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The Ewald dynamical diffraction theory – ninety years later

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Diffraction on a crystalline slab formed by point-like scattering centres is treated as a multiple scattering problem based on the Ewald equations. Using general results expressed in a lucid matrix form, the two-beam solution for both coplanar and non-coplanar cases valid near and far from Bragg peaks is found and a detailed comparison of the final formulae obtained with those following from Laue's theory is performed.

1. Introduction

Ninety years ago, from 1912 to 1916, P. P. Ewald was developing the fundamentals of the theory, now called the Ewald dynamical theory of diffraction [see original papers by Ewald (1916, 1917) and a memorial volume for P. P. Ewald (Cruickshank *et al.*, 1992)]. Ewald considered a crystal as a three-dimensional array of electric dipoles fixed at the lattice points. Oscillating dipoles generate electromagnetic fields, which, superimposed upon the external wave, force dipoles to oscillate. The fields propagating inside the crystal must be such as to produce excitations of all scatterers that are in full equilibrium with the fields themselves. The problem of Ewald has been the mechanical problem of forced oscillations of a system of electromagnetically coupled oscillators where no boundary conditions appear. Thus, the Ewald discrete dipole model was recently used successfully in surface optics (Dub, 1983; Wijers & Poppe, 1992; de Boeij *et al.*, 1996).

Later, the Ewald concept was applied to neutron scattering where the interaction potential is replaced by the Fermi pseudopotential (Dederichs, 1972; Sears, 1989). The Lippmann–Schwinger equation for the multiple scattering on a system of δ-function potentials yields a self-consistent system of equations, which are the quantum-mechanical analogue of equations first introduced by Ewald to describe the multiple scattering of electromagnetic radiation.

On the other hand, in the dynamical theory of diffraction of Bethe and von Laue, the crystal is considered to be a continuum described by the periodic potential. Since the potential is discontinuous at the surface of the sample volume V, one must find separate solutions inside and outside V and then match the exterior and interior solutions by boundary conditions. The mathematical solution of the problem based on a macroscopic and phenomenological procedure raises the question about the nature of the border surface and, as pointed out by von Laue (1941), the boundary conditions problem is 'the weakest point of the theory'. The boundary conditions problem was also mentioned by other authors (Pinsker, 1978; Authier, 2001; Dub & Litzman, 2001*b*). Furthermore, as pointed out by Sears (1989): 'The accuracy of the results obtained by the Laue method is limited by the accuracy of the elementary expressions for the optical potential, which neglects local-field effects. This limitation is overcome in the Ewald method, which ... consists in finding a systematic self-consistent solution of the Ewald equations. In the Ewald method the local-field effects are taken rigorously into account.'

Ewald's theory has been mostly connected with the theory of dispersion (Authier, 2001, pp. 41–48) and detailed comparison of the dispersion theories by Ewald and Laue was done by Wagenfeld (1968). On the other hand, authors interested in the theory of reflection and diffraction have adopted the Laue method (see *e.g.* Rauch & Petraschek, 1978; Sears, 1989; Authier, 2001). In our series of papers (Litzman & Rózsa, 1977; Litzman, 1978, 1980, 1986; Litzman & Dub, 1990; Litzman, 1991; Litzman *et al.*, 1996; Litzman & Mikulík, 1999), however, we have further developed and applied the Ewald concept of the dynamical diffraction theory. In particular, papers by Litzman (1986) and Litzman *et al.* (1996) have been devoted to the problem of the multiple diffraction of neutrons. In Litzman (1986), the solution of the quantum-mechanical Ewald equations was expressed in a lucid matrix form and amplitudes of the diffracted waves were then obtained in well arranged determinant forms, which are valid quite generally. These results may be adopted to deal also with the cases outside the scope of standard dynamical diffraction theory (Litzman & Dub, 1990; Litzman & Mikulík, 1999). In our recent paper (Litzman *et al.*, 1996), the case of a semi-infinite crystal was dealt with, the results obtained being valid for arbitrary angles of incidence, including grazing incidence, Bragg angle near $\pi/2$, near or far from the Bragg peaks. In the present paper, using general derived results, we will treat rigorously the diffraction on a crystalline slab and perform a detailed comparison of results obtained with those following from Laue's theory.

2. Exact multiwave formulae for the reflection and transmission of neutrons on a crystal slab

2.1. Geometrical theory

Let us consider the scattering of neutrons on a system of point scatterers forming a slab

$$\mathbf{R}_\mathbf{m} = m_1\mathbf{a}_1 + m_2\mathbf{a}_2 + m_3\mathbf{a}_3, \quad \mathbf{m} = (m_1, m_2, m_3),$$
$$m_1, m_2 = 0, \pm 1, \pm 2, \ldots, \pm\infty, \quad m_3 = 0, 1, 2, \ldots, N. \quad (1)$$

The origin of the orthogonal coordinate system $Oxyz$ lies at the lattice point $(0, 0, 0)$, the plane Oxy coincides with the entrance crystal surface plane $(\mathbf{a}_1, \mathbf{a}_2)$. The axis Oz (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.* $\mathbf{g}_i \cdot \mathbf{a}_k = 2\pi\delta_{ik}$ $(i, k = 1, 2, 3)$, whereas the lattice $(\mathbf{b}_1, \mathbf{b}_2)$ is reciprocal to the two-dimensional lattice $(\mathbf{a}_1, \mathbf{a}_2)$, *i.e.* $\mathbf{b}_i \perp \mathbf{e}_3$, $\mathbf{b}_i \cdot \mathbf{a}_k = 2\pi\delta_{ik}$ $(i, k = 1, 2)$. With $\mathbf{c}^{||}$ and $\mathbf{c}^{\perp}$ denoting the components of the vector $\mathbf{c} = \mathbf{c}^{||} + \mathbf{c}^{\perp}$ parallel and perpendicular to the surface, respectively, we have $\mathbf{g}_1^{||} = \mathbf{b}_1$, $\mathbf{g}_2^{||} = \mathbf{b}_2$, $\mathbf{g}_3^{||} = \mathbf{0}$. Further,

$$f(\mathbf{r}) = A\exp(\mathrm{i}\mathbf{k}\cdot\mathbf{r}) \quad \text{with } k_z > 0 \quad (2)$$

represents the plane wave incident upon the entrance crystal surface.

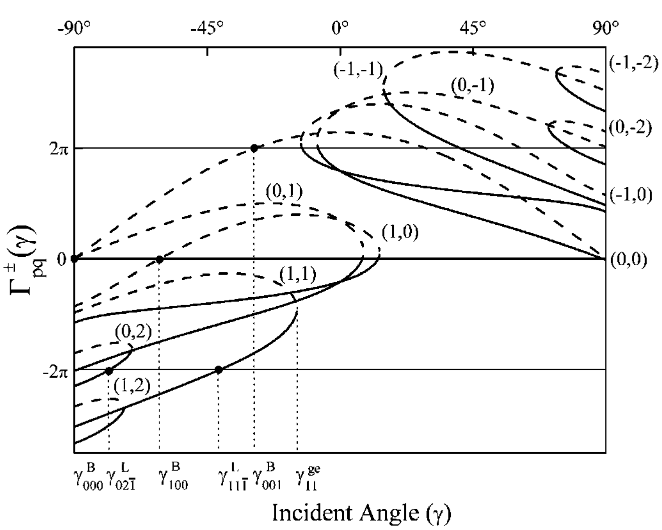

Figure 1
Γ diagrams $\Gamma^{+}_{pq}(\gamma)$ for the Laue geometry (full line) and $\Gamma^{-}_{pq}(\gamma)$ for the Bragg geometry (broken line) for the b.c.c. lattice with $\mathbf{a}_1 = a(1, 0, 0)$, $\mathbf{a}_2 = a(0, 1, 0)$, $\mathbf{a}_3 = (a/2)(1, 1, 1)$, $a/\lambda = 0.875$ and $\mathbf{k}^{||}$ parallel to $\mathbf{a}_1 + 2\mathbf{a}_2$, $\mathbf{a}_1$ and $\mathbf{a}_2$ lying in the crystal surface plane. For (p, q) other than those given in the figure, the values of K_{pqz} from (4) are purely imaginary in the whole interval of γ. The angle γ^{L}_{pql} or γ^{B}_{pql} is the angle of incidence, for which the Bragg condition (8*a*) or (8*b*) for the Laue or Bragg geometry, respectively, is satisfied. Diffractions with $(p, q) = (0, 0)$, $(1, 2)$ and $(-1, -2)$ are coplanar and the others are non-coplanar. $\Gamma^{-}_{00}(\gamma)$ corresponds to the specularly reflected wave.

