k}_g are

decomposed into components such as (p_t, τ) , $(k\gamma_0, \kappa_0)$ and $(k\gamma_g, \kappa_g)$ respectively, where γ_0 and γ_g are the direction cosines of $\bar{\mathbf{k}}_0$ and $\bar{\mathbf{k}}_g$ with respect to the direction t , and κ_0 and κ_g are the components in the plane perpendicular to t .

The matrix elements are then,

$$\mathbf{L}_{00}(p_t, \tau) = -2\{k\gamma_0 p_t + (\kappa_0 \cdot \tau)\}, \quad (21 a)$$

$$\mathbf{L}_{gg}(p_t, \tau) = -2\{k\gamma_g p_t + (\kappa_g \cdot \tau)\}, \quad (21 b)$$

$$\mathbf{L}_{0g}(p_t, q_t; \tau, \sigma) = C k^2 \chi_{-g} \beta(p_t - q_t, \tau - \sigma), \quad (21 c)$$

$$\mathbf{L}_{g0}(p_t, q_t; \tau, \sigma) = C k^2 \chi_g \alpha(p_t - q_t, \tau - \sigma). \quad (21 d)$$

In the following, the variables τ and σ are fixed. The only running variables to be considered are p_t and q_t .

By taking the one-dimensional Fourier transform of Eqs. (12 a and b) with respect to p_t , one obtains

$$2\left\{i k^{-1} \gamma_0 \frac{\partial}{\partial t} - (\kappa_0 \cdot \tau)/k^2\right\} \mathbf{D}_0(t; \tau) + C \chi_{-g} \sum_{\sigma} B(t; \tau - \sigma) \mathbf{D}_g(t; \sigma) = 0, \quad (22 a)$$

$$2\left\{i k^{-1} \gamma_g \frac{\partial}{\partial t} - (\kappa_g \cdot \tau)/k^2\right\} \mathbf{D}_g(t; \tau) + C \chi_g \sum_{\sigma} A(t; \tau - \sigma) \mathbf{D}_0(t; \sigma) = 0 \quad (22 b)$$

where
$$\mathbf{D}_0(t; \tau) = \sum_{p_t} \mathbf{D}_0(p_t; \tau) \exp\{2\pi i(p_t \cdot t)\} = \sum_s \mathbf{D}_0(\mathbf{r}) \exp\{-2\pi i(\tau \cdot \mathbf{s})\}, \quad (23 a, b)$$

the variable \mathbf{s} being the component of \mathbf{r} perpendicular to the direction t , and

$$A(t; \eta) = \sum_{p_t} \alpha(p_t; \eta) \exp\{2\pi i(p_t \cdot t)\} = \sum_s \exp\{2\pi i G(\mathbf{r})\} \exp\{-2\pi i(\eta \cdot \mathbf{s})\}. \quad (24 a, b)$$

Similar equations for $\mathbf{D}_g(t; \tau)$ and $B(t; \eta)$ can be derived.

The expressions (22) can be written in the matrix form

$$i k^{-1} \frac{\partial}{\partial t} \begin{pmatrix} \tilde{\mathbf{D}}_0(t; \tau) \\ \tilde{\mathbf{D}}_g(t; \tau) \end{pmatrix} = \begin{pmatrix} \mathbf{H}_{00}(t) & \mathbf{H}_{0g}(t) \\ \mathbf{H}_{g0}(t) & \mathbf{H}_{gg}(t) \end{pmatrix} \begin{pmatrix} \tilde{\mathbf{D}}_0(t; \sigma) \\ \tilde{\mathbf{D}}_g(t; \sigma) \end{pmatrix}, \quad (25)$$

where the matrix elements are given as follows;

$$\langle \tau | \mathbf{H}_{00}(t) | \tau \rangle = (\kappa_0 \cdot \tau)/k^2 \gamma_0, \quad \langle \tau | \mathbf{H}_{gg}(t) | \tau \rangle = (\kappa_g \cdot \tau)/k^2 \gamma_g, \quad (26 a, b)$$

$$\langle \tau | \mathbf{H}_{0g}(t) | \sigma \rangle = -C \chi_{-g} B(t; \tau - \sigma)/2 \gamma_0, \quad \langle \tau | \mathbf{H}_{g0}(t) | \sigma \rangle = -C \chi_g A(t; \tau - \sigma)/2 \gamma_g. \quad (26 c, d)$$

