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Ewald's and Bethe–Laue's Conceptions in the Conventional and Extended Dynamical Theory of Diffraction

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Abstract

Ewald's conception of the dynamical theory of diffraction permits the dispersion equation to be written in a simple analytical form. Bragg reflection, grazing incidence, Bragg reflection at grazing incidence and different n-beam approximations differ in the number of confluent poles of this dispersion equation. The differences between Ewald's and Bethe-Laue's theory are discussed.

1. Introduction

The dynamical theory of diffraction (or the theory of multiple scattering) of radiation in crystals is connected with the names of P. P. Ewald, H. Bethe and M. von Laue.

In the so-called 'conventional' dynamical theory of diffraction, some approximations are used which means that the final formulae are not valid in some extreme cases. This unfavorable situation occurs, for example, when the Bragg angle is near $\pi/2$, at grazing incidence, or at skew reflection. The usual extended dynamical theory of diffraction tries to remove these difficulties by making the von Laue conventional theory more precise (Afanas'ev & Melkonyan, 1983; Bedyńska, 1974; Brümmer, Höche & Nieber, 1979; Härtwig 1977). But this endeavor, after a more exact solution of the diffraction problem, also supplies an incentive for a new study of Ewald's fundamental ideas (Ewald, 1916, 1917).

In the following we shall deal with the scattering of particles on a periodic system of Fermi delta potentials which correspond to the diffraction of neutrons on crystals, using the quantum-mechanical generalization of Ewald's theory. But as the ideas of the electrical dipole and electromagnetic waves are more familiar than the T matrix and de Broglie's waves, we explain first the fundamental ideas of Ewald's procedure on the problem of diffraction of light in a crystal.

2. Fundamental equations of Ewald's extended theory

Ewald's starting point was different from that of Bethe and Laue. The aim of Ewald in 1910 (*i.e.* before the experimental discovery of X-ray diffraction) was to support by optical theoretical studies the hypothesis for the existence of the crystal lattice. Thus it was quite natural to consider the crystal as a discrete system of classical electrical vibrating dipoles

$$\mathbf{p}_\mathbf{m}(t) = \mathbf{p}_\mathbf{m} \exp(-i\omega t) \tag{2.1}$$

fixed at the lattice points

$$\mathbf{R}_\mathbf{m} = m_1\mathbf{a}_1 + m_2\mathbf{a}_2 + m_3\mathbf{a}_3, \quad m_1, m_2, m_3 = 0, \pm 1, \ldots, \pm\infty, \tag{2.2}$$

of a crystal lattice. The dipoles are coupled with retarding electromagnetic forces. An external electromagnetic wave

$$\mathbf{E}_{\rm inc} = \mathbf{f} \exp(-i\omega t + i\mathbf{kr}) \tag{2.3}$$

excites the mechanical vibrations of this system of coupled dipoles. The electromagnetic waves generated by oscillating dipoles - and superposed on the incident wave - are registered outside the crystal as the reflected and transmitted waves. Thus the problem of Ewald was in fact the mechanical problem of forced oscillations of a system of electromagnetically coupled oscillators.

Let us formulate the above ideas in a mathematical form (Litzman, 1978, 1980). The electromagnetic field of the oscillating dipole $\mathbf{p}_\mathbf{m}(t)$ is expressed in terms of its Hertz vector

$$\mathbf{Z}(t) = R^{-1}\mathbf{p}(t - R/c) \tag{2.4}$$

in the usual way,

$$\mathbf{E} = [\text{grad div} - (1/c^2)\partial^2/\partial t^2]\mathbf{Z}, \quad \mathbf{H} = c^{-1} \text{ rot } \mathbf{Z}. \tag{2.5}$$

Neglecting the magnetic forces we get for the amplitudes $\mathbf{p}_\mathbf{m}$ of the dipoles (2.1) the equations

$$\mathbf{p}_\mathbf{m} = \alpha\left\{ \sum_{\mathbf{n}\neq\mathbf{m}}{}' [(\text{grad div} + k^2)_\mathbf{m}\mathbf{p}_\mathbf{n} \exp(ikR_{\mathbf{mn}})/R_{\mathbf{mn}}] + \mathbf{f}\exp(i\mathbf{kR}_\mathbf{m})\right\}, \tag{2.6}$$

where α is the polarizability, $k = \omega/c$, c is the velocity of light, $R_{\mathbf{mn}} = |\mathbf{R}_\mathbf{m} - \mathbf{R}_\mathbf{n}|$ and in the sum the term $\mathbf{n} = \mathbf{m}$ is omitted.