Owing to the two-dimensional discrete translation symmetry in the surface plane $(\mathbf{a}_1, \mathbf{a}_2)$, the components of the wavevectors parallel to the crystal surface of diffracted waves are of the form

$$\mathbf{k}^{||}_{pq} = \mathbf{k}^{||} + p\mathbf{b}_1 + q\mathbf{b}_2, \quad \mathbf{k}^{||} = \mathbf{k} - k_z\mathbf{e}_3, \quad p, q \text{ being integers.} \quad (3)$$

Then considering merely elastic scattering, the wavevectors $\mathbf{K}^{+}_{pq}(\mathbf{k})$ and $\mathbf{K}^{-}_{pq}(\mathbf{k})$ of the diffracted waves in the Laue (transmission) and Bragg (reflection) geometry, respectively, are given by

$$\mathbf{K}^{\pm}_{pq}(\mathbf{k}) = \mathbf{k}^{||}_{pq} \pm \mathbf{e}_3 K_{pqz}(\mathbf{k}) \quad \text{with } K_{pqz}(\mathbf{k}) = +[k^2 - (\mathbf{k}^{||}_{pq})^2]^{1/2}. \quad (4)$$

Using this notation, $\mathbf{K}^{+}_{00} = \mathbf{k}$ is the wavevector of the incident and forward propagating waves and $\mathbf{K}^{-}_{00}$ is the wavevector of the specularly reflected wave. From (4), it can be seen that there is a finite number, say n, of different couples (p, q) (depending on the wavelength λ of the incident radiation and the angle of incidence γ) yielding $2n$ radiative waves with real $K_{pqz}(\mathbf{k})$. Other (p, q) correspond to non-radiative waves with pure imaginary $K_{pqz}(\mathbf{k})$.

As the wavevectors $\mathbf{K}^{\pm}_{pq}$ are given by (4),[1] two Laue equations are satisfied automatically, *viz* $\mathbf{a}_1 \cdot (\mathbf{k} - \mathbf{K}^{\pm}_{pq}) = -2\pi p$, $\mathbf{a}_2 \cdot (\mathbf{k} - \mathbf{K}^{\pm}_{pq}) = -2\pi q$. Thus, should the incident wave (2) fulfil the Bragg condition, the third Laue equation must be satisfied, *i.e.* for its wavevector $\mathbf{k}_\mathrm{B}$

$$\mathbf{a}_3 \cdot [\mathbf{k}_\mathrm{B} - \mathbf{K}^{+}_{pq}(\mathbf{k}_\mathrm{B})] = 2\pi l \quad \text{(Laue geometry)} \quad (5a)$$

and/or

$$\mathbf{a}_3 \cdot [\mathbf{k}_\mathrm{B} - \mathbf{K}^{-}_{pq}(\mathbf{k}_\mathrm{B})] = 2\pi l \quad \text{(Bragg geometry)} \quad (5b)$$

must hold, the diffraction vector being $p\mathbf{g}_1 + q\mathbf{g}_2 - l\mathbf{g}_3$ with l integer. We introduce

$$\theta^{\pm}_{pq}(\mathbf{k}) = \mathbf{a}_3 \cdot \mathbf{K}^{\pm}_{pq}(\mathbf{k}) = \mathbf{a}^{||}_3 \cdot \mathbf{k}^{||}_{pq} \pm a_{3z}K_{pqz}(\mathbf{k}), \quad (6)$$

so conditions (5*a*) and (5*b*) read

$$\theta^{+}_{00}(\mathbf{k}_\mathrm{B}) - \theta^{+}_{pq}(\mathbf{k}_\mathrm{B}) = 2\pi l \quad \text{(Laue geometry)} \quad (7a)$$
$$\theta^{+}_{00}(\mathbf{k}_\mathrm{B}) - \theta^{-}_{pq}(\mathbf{k}_\mathrm{B}) = 2\pi l \quad \text{(Bragg geometry).} \quad (7b)$$

In most experiments, the plane of incidence and the wavelength are kept constant and only the angle of incidence γ (measured from the inner normal to the surface) varies. All quantities in (6) are then functions of the angle γ and (7*a*) and (7*b*) can be expressed as

$$\Gamma^{+}_{pq}(\gamma^{\mathrm{L}}_{pql}) = 2\pi l \quad (8a)$$

and

$$\Gamma^{-}_{pq}(\gamma^{\mathrm{B}}_{pql}) = 2\pi l, \quad (8b)$$

where

$$\Gamma^{\pm}_{pq}(\gamma) = \theta^{+}_{00}(\gamma) - \theta^{\pm}_{pq}(\gamma). \quad (9)$$

[1] See also equation (84).

Then the diffraction condition may be visualized by 'Γ diagrams'. In Fig. 1, we give the plot of Γ^+_{pq} and Γ^-_{pq} *versus* $\gamma \in (-90^\circ, +90^\circ)$. The intersections of the plots of $\Gamma^+_{pq}(\gamma)$ or $\Gamma^-_{pq}(\gamma)$ with the horizontal straight lines $2\pi l$ give Bragg reflections for the Laue or Bragg geometry, respectively. In particular, since $\Gamma^-_{00}(\pm 90^\circ) = 0$, the total reflection at grazing incidence can be considered as a special case of the symmetrical Bragg reflection (8*b*) with $(p, q) = (0, 0)$ and $l = 0$ (see Litzman, 1991). Furthermore, the points (*e.g.* γ^{ge}_{11}) where Γ diagrams for the Laue geometry Γ^+_{pq} and for the Bragg geometry Γ^-_{pq} stick together, and thus $\theta^+_{pq} \to \theta^-_{pq}$, should be mentioned since it happens if $K_{pqz} \to 0$, which indicates grazing emergence.

2.2. Quantum-mechanical analogue of Ewald's theory for the diffraction of neutrons

The Ewald dynamical diffraction theory, generalized to quantum mechanics, yields the following equations for the wavefunction $\Psi(\mathbf{r})$ describing the diffraction of neutrons on a crystal slab formed by identical point-like scattering centres (Dederichs, 1972; Sears, 1989):

$$\Psi(\mathbf{r}) = f(\mathbf{r}) - \sum_{\mathbf{n}} Q \frac{\exp(\mathrm{i}k|\mathbf{r} - \mathbf{R_n}|)}{|\mathbf{r} - \mathbf{R_n}|} \Phi^{\mathbf{n}}(\mathbf{R_n}) \qquad (10a)$$

with

$$\Phi^{\mathbf{m}}(\mathbf{R_m}) = f(\mathbf{R_m}) - \sum_{\mathbf{n}\neq\mathbf{m}}{}' Q \frac{\exp(\mathrm{i}k|\mathbf{R_m} - \mathbf{R_n}|)}{|\mathbf{R_m} - \mathbf{R_n}|} \Phi^{\mathbf{n}}(\mathbf{R_n}). \qquad (10b)$$

$\Psi(\mathbf{r})$ is the total field at the point $\mathbf{r}$, $\Phi^{\mathbf{m}}(\mathbf{R_m})$ is the field incident on the scatterer at $\mathbf{R_m}$ (local field) and $f(\mathbf{r})$ represents the incident wave (2). The point-like scattering centres are described by the scattering length

$$Q = (Q_0^{-1} + \mathrm{i}k)^{-1}, \qquad (11)$$

where $\operatorname{Im} Q_0 < 0$. In the case without absorption, which will be considered in the following, this condition should be understood in the limit $\operatorname{Im} Q_0 \to 0^-$. The theory is applicable for both positive and negative scattering lengths. Nevertheless, in the following we will consider the most common case with $Q_0 > 0$.