Equation (25) is the basic equation in the scattering matrix theory. The selection of the coordinate (t) is arbitrary as mentioned above. The present choice is convenient for the plane-wave theory with the boundary condition of the plane entrance surface. When we are concerned with the spherical wave theory with a point source on or near the entrance surface, it is convenient to take z along the net plane within the reflection plane determined by \mathbf{k}_0 and \mathbf{k}_g . In this paper, however, we shall not discuss the details of the boundary conditions.

§ 5. Various Representations of the T Equation

To derive the arguments of this section it is convenient to write Eqs. (20) in terms of two-by-two matrices. The expression will be given below [see

Equation (31)]. The equation resembles the Hamiltonian form of the quantum-mechanical equation for the motion of a single particle system, if one notices the formal correspondences

$$k^{-1} \rightarrow \hbar \quad (\text{Planck's constant}/2\pi), \quad (27 a)$$

$$c \rightarrow \text{light velocity}, \quad (27b)$$

$$z \rightarrow \text{time variable}. \quad (27c)$$

Keeping this analogy in mind, one can write Eq. (20) in various forms. In fact, if the equation of motion is given in the form

$$i\hbar \partial\psi/\partial t = \mathbf{H}\psi, \quad (28)$$

the equivalent one is obtained by the transformation

$$\varphi = \mathbf{S}\psi. \quad (29)$$

The transformed equation must be

$$i\hbar \partial\varphi/\partial t = [\mathbf{S}\mathbf{H}\mathbf{S}^{-1} + i\hbar (\partial\mathbf{S}/\partial t)\mathbf{S}^{-1}] \varphi. \quad (30)$$

Obviously, in our particular problem, the matrix \mathbf{S} must be a two-by-two matrix, and ψ and φ are vectors having two components.

Here, two categories of the transformation are conceivable. One is generated by either a diagonal or skew matrix. In this case, each component of the state vector represents either the O or G wave. For this reason, the representation is called the "O-G representation". The second one is generated by a more general matrix. After the transformation, the components of the state vector become a combination of O and G waves. For this reason, the representation obtained in this way is called a "combination representation". We shall not mention here the combination representation since it is not so valuable in the case of T equations. Some "combination representations" are useful for S equations (see 1963 papers in Reference ¹).

1. Equations (20) can be written as follows by the use of the Pauli matrix ^{*}.

$$ik^{-1} \partial \mathbf{D} / \partial z = \left[ik^{-1} c \boldsymbol{\sigma}_z \frac{\partial}{\partial x} + m_1 c^2 \boldsymbol{\sigma}_x \exp\{2\pi i(G_1 \sigma_z)\} + im_2 c^2 \boldsymbol{\sigma}_x \exp\{2\pi i(G_2 \sigma_z)\} \right] \mathbf{D}, \quad (31)$$

where \mathbf{D} is the column vector having the components $\mathbf{D}_0(\mathbf{r})$ and $\mathbf{D}_g(\mathbf{r})$, and m_1, m_2 and G_1, G_2 are defined by the Fourier transforms of $\text{Re}(\chi) = \chi'$

^{*}

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

In Eq. (31), the following identity is employed.

$$\begin{pmatrix} 0 & e^{-i\delta} \\ e^{i\delta} & 0 \end{pmatrix} = \sigma_x \cdot \exp\{i\delta \sigma_z\} = \exp\{-i\delta \sigma_z\} \cdot \sigma_x \\ = \cos \delta \cdot \sigma_x + \sin \delta \cdot \sigma_y.$$

and $\text{Im}(\chi) = \chi''$ as follows:

$$m_1 = \frac{1}{2} |\chi_g'| C (\cos \Theta_B / \sin^2 \Theta_B), \quad (32a)$$

$$m_2 = \frac{1}{2} |\chi_g''| C (\cos \Theta_B / \sin^2 \Theta_B), \quad (32b)$$