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Thus the first task of Ewald's theory is to find the solutions of the infinitely great system of non-homogeneous algebraic equations (2.6). These can be found in the form of 'dipole waves'

$$\mathbf{p}_\mathbf{m}(\boldsymbol{\kappa}_j) = \mathbf{u}_j \exp(i\boldsymbol{\kappa}_j\mathbf{R}_\mathbf{m}). \tag{2.7}$$

It is important to be clear that (2.7) is simply a kinematical description of a steady state of oscillation of dipoles and not an electromagnetic wave running through the medium in which the dipoles are situated. The electromagnetic field generated by the 'dipole wave' (2.7) is derived again from its Hertz potential

$$\mathbf{Z}(\mathbf{R})_j = \sum_\mathbf{m} [\mathbf{p}_\mathbf{m}(\boldsymbol{\kappa}_j)/|\mathbf{R}-\mathbf{R}_\mathbf{m}|] \times \exp[-i\omega t + i\omega|\mathbf{R}-\mathbf{R}_\mathbf{m}|/c] \tag{2.8}$$

by means of (2.5).

Thus, the electromagnetic field outside the crystal is given by the superposition

$$\mathbf{E} = \mathbf{f}\exp(-i\omega t + i\mathbf{k}\mathbf{r}) + \sum_j [\text{grad div} - c^{-2}\,\partial^2/\partial t^2]\mathbf{Z}_j. \tag{2.9}$$

The procedure for the solution of (2.6) was explained in previous papers (Litzman, 1978, 1980).

The generalization of Ewald's classical dynamical theory of the diffraction of light to the quantum-mechanical problem of the diffraction of particles was handled by Lax (1951) and its application to the diffraction of neutrons can be found, for example, in Dederichs (1972) or Sears (1989). In this theory the crystal diffraction centers are characterized not by the classical dipole moments $\mathbf{p}_\mathbf{m}(t)$ but by the quantum-mechanical $T_\mathbf{m}$ matrices

$$T_\mathbf{m}(\mathbf{r},\mathbf{r}') = (\hbar^2/2m)4\pi Q\delta(\mathbf{r}-\mathbf{R}_\mathbf{m})\delta(\mathbf{r}'-\mathbf{R}_\mathbf{m}). \tag{2.10}$$

Q is the scattering length.

Now let us recall briefly the main results of our previous papers on the dynamical theory of diffraction of particles on a periodic system of point scatterers [Fermi δ potentials (2.10)] (Litzman, 1986; Litzman & Dub 1990). We shall deal with the diffraction on a simple lattice forming a semi-infinite crystal

$$\begin{gathered}\mathbf{R}_\mathbf{m} = m_1\mathbf{a}_1 + m_2\mathbf{a}_2 + m_3\mathbf{a}_3,\\ \mathbf{m} = (m_1, m_2, m_3),\\ m_1, m_2 = 0, \pm1, \pm2, \ldots, \pm\infty,\\ m_3 = 0, 1, 2, \ldots, \infty,\end{gathered} \tag{2.11}$$