Because of the two-dimensional translational symmetry of our problem, the solution of (10*b*) can be expressed as a superposition of plane waves

$$\begin{aligned}\Phi^{n_1 n_2 n_3}(\mathbf{R_n}) &= \exp[\mathrm{i}\mathbf{k}^{||} \cdot (n_1\mathbf{a}_1 + n_2\mathbf{a}_2)] \sum_j \frac{|\mathbf{a}_1 \times \mathbf{a}_2|}{2\pi\mathrm{i}} c_j \exp(\mathrm{i}n_3\psi_j) \\ &= \sum_j \frac{|\mathbf{a}_1 \times \mathbf{a}_2|}{2\pi\mathrm{i}} c_j \exp(\mathrm{i}\tilde{\mathbf{k}}_j \cdot \mathbf{R_n}) \qquad (12a)\end{aligned}$$

with the wavevectors

$$\tilde{\mathbf{k}}_j = \mathbf{k}^{||} + (1/2\pi)(\psi_j - \mathbf{k}^{||} \cdot \mathbf{a}_3)\mathbf{g}_3 = \mathbf{k}^{||} + \tilde{k}_{jz}\mathbf{e}_3, \quad \textit{i.e.} \quad \psi_j = \mathbf{a}_3 \cdot \tilde{\mathbf{k}}_j, \qquad (12b)$$

characterizing the local field.

Substituting the *Ansatz* (12*a*) into (10*b*), we get the following.

(i) The dispersion relation for the parameters ψ_j:

$$\frac{1}{Q} + S'(\mathbf{k}) + \frac{2\pi\mathrm{i}a_{3z}}{|\mathbf{a}_1 \times \mathbf{a}_2|} \sum_{pq} \left\{ \frac{1}{a_{3z}K_{pqz}} \left[\frac{\exp(\mathrm{i}\theta^+_{pq})}{\exp(\mathrm{i}\psi) - \exp(\mathrm{i}\theta^+_{pq})} + \frac{\exp(-\mathrm{i}\theta^-_{pq})}{\exp(-\mathrm{i}\psi) - \exp(-\mathrm{i}\theta^-_{pq})} \right] \right\} = 0, \qquad (13)$$

where poles $\theta^\pm_{pq}$ are given by (6) and

$$S'(\mathbf{k}) = \sum_{(n_1,n_2)\neq(0,0)} \frac{\exp(\mathrm{i}k|n_1\mathbf{a}_1 + n_2\mathbf{a}_2|)}{|n_1\mathbf{a}_1 + n_2\mathbf{a}_2|} \exp[\mathrm{i}\mathbf{k}^{||} \cdot (n_1\mathbf{a}_1 + n_2\mathbf{a}_2)] \qquad (14a)$$

is the well known two-dimensional interplanar Ewald optical lattice sum (Dub & Litzman, 1983), the imaginary part of which is

$$\operatorname{Im} S'(\mathbf{k}) = \frac{2\pi}{|\mathbf{a}_1 \times \mathbf{a}_2|} \sum_{K^2_{pqz}>0} \frac{1}{K_{pqz}} - k. \qquad (14b)$$

(ii) The inhomogeneous system of linear algebraic equations for the amplitudes c_j:

$$\mathbf{Hc} = -Ak_z \frac{\exp(-\mathrm{i}\theta^+_{00})}{Q} \mathbf{e}, \qquad (15)$$

where

$$\mathbf{c} = \|c_1, c_2, \ldots, c_{2n}\|^{\mathrm{T}} \quad \text{and} \quad \mathbf{e} = \|1, 0, 0, \ldots, 0\|^{\mathrm{T}}$$

are column vectors and $\mathbf{H}$ is square matrix of order $2n$,

$$
\mathbf{H} = \left\| \begin{array}{cccc|cccc}
\frac{1}{x_{00}^{+} - y_{00}^{+}} & \frac{1}{x_{pq}^{+} - y_{00}^{+}} & \frac{1}{x_{gh}^{+} - y_{00}^{+}} \cdots & \frac{1}{x_{uv}^{+} - y_{00}^{+}} & \frac{1}{x_{00}^{-} - y_{00}^{+}} & \frac{1}{x_{pq}^{-} - y_{00}^{+}} & \frac{1}{x_{gh}^{-} - y_{00}^{+}} \cdots & \frac{1}{x_{uv}^{-} - y_{00}^{+}} \\
\frac{1}{x_{00}^{+} - y_{pq}^{+}} & \frac{1}{x_{pq}^{+} - y_{pq}^{+}} & \frac{1}{x_{gh}^{+} - y_{pq}^{+}} \cdots & \frac{1}{x_{uv}^{+} - y_{pq}^{+}} & \frac{1}{x_{00}^{-} - y_{pq}^{+}} & \frac{1}{x_{pq}^{-} - y_{pq}^{+}} & \frac{1}{x_{gh}^{-} - y_{pq}^{+}} \cdots & \frac{1}{x_{uv}^{-} - y_{pq}^{+}} \\
\frac{1}{x_{00}^{+} - y_{gh}^{+}} & \frac{1}{x_{pq}^{+} - y_{gh}^{+}} & \frac{1}{x_{gh}^{+} - y_{gh}^{+}} \cdots & \frac{1}{x_{uv}^{+} - y_{gh}^{+}} & \frac{1}{x_{00}^{-} - y_{gh}^{+}} & \frac{1}{x_{pq}^{-} - y_{gh}^{+}} & \frac{1}{x_{gh}^{-} - y_{gh}^{+}} \cdots & \frac{1}{x_{uv}^{-} - y_{gh}^{+}} \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
\frac{1}{x_{00}^{+} - y_{uv}^{+}} & \frac{1}{x_{pq}^{+} - y_{uv}^{+}} & \frac{1}{x_{gh}^{+} - y_{uv}^{+}} \cdots & \frac{1}{x_{uv}^{+} - y_{uv}^{+}} & \frac{1}{x_{00}^{-} - y_{uv}^{+}} & \frac{1}{x_{pq}^{-} - y_{uv}^{+}} & \frac{1}{x_{gh}^{-} - y_{uv}^{+}} \cdots & \frac{1}{x_{uv}^{-} - y_{uv}^{+}} \\
\hline
\frac{(x_{00}^{+})^{N+1}}{x_{00}^{+} - y_{00}^{-}} & \frac{(x_{pq}^{+})^{N+1}}{x_{pq}^{+} - y_{00}^{-}} & \frac{(x_{gh}^{+})^{N+1}}{x_{gh}^{+} - y_{00}^{-}} \cdots & \frac{(x_{uv}^{+})^{N+1}}{x_{uv}^{+} - y_{00}^{-}} & \frac{(x_{00}^{-})^{N+1}}{x_{00}^{-} - y_{00}^{-}} & \frac{(x_{pq}^{-})^{N+1}}{x_{pq}^{-} - y_{00}^{-}} & \frac{(x_{gh}^{-})^{N+1}}{x_{gh}^{-} - y_{00}^{-}} \cdots & \frac{(x_{uv}^{-})^{N+1}}{x_{uv}^{-} - y_{00}^{-}} \\
\frac{(x_{00}^{+})^{N+1}}{x_{00}^{+} - y_{pq}^{-}} & \frac{(x_{pq}^{+})^{N+1}}{x_{pq}^{+} - y_{pq}^{-}} & \frac{(x_{gh}^{+})^{N+1}}{x_{gh}^{+} - y_{pq}^{-}} \cdots & \frac{(x_{uv}^{+})^{N+1}}{x_{uv}^{+} - y_{pq}^{-}} & \frac{(x_{00}^{-})^{N+1}}{x_{00}^{-} - y_{pq}^{-}} & \frac{(x_{pq}^{-})^{N+1}}{x_{pq}^{-} - y_{pq}^{-}} & \frac{(x_{gh}^{-})^{N+1}}{x_{gh}^{-} - y_{pq}^{-}} \cdots & \frac{(x_{uv}^{-})^{N+1}}{x_{uv}^{-} - y_{pq}^{-}} \\
\frac{(x_{00}^{+})^{N+1}}{x_{00}^{+} - y_{gh}^{-}} & \frac{(x_{pq}^{+})^{N+1}}{x_{pq}^{+} - y_{gh}^{-}} & \frac{(x_{gh}^{+})^{N+1}}{x_{gh}^{+} - y_{gh}^{-}} \cdots & \frac{(x_{uv}^{+})^{N+1}}{x_{uv}^{+} - y_{gh}^{-}} & \frac{(x_{00}^{-})^{N+1}}{x_{00}^{-} - y_{gh}^{-}} & \frac{(x_{pq}^{-})^{N+1}}{x_{pq}^{-} - y_{gh}^{-}} & \frac{(x_{gh}^{-})^{N+1}}{x_{gh}^{-} - y_{gh}^{-}} \cdots & \frac{(x_{uv}^{-})^{N+1}}{x_{uv}^{-} - y_{gh}^{-}} \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
\frac{(x_{00}^{+})^{N+1}}{x_{00}^{+} - y_{uv}^{-}} & \frac{(x_{pq}^{+})^{N+1}}{x_{pq}^{+} - y_{uv}^{-}} & \frac{(x_{gh}^{+})^{N+1}}{x_{gh}^{+} - y_{uv}^{-}} \cdots & \frac{(x_{uv}^{+})^{N+1}}{x_{uv}^{+} - y_{uv}^{-}} & \frac{(x_{00}^{-})^{N+1}}{x_{00}^{-} - y_{uv}^{-}} & \frac{(x_{pq}^{-})^{N+1}}{x_{pq}^{-} - y_{uv}^{-}} & \frac{(x_{gh}^{-})^{N+1}}{x_{gh}^{-} - y_{uv}^{-}} \cdots & \frac{(x_{uv}^{-})^{N+1}}{x_{uv}^{-} - y_{uv}^{-}}
\end{array} \right\|, \qquad (16)
$$