$$G_1 = G + \varphi_1 / 2\pi, \quad \varphi_1 = \arg(\chi_g'), \quad (33a, b)$$

$$G_2 = G + \varphi_2 / 2\pi, \quad \varphi_2 = \arg(\chi_g''). \quad (34a, b)$$

2a. O-G representation. By the use of the matrices

$$\mathbf{S}_a = \exp\{\pi i(G_1 \sigma_z)\}, \quad \mathbf{S}_a^{-1} = \exp\{-\pi i(G_1 \sigma_z)\}, \quad (35a, b)$$

one obtains from Equation (31):

$$ik^{-1} \left[\frac{\partial}{\partial z} + i\pi c \frac{\partial G}{\partial x} \right] \mathbf{D}_a = \left[ik^{-1} c \sigma_z \left(\frac{\partial}{\partial x} + i\frac{\pi}{c} \frac{\partial G}{\partial z} \right) + m_1 c^2 \sigma_x + im_2 c^2 \boldsymbol{\Sigma} \right] \mathbf{D}_a, \quad (36)$$

$$\text{where } \boldsymbol{\Sigma} = \sigma_x \cdot \exp\{i(\varphi_2 - \varphi_1) \sigma_z\}. \quad (37)$$

For the comparison with the field equation for a relativistic particle, it is convenient to use the notations

$$\pi c \partial G / \partial x = k e V, \quad \pi \partial G / \partial z = -k e A_x. \quad (38a, b)$$

Then, (V, A_x) can be interpreted as the scalar and vector potentials in electrodynamics. In fact, they satisfy a relation similar to the Lorentz condition

$$(1/c) \partial V / \partial z + \partial A_x / \partial x = 0. \quad (39)$$

2b. O-G representation; Gauge transformation. By the use of the matrices

$$\mathbf{S}_b = \exp\{-ik e U/c\} \mathbf{S}_a, \quad \mathbf{S}_b^{-1} = \mathbf{S}_a^{-1} \exp\{ik e U/c\}. \quad (40a, b)$$

Equation (31) can be transformed as

$$ik^{-1} (\partial / \partial z + ik e \bar{V}) \mathbf{D}_b = [ik^{-1} c \sigma_z (\partial / \partial x + ik e \bar{A}_x / c) + m_1 c^2 \sigma_x + im_2 c^2 \boldsymbol{\Sigma}] \mathbf{D}_b \quad (41)$$

where

$$\bar{V} = V + (1/c) \partial U / \partial z, \quad \bar{A}_x = A_x - (\partial / \partial x) U. \quad (42a, b)$$

In electrodynamics, U is usually restricted so as to satisfy the wave equation

$$\partial^2 U / \partial x^2 - (1/c^2) \partial^2 U / \partial z^2 = 0 \quad (43)$$

from the requirement that (\bar{V}, \bar{A}_x) also has to satisfy the Lorentz condition (39) or equivalently Equations (38). In diffraction problems, however, this

requirement is not necessarily postulated. It is worth noticing that one can always take either V or A_x as zero by taking a suitable function $U(x, z)$.

In particular, if one takes $U(x, z)$ as

$$k e U/c = \pi G, \quad (44)$$

one can immediately see from Eqs. (38) and (42) that

$$\bar{V} = V - A_x, \quad \bar{A}_x = A_x - V. \quad (45 a, b)$$

Then, Eq. (41) is reduced to (non-absorbing case)

$$i k^{-1} \begin{pmatrix} \left\{ \frac{\partial}{\partial z} - c \frac{\partial}{\partial x} \right\} + 2\beta & 0 \\ 0 & \left\{ \frac{\partial}{\partial z} + c \frac{\partial}{\partial x} \right\} \end{pmatrix} \mathbf{D}_b = \begin{pmatrix} 0 & m_1 c^2 \\ m_1 c^2 & 0 \end{pmatrix} \mathbf{D}_b \quad (46)$$

where

$$\beta = k e (V - A_x) = \pi c (\partial G / \partial x + (1/c) \partial G / \partial z). \quad (47)$$

Equation (46) was originally obtained by Takagi³.