and $a_{3z} > 0$. The origin of the orthogonal coordinate system lies at the lattice point $(0, 0, 0)$, the plane $0xy$ coincides with the crystal surface plane $(\mathbf{a}_1, \mathbf{a}_2)$. The axis $0z$ (the unit vector $\mathbf{e}_3$) and the vector $\mathbf{a}_1\times\mathbf{a}_2$ point into the crystal. The lattice $(\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3)$ is reciprocal to the three-dimensional lattice $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)$, *i.e.* $\mathbf{g}_i\mathbf{a}_j = 2\pi\delta_{ij}$, $i, j = 1, 2, 3$, whereas the lattice $(\mathbf{b}_1, \mathbf{b}_2)$ is reciprocal to the two-dimensional lattice $(\mathbf{a}_1, \mathbf{a}_2)$, *i.e.* $\mathbf{b}_i\mathbf{a}_j = 2\pi\delta_{ij}$, $\mathbf{b}_i \perp \mathbf{e}_3$, $i, j = 1, 2$. Further, $\mathbf{c}''$ and $\mathbf{c}^\perp$ denote the components of the vector $\mathbf{c} = \mathbf{c}'' + \mathbf{c}^\perp$ parallel and perpendicular to the crystal surface, respectively. Then, $\mathbf{b}_1 = \mathbf{g}_1''$, $\mathbf{b}_2 = \mathbf{g}_2''$, $\mathbf{g}_3'' = 0$.

Let $\mathbf{k}$ be the wavevector of the incident wave, $k_z > 0$. We assign to this vector $\mathbf{k}$ and to each (p, q), where p, q are integers, three other vectors $\mathbf{k}''_{pq}$ and $\mathbf{K}^\pm_{pq}(\mathbf{k})$ as follows:

$$\mathbf{k}''_{pq} = \mathbf{k}'' + p\mathbf{b}_1 + q\mathbf{b}_2 \tag{2.12a}$$

$$\mathbf{K}^\pm_{pq}(\mathbf{k}) = \mathbf{k}''_{pq} \pm \mathbf{e}_3 K_{pqz}(\mathbf{k}), \tag{2.12b}$$

where

$$K_{pqz}(\mathbf{k}) = +[k^2 - (\mathbf{k}''_{pq})^2]^{1/2}. \tag{2.12c}$$

This means that

$$|\mathbf{K}^\pm_{pq}(\mathbf{k})| = k. \tag{2.12d}$$

For $(p, q) = (0, 0)$, $\mathbf{K}^+_{00}(\mathbf{k}) = \mathbf{k}$ and $K_{00z}(k) = k_z$ hold. Further, we define $\theta^\pm_{pq}$ as

$$\theta^\pm_{pq} \equiv \theta^\pm_{pq}(\mathbf{k}) = \mathbf{a}_3\mathbf{K}^\pm_{pq}(k) = \mathbf{a}_3''\mathbf{k}''_{pq} \pm a_{3z}K_{pqz}(k). \tag{2.12e}$$

Now let us write equations for the diffraction of de Broglie's wave $f\exp(i\mathbf{k}\mathbf{r})$ on the periodic system of δ potentials at the lattice points (2.11). The wave function $\Psi(\mathbf{r})$ describing the diffraction of particles is

$$\Psi(\mathbf{r}) = f\exp(i\mathbf{k}\mathbf{r}) - \sum_\mathbf{n} Q\{[\exp(ik|\mathbf{r}-\mathbf{R}_\mathbf{n}|)]/|\mathbf{r}-\mathbf{R}_\mathbf{n}|\} \times \varphi^\mathbf{n}(\mathbf{R}_\mathbf{n}), \tag{2.13}$$

which is the superposition of the incident plane wave $f\exp(i\mathbf{k}\mathbf{r})$ and the spherical waves excited by the point scatterers forming the crystal (2.11). The diffraction amplitude of the nth atom is $Q\varphi^\mathbf{n}(\mathbf{R}_\mathbf{n})$, where Q is the diffraction length of the scatterers (atoms), and the 'effective field' $\varphi^\mathbf{n}(\mathbf{R}_\mathbf{n})$ incident on the nth atom must satisfy

$$\varphi^\mathbf{n}(\mathbf{R}_\mathbf{n}) = f\exp(i\mathbf{k}\mathbf{R}_\mathbf{n}) - \sum_{\mathbf{m}\neq\mathbf{n}}{}' Q\{[\exp(ik|\mathbf{R}_\mathbf{m}-\mathbf{R}_\mathbf{n}|)]/|\mathbf{R}_\mathbf{m}-\mathbf{R}_\mathbf{n}|\} \times \varphi^\mathbf{m}(\mathbf{R}_\mathbf{m}). \tag{2.14}$$

It can be seen that (2.14) for neutrons is quite analogous to (2.6) for photons after omitting in the latter the operator (grad div + k^2). This also holds for (2.13) and (2.9), (2.8).