where the following notation has been used

$$y_{kl}^{\pm} = \exp(\mathrm{i}\theta_{kl}^{\pm}), \qquad (17a)$$

for all n real θ_{kl}^{+} and all n real θ_{kl}^{-}, and

$$x_{kl}^{\pm} = \exp(\mathrm{i}\psi_{kl}^{\pm}) \qquad (17b)$$

with ψ_{kl}^{+} and ψ_{kl}^{-} being solutions of the dispersion relation (13).

Inserting the plane-wave superposition (12*a*) with the amplitudes c_j given by (15) into (10*a*), we get the external wavefunctions $\Psi^{<}(\mathbf{r})$ and $\Psi^{>}(\mathbf{r})$ above ($z < 0$) and below ($z > Na_{3z}$) the crystalline slab, respectively (Litzman, 1986),

$$
\begin{aligned}
\Psi^{<}(\mathbf{r}) &= A\exp(\mathrm{i}\mathbf{k}\cdot\mathbf{r}) - Ak_z\exp(-i\mathbf{k}\cdot\mathbf{a}_3) \\
&\quad \times \sum_{pq}\left[\left(\frac{1}{K_{pqz}}\right)\frac{\det\mathbf{M}_{pq}^{-}}{\det\mathbf{H}}\exp(\mathrm{i}\theta_{pq}^{-})\exp(\mathrm{i}\mathbf{K}_{pq}^{-}\cdot\mathbf{r})\right] \\
&= A\exp(\mathrm{i}\mathbf{k}\cdot\mathbf{r}) - \sum_{pq}\Psi_{pq}^{<}(\mathbf{r}) \qquad (18a)
\end{aligned}
$$

$$
\begin{aligned}
\Psi^{>}(\mathbf{r}) &= Ak_z\exp(-i\mathbf{k}\cdot\mathbf{a}_3)\sum_{pq}\left[\left(\frac{1}{K_{pqz}}\right)\frac{\det\mathbf{M}_{pq}^{+}}{\det\mathbf{H}}\right. \\
&\quad \left.\times\exp(-iN\theta_{pq}^{+})\exp(i\mathbf{K}_{pq}^{+}\cdot\mathbf{r})\right] \\
&= \sum_{pq}\Psi_{pq}^{>}(\mathbf{r}). \qquad (18b)
\end{aligned}
$$

The matrices $\mathbf{M}_{pq}^{-}$ and $\mathbf{M}_{pq}^{+}$ of order $2n$ differ from the matrix $\mathbf{H}$ defined by (16) in the first row only. Their first rows read

$$
\|(\mathbf{M}_{pq}^{-})_{1,j}\| = \left\| \frac{1}{x_{00}^{+} - y_{pq}^{-}} \quad \frac{1}{x_{pq}^{+} - y_{pq}^{-}} \quad \frac{1}{x_{gh}^{+} - y_{pq}^{-}} \quad \cdots \quad \frac{1}{x_{uv}^{+} - y_{pq}^{-}} \;\middle|\; \frac{1}{x_{00}^{-} - y_{pq}^{-}} \quad \frac{1}{x_{pq}^{-} - y_{pq}^{-}} \quad \frac{1}{x_{gh}^{-} - y_{pq}^{-}} \quad \cdots \quad \frac{1}{x_{uv}^{-} - y_{pq}^{-}} \right\| \qquad (19a)
$$

$$
\|(\mathbf{M}_{pq}^{+})_{1,j}\| = \left\| \frac{(x_{00}^{+})^{N+1}}{x_{00}^{+} - y_{pq}^{+}} \quad \frac{(x_{pq}^{+})^{N+1}}{x_{pq}^{+} - y_{pq}^{+}} \quad \frac{(x_{gh}^{+})^{N+1}}{x_{gh}^{+} - y_{pq}^{+}} \quad \cdots \quad \frac{(x_{uv}^{+})^{N+1}}{x_{uv}^{+} - y_{pq}^{+}} \;\middle|\; \frac{(x_{00}^{-})^{N+1}}{x_{00}^{-} - y_{pq}^{+}} \quad \frac{(x_{pq}^{-})^{N+1}}{x_{pq}^{-} - y_{pq}^{+}} \quad \frac{(x_{gh}^{-})^{N+1}}{x_{gh}^{-} - y_{pq}^{+}} \quad \cdots \quad \frac{(x_{uv}^{-})^{N+1}}{x_{uv}^{-} - y_{pq}^{+}} \right\|. \qquad (19b)
$$

Equations (18*a*), (18*b*) are the exact multiple-beam solution of Ewald's equations (10*a*), (10*b*), which are valid for any angle of incidence and both coplanar and non-coplanar diffractions. To apply them, it is necessary to find solutions of the dispersion relation (13) and then to evaluate quotients $\det\mathbf{M}_{pq}^{-}/\det\mathbf{H}$ and $\det\mathbf{M}_{pq}^{+}/\det\mathbf{H}$.