§ 6. Discussion and Summary

First, the Maxwell equation is transformed to a set of linear equations for the Fourier amplitudes of the field vectors. No approximation is required. From this fundamental equation, the dynamical diffraction theory for distorted crystals is systematically derived by the Fourier transform. The S equation is characterized as a mixed representation of the wave equation in terms of a real variable and a two-dimensional reciprocal space vector. On the other hand, the Takagi-Taupin equation is charac-

terized as a representation in terms of real variables. The essential approximation involved is to assume the Ewald sphere as a contact plane surface at the reciprocal lattice points \bar{O} and \bar{G} . For this reason, the scattering matrix theory and Takagi-Taupin's theory are equivalent.

The Eikonal theory⁶ needs further approximation which neglects inter-branch and intra-branch jumping of the dispersion point. Only the continuous migration on the dispersion surface is concerned. Thus, the concept of the ray is allowed. The trajectory of the ray obeys the relativistic equation of motion^{6,7} provided that the space variable z along the net plane is interpreted as a time variable. Recently, Indenbom and Chukhovskii⁸ derived the Eikonal theory from the T equation, although it has been originally derived directly from the Maxwell equation. This suggests that the T equation must be a kind of wave-mechanical equation for a relativistic particle. In real physics, Klein-Gordon and Dirac equations are proposed for describing a relativistic particle. If one takes into account lattice distortions in diffraction theory, i.e. potential fields in the analogy to electrodynamics, the T equation turns out to be analogous to the Dirac equation rather than to the Klein-Gordon equation*. Since it is sufficient for our purpose to consider one-dimensional motion analogous to electrodynamics, only the concept of positive and negative charge is to be introduced and the concept of spin is not required. It seems promising for the further development of the theory to apply some mathematical techniques used for solving the Dirac equation in the classical and quantum mechanical field theory.

* Although the dispersion equation (energy-momentum relation) is identical both for the Klein-Gordon and Dirac equations, the wave equations are different in the mathematical structure. The Hamiltonians in the wave mechanical treatments must be taken in the different forms (see, for example, H. Feshbach and F. Villars, *Rev. Mod. Physics* **30**, 24 [1958]). In this respect, the present author has a different view from Kambe's interpretation of Eq. (73) in his second paper⁷.

¹ The terminology of "scattering matrix" is different from what is meant in quantum-mechanical scattering theory, although the basic idea is similar. The first introduction of a scattering matrix in the sense of this paper is due to L. Sturkey (*Acta Cryst.* **10**, 858 [1957]; *Proc. Phys. Soc. London* **20**, 321 [1962]). He was mainly interested in the many-beam problems in electron diffraction. Although one has to trace back to C. G. Darwin's masterpiece (*Phil. Mag.* **27**, 325 and 675 [1914]), the matrix formulation for distorted crystals was presented by the present author (*Acta Cryst.* **16**, 276 and 282 [1963]) in X-ray cases.

² P. B. Hirsch, A. Howie, R. B. Nicholson, D. W. Pashley, and H. J. Whelan, *Electron Microscopy of Thin Crystals*, Butterworths, London 1965. — S. Amelinckx, *Sol. State Phys.*, Supplement **6**, Academic Press, New York 1964. — S. Amelinckx, R. Gevers, G. Renault, and J. Van Landuyt, *Modern Diffraction and Imaging Techniques in Material Science*, North Holland, Amsterdam 1970.

³ S. Takagi, *Acta Cryst.* **15**, 1311 [1962]; *J. Phys. Soc. Japan* **26**, 1239 [1969].

⁴ D. Taupin, *Bull. Soc. Franç. Minér. Crist.* **87**, 469 [1964].

⁵ A. Authier, *Advances in X-ray Analysis* **10**, 9 [1967].

⁶ N. Kato, *J. Phys. Soc. Japan* **18**, 1785 [1963]; **19**, 67, 971 [1964].

⁷ K. Kambe, *Z. Naturforsch.* **20 a**, 770 [1965]; **23 a**, 25 [1968].

⁸ V. L. Indenbom and F. N. Chukhovskii, *Sov. Phys. Crystallography* **16**, 972 [1972].