The solution of the infinite system of non-homogeneous algebraic equations (2.14) has the form

$$\varphi^\mathbf{n}(\mathbf{R}_\mathbf{n}) = \sum_j c_j' \exp(i\boldsymbol{\kappa}_j\mathbf{R}_\mathbf{n}), \qquad \operatorname{Im}\boldsymbol{\kappa}_j > 0, \tag{2.15}$$

where

$$\boldsymbol{\kappa}_j = \mathbf{k}'' + (1/2\pi)(\psi_j - \mathbf{k}''\mathbf{a}_3'')\mathbf{g}_3. \tag{2.16}$$

Quantities ψ_j appearing in (2.16) are solutions of the 'dispersion relation' (Litzman, 1986).

$$1+QS'(\mathbf{k}'') -\sum_{pq} b_{pq}\{\exp(i\theta^+_{pq})/[\exp(i\psi)-\exp(i\theta^+_{pq})] +\exp(-i\theta^-_{pq})/[\exp(-i\psi)-\exp(-i\theta^-_{pq})]\} =0, \quad (2.17)$$

in which $S'(\mathbf{k}'')$ is the two-dimensional lattice sum

$$S'(\mathbf{k}'')=\sum_{(n_1,n_2\neq 00)}' \{\exp(ik|n_1\mathbf{a}_1+n_2\mathbf{a}_2|)/|n_1\mathbf{a}_1+n_2\mathbf{a}_2| \times \exp[i\mathbf{k}''(n_1\mathbf{a}_1+n_2\mathbf{a}_2)]\} \quad (2.18)$$

and

$$b_{pq}=-2\pi iQ/|\mathbf{a}_1\times\mathbf{a}_2|K_{pqz}. \quad (2.19)$$

The explicit form of the coefficients c'_j in (2.15) is unimportant for this paper.

Since the translational symmetry of our problem in the directions of the vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ is preserved it is clear that the wavevectors of the reflected particles are the vectors $\mathbf{K}^-_{pq}$ (2.12*b*) only. Introducing (2.15) into (2.13) we have deduced for the reflectivity $\mathcal{R}(\mathbf{K}^-_{rs})$ in the direction of the vector $\mathbf{K}^-_{rs}$ the formula

$$\mathcal{R}(\mathbf{K}^-_{rs})=|R_1(\mathbf{K}^-_{rs})|^2|R_2(\mathbf{K}^-_{rs})|^2k_z/K_{rsz}, \quad (2.20)$$

where

$$R_1(\mathbf{K}^-_{rs})=\frac{\exp(i\psi_1)-\exp(i\theta^+_{00})}{\exp(i\psi_1)-\exp(i\theta^-_{rs})}, \quad (2.21)$$

$$R_2(\mathbf{K}^-_{rs})=\prod_{j\neq 1}' \frac{\exp(i\psi_j)-\exp(i\theta^+_{00})}{\exp(i\psi_j)-\exp(i\theta^-_{rs})} \times\frac{\exp(i\theta^+_j)-\exp(i\theta^-_{rs})}{\exp(i\theta^+_j)-\exp(i\theta^+_{00})}. \quad (2.22)$$

The details of the derivations of the above formulae can be found in Litzman (1986). In (2.21), (2.22) only the solutions of (2.17) with $\operatorname{Im}\psi_j>0$ are used. Although (2.20) is invariant to the permutation of indices j, for practical cases it is advantageous to denote the solution ψ that is near to the pole θ^+_{rs} as ψ_{rs} and $\psi_{00}=\psi_1$.

Similar formulae to those above were deduced for the reflection of light on a periodic system of dipoles (Litzman & Rózsa, 1990). The paper by Avron, Grossman & Høegh-Krohn (1983) should also be mentioned in this connection.