3. Dispersion relation

The dispersion relation (13) which is of crucial importance for the dynamical theory of diffraction was discussed in detail in our previous paper (Litzman *et al.*, 1996). Let us recall the most important general results. First we recall that (13) may be brought into the following form appropriate for finding its solutions

$$L^{>}(\psi) + L^{<}(\psi) = h_0\{1 + Q_0\mathrm{Re}[S'(\mathbf{k})]\} \qquad (20)$$

with

$$L^{>}(\psi) = -\frac{1}{2}\sum_{\substack{pq\\K^2_{pqz}>0}}^{(n)} \frac{1}{a_{3z}K_{pqz}} \frac{\sin(a_{3z}K_{pqz})}{\sin[(\psi-\theta^+_{pq})/2]\sin[(\psi-\theta^-_{pq})/2]} \quad (21a)$$

$$L^{<}(\psi) = \sum_{\substack{pq\\K^2_{pqz}<0}} \frac{1}{a_{3z}|K_{pqz}|}\left[\frac{\exp(-a_{3z}|K_{pqz}|)-\cos(\psi-\mathbf{a}^{||}_3\cdot\mathbf{k}^{||}_{pq})}{\cosh(a_{3z}|K_{pqz}|)-\cos(\psi-\mathbf{a}^{||}_3\cdot\mathbf{k}^{||}_{pq})}\right] \quad (21b)$$

being the finite and rapidly convergent infinite sums over all (pq) for which K_{pqz} is real and purely imaginary, respectively. Furthermore,

$$h_0 = \frac{|\mathbf{a}_1\times\mathbf{a}_2|}{2\pi a_{3z}Q_0} \quad (22)$$

and the term $Q_0\mathrm{Re}[S'(\mathbf{k})]$, being of order $1/h_0$, can be neglected for $h_0 \gg 1$. It is worth noting that the right-hand side of (20) is real because in the dispersion relation (13) the imaginary part of $1/Q$, being equal to k, cancels exactly with the term $-k$ in the imaginary part (14b) of the interplanar lattice sum, which results from the fact that the local-field effects are taken rigorously into account.[2] If we put Q_0 equal to the bound scattering length, the parameter h_0 is related to ξ defined by equation (3.1.7) in Sears (1989) by[3]

$$h_0 = \frac{2}{\xi a^2_{3z}k^2}. \quad (23)$$

The function on the left-hand side of (20) has poles for $\theta^+_{pq}+2\pi m$ and $\theta^-_{pq}+2\pi m$, the positions of which are given by the geometry and the wavelength only, whereas the right-hand side of (20) depends on the strength of the interaction between neutron and scattering centres. Thus, each solution of the dispersion relation may be associated with one pole θ^+_{pq} and/or θ^-_{pq}. We denote them by ψ^+_{pq} and ψ^-_{pq}, respectively. The distance $|\psi^+_{pq}-\theta^+_{pq}|$ and/or $|\psi^-_{pq}-\theta^-_{pq}|$ is the smaller the greater the value of h_0. Considering neutron diffraction where $h_0 \gg 1$, each solution $\psi^+_{pq}(\psi^-_{pq})$ lies 'very' near the corresponding pole $\theta^+_{pq}(\theta^-_{pq})$. In the simplest case when the pole θ^+_{pq} and/or θ^-_{pq} is far (mod 2π) from any other poles, we get directly from (13)

$$\exp(\mathrm{i}\psi^{\pm}_{pq}) = \exp(\mathrm{i}\theta^{\pm}_{pq})[1\pm \mathrm{i}\beta_{pq}+O(h_0^{-2})], \quad (24)$$

where

$$\beta_{pq} = -\frac{1}{h_0 a_{3z}K_{pqz}} = -\frac{\xi a_{3z}k^2}{2K_{pqz}}. \quad (25)$$

The more complicated problem arises when some poles of dispersion relation almost coincide (mod 2π). Special attention should be paid to the confluence of two particular poles, namely $\theta^+_{rs}(\mathbf{k})$ and $\theta^+_{00}(\mathbf{k})$ and/or $\theta^-_{rs}(\mathbf{k})$ and $\theta^+_{00}(\mathbf{k})$, the former representing the Bragg diffraction condition for the Laue geometry and the latter for the Bragg geometry.

[2] In the electromagnetic case, the Lorentz radiation damping $i(2/3)k^3$ is also cancelled by the imaginary part of the optical lattice sum (Vlieger, 1973; Litzman & Dub, 1982).

[3] See §5.

(i) *Laue geometry*

Let us consider the two poles θ^+_{00} and θ^+_{rs},

$$\theta^+_{00}-\theta^+_{rs} = 2\pi l + \mu^l_{00,rs}, \quad |\mu^l_{00,rs}|<\pi \quad \text{and } l \text{ is an integer}, \quad (26)$$

which may coincide when $\mu^l_{00,rs}\to 0$, and it is assumed that the other poles are well separated from both θ^+_{00} and θ^+_{rs} (mod 2π). In the following, we will use the simple notation $\mu^l_{00,rs}=\mu$.

Then we separate the terms corresponding to the poles θ^+_{00} and θ^+_{rs} in (13), converting it into the form

$$\mathrm{i}\beta_{00}\frac{\exp(\mathrm{i}\theta^+_{00})}{\exp(\mathrm{i}\psi)-\exp(\mathrm{i}\theta^+_{00})} + \mathrm{i}\beta_{rs}\frac{\exp(\mathrm{i}\theta^+_{rs})}{\exp(\mathrm{i}\psi)-\exp(\mathrm{i}\theta^+_{rs})} = G_{00,rs}(\psi), \quad (27)$$

where β_{pq} is given by (25) and

$$G_{00,rs}(\psi) = 1+\sigma_{00,rs}(\psi) - \mathrm{i}\frac{\beta_{00}+\beta_{rs}}{2} \quad (28a)$$

with

$$\begin{aligned}\sigma_{00,rs}(\psi) &= Q_0\mathrm{Re}[S'(\mathbf{k})] + \beta_{00}\frac{\sin(\psi-\theta^-_{00})}{2[1-\cos(\psi-\theta^-_{00})]} \\ &\quad + \beta_{rs}\frac{\sin(\psi-\theta^-_{rs})}{2[1-\cos(\psi-\theta^-_{rs})]} + \frac{1}{2h_0}\sum_{\substack{uv\\(uv)\neq(00)\\(uv)\neq(rs)\\K^2_{uvz}>0}}{}' \left\{\frac{1}{a_{3z}K_{uvz}} \right.\\ &\quad \left.\times\frac{\sin(a_{3z}K_{uvz})}{\sin[(\psi-\theta^+_{uv})/2]\sin[(\psi-\theta^-_{uv})/2]}\right\} - \frac{1}{h_0}L^{<}(\psi).\end{aligned} \quad (28b)$$

As the term $Q_0\mathrm{Re}[S'(\mathbf{k})]$ is of order $1/h_0$, the value of the function $\sigma_{00,rs}(\psi)$, having poles for all θ^+_{mn} and θ^-_{mn}, except θ^+_{00} and θ^+_{rs}, is, outside the poles θ^+_{mn} and θ^-_{mn}, of order $1/h_0$.

To find solutions of (27), ψ^+_{00} and ψ^+_{rs}, which are associated with the poles θ^+_{00} and θ^+_{rs}, let us put on the left-hand side of (27) $x=\exp(i\psi)$ and formally solve for x the quadratic equation obtained. Then, after some lengthy but easy algebra, dispersion relation (27) yields two equations:

$$\begin{aligned}\exp(\mathrm{i}\psi^+_{00}) = \exp(\mathrm{i}\theta^+_{00})\Bigg\{1-\frac{\mathrm{i}}{G_{00,rs}(\psi^+_{00})}\Bigg[&(\beta_{00}\beta_{rs})^{1/2}\tilde{Z}^-_{00,rs}(\psi^+_{00}) \\ &\times\exp\left(\mathrm{i}\frac{\theta^+_{rs}-\theta^+_{00}}{2}\right)-\beta_{00}\Bigg]\Bigg\}\end{aligned} \quad (29a)$$

and

$$\begin{aligned}\exp(\mathrm{i}\psi^+_{rs}) = \exp(\mathrm{i}\theta^+_{rs})\Bigg\{1+\frac{\mathrm{i}}{G_{00,rs}(\psi^+_{rs})}\Bigg[&(\beta_{00}\beta_{rs})^{1/2}\tilde{Z}^-_{00,rs}(\psi^+_{rs}) \\ &\times\exp\left(\mathrm{i}\frac{\theta^+_{00}-\theta^+_{rs}}{2}\right)+\beta_{rs}\Bigg]\Bigg\},\end{aligned} \quad (29b)$$

where

$$\tilde{Z}^-_{00,rs}(\psi) = Z_{00,rs}(\psi) - \mathrm{s}[Z_{00,rs}(\psi)][Z^2_{00,rs}(\psi)+1]^{1/2} \quad (30)$$

with

$$Z_{00,rs}(\psi) = \frac{1}{2(\beta_{00}\beta_{rs})^{1/2}} \left\{ (\beta_{00} - \beta_{rs}) \cos\left(\frac{\theta_{00}^+ - \theta_{rs}^+}{2}\right) + 2\mathrm{Re}[G_{00,rs}(\psi)] \sin\left(\frac{\theta_{00}^+ - \theta_{rs}^+}{2}\right) \right\}. \quad (31)$$

Here and in the following s(X) means the sign of X. Let us note that for $\tilde{Z}^-_{00,rs}(\psi)$ the condition $|\tilde{Z}^-_{00,rs}(\psi)| \le 1$ holds.

Next we will look for appropriate approximations in (29a), (29b). The right-hand side of (29a) and/or (29b) depends on ψ^+_{00} and/or ψ^+_{rs} through $\sigma_{00,rs}(\psi)$. As ψ^+_{00} and ψ^+_{rs} are near to the poles θ^+_{00} and θ^+_{rs}, both $\sigma_{00,rs}(\psi^+_{00})$ and $\sigma_{00,rs}(\psi^+_{rs})$ are very small (of order $1/h_0$) and, therefore, we may put in (29a) and (29b) $G_{00,rs}(\psi) = 1 + O(h_0^{-1})$. In this approximation, (29a) and (29b) yield

$$\exp(\mathrm{i}\psi^+_{00}) = \exp(\mathrm{i}\theta^+_{00}) \left\{ 1 - \mathrm{i}\left[(\beta_{00}\beta_{rs})^{1/2}(-1)^l \tilde{Z}^-_{00,rs} \times \exp\left(-\mathrm{i}\frac{\mu}{2}\right) - \beta_{00} \right] + O(h_0^{-2}) \right\} \quad (32a)$$

and

$$\exp(\mathrm{i}\psi^+_{rs}) = \exp(\mathrm{i}\theta^+_{rs}) \left\{ 1 + \mathrm{i}\left[(\beta_{00}\beta_{rs})^{1/2}(-1)^l \tilde{Z}^-_{00,rs} \times \exp\left(\mathrm{i}\frac{\mu}{2}\right) + \beta_{rs} \right] + O(h_0^{-2}) \right\}, \quad (32b)$$

where μ has been introduced by (26) and $\tilde{Z}^-_{00,rs}$ (not depending on ψ) is given by (30) with $Z_{00,rs}(\psi)$ being replaced by

$$Z_{00,rs} \equiv Z_{rs} = \frac{(-1)^l}{2(\beta_{00}\beta_{rs})^{1/2}} \left\{ (\beta_{00} - \beta_{rs}) \cos\left(\frac{\mu}{2}\right) + 2\sin\left(\frac{\mu}{2}\right) \right\}, \quad (33)$$

which now does not depend on ψ. It is worth noting that if μ increases, which means that the poles become separated, $\tilde{Z}^-_{00,rs}$ goes to zero and consequently (32a) and (32b) reduce to (24).

On the other hand, for Bragg reflection, where $\mu \to 0$, (33) may be approximated by

$$Z^{(0)}_{00,rs} = \frac{(-1)^l}{2(\beta_{00}\beta_{rs})^{1/2}} \left[(\beta_{00} - \beta_{rs}) + \mu \right] = (-1)^l z_{rsl}, \quad (34)$$

which depends linearly on the parameter μ expressing the deviation from the Bragg diffraction condition. As $\beta_{pq} = O(h_0^{-1})$ and $|\tilde{Z}^-_{00,rs}| \le 1$, (32$a$) and (32$b$) yield, respectively,

$$\psi^+_{00} - \theta^+_{00} = \beta_{00} - (\beta_{00}\beta_{rs})^{1/2}[z_{rsl} - \mathrm{s}(z_{rsl})(z^2_{rsl} + 1)^{1/2}] \quad (35a)$$

and

$$\psi^+_{rs} - \theta^+_{00} = \beta_{00} - (\beta_{00}\beta_{rs})^{1/2}[z_{rsl} + \mathrm{s}(z_{rsl})(z^2_{rsl} + 1)^{1/2}]. \quad (35b)$$

From (35a) and (35b), it can be seen that when the sign of z_{rsl} is changed the solutions ψ^+_{00} and ψ^+_{rs} interchange.

If the reflected wave does lie in the plane of incidence (coplanar diffraction), the parameter μ is related to the departure $\Delta\Theta$ from Bragg's incidence of the incident wave (see Appendix A) by

$$\mu = -a_{3z}k^2 \frac{1}{K_{rsz}} \sin 2\Theta_{\rm B}\Delta\Theta, \quad (36)$$

where $\Theta_{\rm B}$ is the Bragg angle. Then substituting μ from (36) and β_{pq} from (25) into (34), we get

$$z_{rsl} = -\frac{1}{2}\left[\left(\frac{K_{rsz}}{k_z}\right)^{1/2} - \left(\frac{k_z}{K_{rsz}}\right)^{1/2} + \frac{2}{\xi}\left(\frac{k_z}{K_{rsz}}\right)^{1/2} \sin 2\Theta_{\rm B}\Delta\Theta \right]. \quad (37)$$

(ii) *Bragg geometry*

Now we will consider the two poles θ^+_{00} and θ^-_{rs} related by

$$\theta^+_{00} - \theta^-_{rs} = 2\pi l + \eta^l_{00,rs}, \quad |\eta^l_{00,rs}| < \pi \quad \text{and } l \text{ is an integer}, \quad (38)$$

which may coincide when $\eta^l_{00,rs} \to 0$, and again suppose that the other poles are well separated from both θ^+_{00} and θ^-_{rs}. In the following, we will again use the simple notation $\eta^l_{00,rs} = \eta$.