3. The comparison of Ewald's and Bethe–Laue's procedures

In the dynamical theory of diffraction of Bethe (1928) and Laue (1948), the crystal is considered as a continuous medium. Thus, applying this method to the diffraction of neutrons we have to solve the Schrödinger equation

$$[-(\hbar^2/2m)\Delta+V(\mathbf{r})]\psi=E\psi \quad (3.1)$$

with the periodic potential $V(\mathbf{r})=V(\mathbf{r}+\mathbf{R}_m)$, *i.e.*

$$V(\mathbf{r})=\sum_{\mathbf{G}} V(\mathbf{G})\exp(i\mathbf{Gr}), \quad (3.2)$$

where $\mathbf{G}$ are vectors of the reciprocal lattice $\{\mathbf{g}_1,\mathbf{g}_2,\mathbf{g}_3\}$. From the Bloch theorem we write the solution of (3.1) as

$$\psi_{\boldsymbol{\kappa}}(\mathbf{r})=\sum_{\mathbf{G}} C_{\boldsymbol{\kappa}}(\mathbf{G})\exp[i(\boldsymbol{\kappa}+\mathbf{G})\mathbf{r}]. \quad (3.3)$$

By well known procedures (Sears, 1989; Rauch & Petrascheck, 1978) we get for the unknown vectors $\boldsymbol{\kappa}$ and for the expansion coefficients $C_{\boldsymbol{\kappa}}(\mathbf{G})$ the following system of homogeneous equations:

$$[E-V(0)-(\hbar^2/2m)(\boldsymbol{\kappa}+\mathbf{G})^2]C_{\boldsymbol{\kappa}}(\mathbf{G}) =\sum_{\mathbf{G}'\neq\mathbf{G}} V(\mathbf{G}-\mathbf{G}')C_{\boldsymbol{\kappa}}(\mathbf{G}'). \quad (3.4)$$

The determinant of the infinitely great system of algebraic equations (3.4) will be denoted as $\mathcal{D}(\boldsymbol{\kappa})$ and the equation for the unknown vector $\boldsymbol{\kappa}$,

$$\mathcal{D}(\boldsymbol{\kappa})=0, \quad (3.5)$$

is called the dispersion equation. Its solutions

$$\boldsymbol{\kappa}_1,\boldsymbol{\kappa}_2,\ldots,\boldsymbol{\kappa}_j,\ldots \quad (3.6)$$

determine the wavevectors of the de Broglie waves which can propagate through the infinite crystal [see (3.3)].

If the external wave $f\exp(i\mathbf{kr})$ impinges on a semi-infinite crystal bordered by the surface $0xy$, the wavevectors $\boldsymbol{\kappa}_j$ of the waves inside the crystal must satisfy besides (3.5) the conditions

$$\boldsymbol{\kappa}_j=\mathbf{k}-k\delta_j\mathbf{e}_3. \quad (3.7)$$

Introducing (3.7) into (3.5) we get the fundamental equation of Bethe–Laue's theory

$$\mathcal{D}(\delta)=0 \quad (3.8)$$

for the evaluation of the wavevectors of de Broglie's waves in the crystal.

Of course, as the order of the determinant of the system (3.4) is infinite, it is not possible to write (3.5) in an explicit form and approximate procedures should be applied. If the wavevector $\mathbf{k}_B$ of the incident wave satisfies the Bragg reflection condition for one vector $\mathbf{G}$ of the reciprocal lattice only, *i.e.*

$$(\mathbf{k}_B+\mathbf{G})^2=k^2, \qquad \mathbf{G}=r\mathbf{g}_1+s\mathbf{g}_2-n\mathbf{g}_3, \quad r, s, n \text{ are integers}, \quad (3.9)$$

the two-beam approximation is used and the system (3.4) is reduced to

$$[E-V(0)-(\hbar^2/2m)\boldsymbol{\kappa}^2]C_{\boldsymbol{\kappa}}(0)=V(-\mathbf{G})C_{\boldsymbol{\kappa}}(\mathbf{G}) \quad (3.10)$$
$$[E-V(0)-(\hbar^2/2m)(\boldsymbol{\kappa}+\mathbf{G})^2]C_{\boldsymbol{\kappa}}(\mathbf{G})=V(\mathbf{G})C_{\boldsymbol{\kappa}}(0).$$

Then (3.8) is of second order in the conventional theory (Sears, 1989; Rauch & Petrascheck, 1978) and of fourth order in the extended one (Bedyńska, 1974).