Analogously to the Laue geometry, we separate the terms corresponding to the poles θ^+_{00} and θ^-_{rs} in (13) converting it into the form

$$\mathrm{i}\beta_{00}\frac{\exp(\mathrm{i}\theta^+_{00})}{\exp(\mathrm{i}\psi) - \exp(\mathrm{i}\theta^+_{00})} + \mathrm{i}\beta_{rs}\frac{\exp(-\mathrm{i}\theta^-_{rs})}{\exp(-\mathrm{i}\psi) - \exp(-\mathrm{i}\theta^-_{rs})} = F_{00,rs}(\psi), \quad (39)$$

where β_{pq} is given by (25) and

$$F_{00,rs}(\psi) = 1 + \varphi_{00,rs}(\psi) - \mathrm{i}\frac{\beta_{00} + \beta_{rs}}{2} \quad (40a)$$

with

$$\varphi_{00,rs}(\psi) = Q_0\mathrm{Re}[S'(\mathbf{k})] + \beta_{00}\frac{\sin(\psi - \theta^-_{00})}{2[1 - \cos(\psi - \theta^-_{00})]} - \beta_{rs}\frac{\sin(\psi - \theta^+_{rs})}{2[1 - \cos(\psi - \theta^+_{rs})]} + \frac{1}{2h_0}\sideset{}{'}\sum_{\substack{uv \\ (uv)\neq(00) \\ (uv)\neq(rs) \\ K^2_{uvz}>0}} \left\{ \frac{1}{a_{3z}K_{uvz}} \times \frac{\sin(a_{3z}K_{uvz})}{\sin[(\psi - \theta^+_{uv})/2]\sin[(\psi - \theta^-_{uv})/2]} \right\} - \frac{1}{h_0}L^<(\psi), \quad (40b)$$

which has poles for all θ^+_{mn} and θ^-_{mn} except θ^+_{00} and θ^-_{rs} and is, outside the poles θ^+_{mn} and θ^-_{mn}, of order $1/h_0$.

Next we proceed quite analogously as in the Laue geometry. Then, in the approximation $F_{00,rs}(\psi) = 1 + O(h_0^{-1})$, we get

$$\exp(\mathrm{i}\psi^+_{00}) = \exp(\mathrm{i}\theta^+_{00}) \left\{ 1 - \mathrm{i}\left[(\beta_{00}\beta_{rs})^{1/2}(-1)^l \tilde{Y}^-_{00,rs} \times \exp\left(-\mathrm{i}\frac{\eta}{2}\right) - \beta_{00} \right] + O(h_0^{-2}) \right\} \quad (41a)$$

and

$$\exp(\mathrm{i}\psi^-_{rs}) = \exp(\mathrm{i}\theta^-_{rs}) \left\{ 1 + \mathrm{i}\left[(\beta_{00}\beta_{rs})^{1/2}(-1)^l \tilde{Y}^-_{00,rs} \times \exp\left(\mathrm{i}\frac{\eta}{2}\right) - \beta_{rs} \right] + O(h_0^{-2}) \right\}, \quad (41b)$$

where

$$\tilde{Y}^{-}_{00,rs} = Y_{00,rs} - \mathrm{s}(Y_{00,rs})(Y^2_{00,rs} - 1)^{1/2} \tag{42}$$

with

$$Y_{00,rs} \equiv Y_{rs} = \frac{(-1)^l}{2(\beta_{00}\beta_{rs})^{1/2}}\left[(\beta_{rs} + \beta_{00})\cos\left(\frac{\eta}{2}\right) + 2\sin\left(\frac{\eta}{2}\right)\right]. \tag{43}$$

It is worth noting that for $\tilde{Y}^{-}_{00,rs}$ defined by (42) the condition $|\tilde{Y}^{-}_{00,rs}(\psi)| \leq 1$ holds and if η increases $\tilde{Y}^{-}_{00,rs}$ goes to zero and consequently (41*a*) and (41*b*) reduce to (24).

Finally, for the Bragg reflection, where $\eta \to 0$, from (41*a*) and (41*b*) it follows, respectively, that

$$\psi^{+}_{00} - \theta^{+}_{00} = \beta_{00} - (\beta_{00}\beta_{rs})^{1/2}[y_{rsl} - \mathrm{s}(y_{rsl})(y^2_{rsl} - 1)^{1/2}] \tag{44a}$$

and

$$\psi^{-}_{rs} - \theta^{+}_{00} = \beta_{00} - (\beta_{00}\beta_{rs})^{1/2}[y_{rsl} + \mathrm{s}(y_{rsl})(y^2_{rsl} - 1)^{1/2}], \tag{44b}$$

where

$$y_{rsl} = \frac{1}{2(\beta_{00}\beta_{rs})^{1/2}}[(\beta_{00} + \beta_{rs}) + \eta] \tag{45}$$

depends, like z_{rsl} defined by (34), linearly on the parameter η expressing the deviation from the Bragg diffraction condition. From (44*a*), (44*b*), it can be seen that when the sign of y_{rsl} is changed the solutions ψ^{+}_{00} and ψ^{-}_{rs} interchange and, moreover, if $|y_{rsl}| < 1$, solutions ψ^{+}_{00} and ψ^{-}_{rs} are complex conjugated.

As in the Laue geometry, in the case of coplanar diffraction the parameter η is related to the departure $\Delta\Theta$ from Bragg's incidence of the incident wave (see Appendix *A*),

$$\eta = +a_{3z}k^2\frac{1}{K_{rsz}}\sin 2\Theta_{\rm B}\Delta\Theta \tag{46}$$

and then y_{rsl} reads

$$y_{rsl} = -\frac{1}{2}\left[\left(\frac{K_{rsz}}{k_z}\right)^{1/2} + \left(\frac{k_z}{K_{rsz}}\right)^{1/2} - \frac{2}{\xi}\left(\frac{k_z}{K_{rsz}}\right)^{1/2}\sin 2\Theta_{\rm B}\Delta\Theta\right]. \tag{47}$$

Let us recall that (35*a*), (35*b*) with z_{rsl} given by (37) and (44*a*), (44*b*) with y_{rsl} given by (47) result from the two-beam dispersion relation for coplanar Bragg reflections in the Laue or Bragg geometry, respectively.

Furthermore, considering (6) and (12*b*), we get

$$\begin{aligned}\psi^{\pm}_{pq} - \theta^{+}_{00} &= \mathbf{a}_3 \cdot \tilde{\mathbf{k}}^{\pm}_{pq} - \mathbf{a}_3 \cdot \mathbf{K}^{+}_{00} \\ &= (\mathbf{a}^{\|}_3 \cdot \mathbf{k}^{\|} + a_{3z}\tilde{k}^{\pm}_{pqz}) - (\mathbf{a}^{\|}_3 \cdot \mathbf{k}^{\|} + a_{3z}k_z) \\ &= a_{3z}(\tilde{k}^{\pm}_{pqz} - k_z).\end{aligned} \tag{48}$$

Thus (35*a*), (35*b*) and (44*a*), (44*b*) give the differences between the *z* components of the wavevectors of the local field and the incident beam.

4. Wavefunctions

The wavefunctions of the diffracted waves are given by (18*a*) and (18*b*) where quotients

$$\det \mathbf{M}^{-}_{pq}/\det \mathbf{H} \quad \text{and} \quad \det \mathbf{M}^{+}_{pq}/\det \mathbf{H} \tag{49}$$

are to be evaluated. First we will analyse qualitatively the values of elements of the matrices $\mathbf{H}$, $\mathbf{M}^{-}_{pq}$ and $\mathbf{M}^{+}_{pq}$. As each solution ψ^{+}_{pq} (ψ^{-}_{pq}) lies 'very' near the corresponding pole θ^{+}_{pq} (θ^{-}_{pq}), all elements on the main diagonal of $\mathbf{H}$ are always of order h_0, whereas the values of its elements outside the main diagonal depend on the respective positions of poles. A similar conclusion holds for the matrices $\mathbf{M}^{-}_{pq}$ and $\mathbf{M}^{+}_{pq}$ which, however, contain in their first rows the large element $1/(x^{-}_{pq} - y^{-}_{pq})$ and/or $(x^{+}_{pq})^{N+1}/(x^{+}_{pq} - y^{+}_{pq})$, respectively, being always of order h_0.