Now let us compare the final results of Ewald's and Bethe–Laue's procedures.

In Ewald's conception, (3.8) is replaced by (2.17) which in contrast to (3.8) has a well arranged analytical form for an arbitrary number of beams. As $|b_{pq}| \ll 1$ and $|QS'| \ll 1$, the solutions ψ_j of (2.17) are near to the poles $\theta^{\pm}_{pq}$. In a semi-infinite crystal the solutions with $\operatorname{Im} \psi_j > 0$ have a physical meaning only.

It can be shown [see Appendix 1 in Litzman & Dub (1990)] that the Bragg reflection condition (3.9) is equivalent to

$$\theta^{+}_{00}(\mathbf{k}_B) = \theta^{-}_{rs}(\mathbf{k}_B) + 2\pi n, \; n \text{ integer}, \qquad (3.11)$$

i.e. to the confluence of two poles in (2.17). At grazing incidence $k_z \simeq -k_z$, thus

$$\theta^{-}_{00} = \mathbf{a}''_3\mathbf{k}'' - a_{3z}k_z \simeq \mathbf{a}''_3\mathbf{k}'' + a_{3z}k_z = \theta^{+}_{00}. \quad (3.12)$$

From this point of view, the grazing incidence is a special case of Bragg reflection (3.11) for $n = 0$ and $(rs) = (00)$. We shall show in another paper that this specularly reflected beam is 'strong' only if the index of refraction is smaller than one. This is true for neutrons but not for electrons handled in Bethe's and Laue's papers (Beth, 1928; Laue, 1948).

The reflectivity (2.20) is an explicit function of the solutions ψ_j of (2.17), whereas in Bethe–Laue's theory a further procedure for determining the coefficients $C_{\kappa}(\mathbf{G})$ in (3.3) (applying the boundary conditions for continuous media) is necessary. Following James (1963) their use is not logically justified when the waves concerned have lengths comparable with atom distances. On the other hand, as (2.14) are algebraic equations for a discrete system, no boundary conditions in Ewald's theory are used.

In Bethe–Laue's theory the formula for the intensity of the reflected ray is expressed as a function of the deviation $\Delta\xi$ of the incident ray from the Bragg reflection position. On the other hand, the parameter measuring the deviation of the incident beam from the Bragg reflection position in (2.20) is not the angle $\Delta\xi$ but the difference [see (3.11)]

$$\eta = \theta^{+}_{00}(\mathbf{k}) - \theta^{-}_{rs}(\mathbf{k}) - 2\pi n, \qquad (3.13)$$

whereby the reflected beam need not lie - as usually supposed when applying Bethe–Laue's conventional theory - in the plane of incidence. Thus, (2.17), (2.20) are valid for skew reflection as well. If the reflected beam does lie in the plane of incidence a simple relation between η and $\Delta\xi$ was deduced (Litzman & Dub, 1990),

$$\eta = \alpha\Delta\xi + \beta(\Delta\xi)^2 + 0(\Delta\xi)^3. \qquad (3.14)$$

It can be shown that the well known two-beam approximate formula of Bethe–Laue's conventional theory for the reflectivity on a semi-infinite crystal can be deduced from the exact one (2.20) (based on Ewald's conception) using the following approximations:

(i) $R_2(K^{-}_{rs}) = 1$ in (2.20); (3.15)

(ii) the exact dispersion equation (2.17) is replaced by an approximate one of the second order in $\exp(i\psi)$ by omitting in the sum $\sum_{pq}$ all terms except those with θ^{-}_{rs} and θ^{+}_{00}. Then using (3.14) and taking into consideration the terms of first order in $\Delta\xi$, we get the usual expression of the conventional Bethe–Laue theory for the intensity of the reflected beam, which of course is not valid for the Bragg angle $\theta_B = \pi/2$. Taking into account in (3.14) the terms of second order in $\Delta\xi$, we get for the intensity a modified formula valid for $\theta_B = \pi/2$ too, which agrees with that deduced by Brümmer, Höche & Nieber (1979) in the extended Laue dynamical theory.

One of the aims of the extended dynamical theory of diffraction is the study of Bragg reflection at grazing incidence. To fulfil all boundary conditions, Laue's theory deals with the dispersion equation (3.8) of fourth order (Härtwig, 1977). In Ewald's conception, for Bragg reflection at grazing incidence, (3.11) and (3.12) are simultaneously valid, which means that at asymmetric reflection three poles of the dispersion equation (2.17) coincide. If the reflected beam is also very near the surface, besides (3.11) and (3.12),

$$\theta^{+}_{rs} \simeq \theta^{-}_{rs} \qquad (3.16)$$

holds, which means that four poles of (2.17) coincide. The approximation (3.15) is then no longer valid. Similar considerations hold for the confluence of the poles of the dispersion equation for different n-beam approximations. We intend to discuss these problems in a future paper.

4. Concluding remarks

The crucial point of the dynamical theory of diffraction is the construction and analysis of the dispersion equation. In Bethe–Laue's theory it has the form (3.8) where $\mathcal{D}$ is the determinant of the infinite system of homogeneous algebraic equations (3.4). Thus it is difficult to write $\mathcal{D}(\delta)$ explicitly. On the other hand, the dispersion equation of Ewald's theory (2.17) has a simple analytical form and can be written immediately. Bragg reflections for different n-beam approximations or at grazing incidence differ in Ewald's conception in the number of confluent poles $\theta^{\pm}_{pq}$ of (2.17) only and the intensity of the reflected beams (2.20) is given explicitly by the solutions ψ_j of (2.17). Formulae (2.17), (2.20), (2.21) and (2.22) are exact and are valid for skew reflection as well. The strength of interaction modifies the value of the constants Q and b_{pq} only.

The case of a crystal of finite thickness was dealt with by Litzman & Rózsa (1990). The dispersion equation (2.17) is the same but the formula for the intensity does not have the simple form (2.20).

In the case of a crystal with s atoms in the basis the dispersion equation has a more complicated form (Litzman, 1986):

$$\det \left\| I - C - \sum_{pq} (\{\exp[i(\theta_{pq}^{-} - \psi)] - 1\}^{-1} B_{pq} + \{\exp[-i(\theta_{pq}^{+} - \psi)] - 1\}^{-1} D_{pq}) \right\|, \quad (4.1)$$

where I, C, B_{pq} and D_{pq} are matrices of order s. Neither the dispersion equation (4.1) nor the formulae for the intensities of the reflected and transmitted waves have been analyzed yet.

The dispersion equation for the diffraction of light on a periodic system of dipoles has a form similar to (4.1) (Litzman, 1978, 1980).

We think that a more profound study of the exact Ewald analytical formulae would be useful to test different approximations used in Bethe–Laue's conventional and extended dynamical theory, not only for neutrons but also for X-rays, as was shown for simple examples in Litzman & Dub (1990) and Litzman & Rózsa (1990).

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Perturbation Theory in High-Energy Transmission Electron Diffraction

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Abstract

A perturbation theory for many-beam high-energy transmission electron diffraction in noncentrosymmetric crystals is described for both the nondegenerate and degenerate cases. This perturbation theory differs from the conventional quantum-mechanical perturbation theory by perturbing the electron wavevectors instead of the total electron energy, which is constant for elastically scattered electrons. The relations between the perturbation theory and some other approximations commonly used in electron diffraction are discussed. It is shown that the few-beam approximation and the Kambe approximation are both applications of degenerate perturbation theory. Finally, as an example, this degenerate perturbation theory is applied to obtain an analytical solution to a four-beam case with two systematic (0 and g) and two nonsystematic (h and l) beams. This four-beam solution shows that the intensity of a four-beam interaction depends on all the four three-phase invariants involved, and also shows that the effects of the g beam on the three-beam interaction of 0, h and l are localized to the region near the Bragg condition of g. This may serve as a guide for future experiments using three-beam interactions for the measurement of structure-factor phases of an unknown structure.

1. Introduction

The formal theory of high-energy electron diffraction in a quantum-mechanical framework was established

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