Taking into account the above qualitative assertion, it is possible to evaluate quotients (49) for particular cases in a defined approximation. To calculate the determinants in (49), the following formula for evaluating the determinant of a symmetrically partitioned square matrix will be used:

$$\begin{aligned}\det \mathbf{A} &= \det\begin{Vmatrix} {}^{11}\mathbf{A} & {}^{12}\mathbf{A} \\ {}^{21}\mathbf{A} & {}^{22}\mathbf{A}\end{Vmatrix} \\ &= (\det {}^{22}\mathbf{A})\det[{}^{11}\mathbf{A} - {}^{12}\mathbf{A}({}^{22}\mathbf{A})^{-1}\,{}^{21}\mathbf{A}],\end{aligned} \tag{50}$$

where ${}^{22}\mathbf{A}$ is a (non-singular) square submatrix of $\mathbf{A}$.

In the following, we will handle the case when by changing the direction of the incident beam one pole only, say θ^{+}_{rs}, in the Laue geometry, and/or θ^{-}_{rs} in the Bragg geometry, may approach θ^{+}_{00}, which yields the Bragg diffraction condition, the other poles being well separated from both θ^{+}_{00} and θ^{+}_{rs}, and/or θ^{-}_{rs}. Thus, in the following we will treat two external waves in the Laue geometry, *viz* one with $\mathbf{K}^{+}_{00} \equiv \mathbf{k}$ and one with $\mathbf{K}^{+}_{rs}$, and two external waves in the Bragg geometry, *viz* one with $\mathbf{K}^{+}_{00} \equiv \mathbf{k}$ and one with $\mathbf{K}^{-}_{rs}$. To evaluate the corresponding quotients (49) by using (50), we express the matrices $\mathbf{H}$, $\mathbf{M}^{+}_{rs}$ and $\mathbf{M}^{-}_{rs}$ in the following block form

$$\mathbf{A} = \begin{Vmatrix} {}^{11}\mathbf{A} & {}^{12}\mathbf{A} \\ {}^{21}\mathbf{A} & {}^{22}\mathbf{A}\end{Vmatrix},$$

where the elements of the submatrix ${}^{11}\mathbf{A}$ may be of order h_0 whereas all matrix elements of ${}^{12}\mathbf{A}$ and ${}^{21}\mathbf{A}$ are always of order 1. The square submatrix ${}^{11}\mathbf{A}$ is therefore of order 2 and reads:

(i) *in the Laue geometry*

$${}^{11}\mathbf{H} = \begin{Vmatrix} \dfrac{1}{x^{+}_{00} - y^{+}_{00}} & \dfrac{1}{x^{+}_{rs} - y^{+}_{00}} \\ \dfrac{1}{x^{+}_{00} - y^{+}_{rs}} & \dfrac{1}{x^{+}_{rs} - y^{+}_{rs}}\end{Vmatrix},$$

$${}^{11}\mathbf{M}^{+}_{rs} = \begin{Vmatrix} \dfrac{(x^{+}_{00})^{N+1}}{x^{+}_{00} - y^{+}_{rs}} & \dfrac{(x^{+}_{rs})^{N+1}}{x^{+}_{rs} - y^{+}_{rs}} \\ \dfrac{1}{x^{+}_{00} - y^{+}_{rs}} & \dfrac{1}{x^{+}_{rs} - y^{+}_{rs}}\end{Vmatrix}$$

and

$${}^{11}\mathbf{M}^{+}_{00} = \begin{Vmatrix} \dfrac{(x^{+}_{00})^{N+1}}{x^{+}_{00} - y^{+}_{00}} & \dfrac{(x^{+}_{rs})^{N+1}}{x^{+}_{rs} - y^{+}_{00}} \\ \dfrac{1}{x^{+}_{00} - y^{+}_{rs}} & \dfrac{1}{x^{+}_{rs} - y^{+}_{rs}}\end{Vmatrix}; \tag{51}$$

(ii) *in the Bragg geometry*

$$^{11}\mathbf{H} = \left\| \begin{matrix} \dfrac{1}{x_{00}^+ - y_{00}^+} & \dfrac{1}{x_{rs}^- - y_{00}^+} \\ \dfrac{(x_{00}^+)^{N+1}}{x_{00}^+ - y_{rs}^-} & \dfrac{(x_{rs}^-)^{N+1}}{x_{rs}^- - y_{rs}^-} \end{matrix} \right\|,$$

$$^{11}\mathbf{M}_{rs}^- = \left\| \begin{matrix} \dfrac{1}{x_{00}^+ - y_{rs}^-} & \dfrac{1}{x_{rs}^- - y_{rs}^-} \\ \dfrac{(x_{00}^+)^{N+1}}{x_{00}^+ - y_{rs}^-} & \dfrac{(x_{rs}^-)^{N+1}}{x_{rs}^- - y_{rs}^-} \end{matrix} \right\|$$

and

$$^{11}\mathbf{M}_{00}^+ = \left\| \begin{matrix} \dfrac{(x_{00}^+)^{N+1}}{x_{00}^+ - y_{00}^+} & \dfrac{(x_{rs}^-)^{N+1}}{x_{rs}^- - y_{00}^+} \\ \dfrac{(x_{00}^+)^{N+1}}{x_{00}^+ - y_{rs}^-} & \dfrac{(x_{rs}^-)^{N+1}}{x_{rs}^- - y_{rs}^-} \end{matrix} \right\|. \qquad (52)$$

We now set out to calculate the external waves for both Laue and Bragg geometries.

(i) *Laue geometry*

As $^{22}\mathbf{H} = {^{22}\mathbf{M}_{rs}^+} = {^{22}\mathbf{M}_{00}^+}$, by using (50) and (51) we get

$$\frac{\det \mathbf{M}_{00}^+}{\det \mathbf{H}} = \frac{\det^{11} \mathbf{M}_{00}^+}{\det^{11} \mathbf{H}} + O(h_0^{-2}) = \frac{\dfrac{x_{00}^+ - y_{rs}^+}{x_{00}^+ - y_{00}^+}(x_{00}^+)^{N+1} - \dfrac{x_{rs}^+ - y_{rs}^+}{x_{rs}^+ - y_{00}^+}(x_{rs}^+)^{N+1}}{\dfrac{x_{00}^+ - y_{rs}^+}{x_{00}^+ - y_{00}^+} - \dfrac{x_{rs}^+ - y_{rs}^+}{x_{rs}^+ - y_{00}^+}} + O(h_0^{-2}), \qquad (53a)$$

which determines the amplitude of the external beam with $\mathbf{K}_{00}^+ \equiv \mathbf{k}$, and

$$\frac{\det \mathbf{M}_{rs}^+}{\det \mathbf{H}} = \frac{\det^{11} \mathbf{M}_{rs}^+}{\det^{11} \mathbf{H}} + O(h_0^{-2}) = \frac{(x_{00}^+)^{N+1} - (x_{rs}^+)^{N+1}}{\dfrac{x_{00}^+ - y_{rs}^+}{x_{00}^+ - y_{00}^+} - \dfrac{x_{rs}^+ - y_{rs}^+}{x_{rs}^+ - y_{00}^+}} + O(h_0^{-2}), \qquad (53b)$$

which determines the amplitude of the external beam with $\mathbf{K}_{rs}^+$.

The fractions $(x_{00}^+ - y_{rs}^+)/(x_{00}^+ - y_{00}^+)$ and $(x_{rs}^+ - y_{rs}^+)/(x_{rs}^+ - y_{00}^+)$ in (53*a*), (53*b*) may be evaluated by using (32*a*), (32*b*). After some algebraic manipulations, we get

$$\frac{x_{00}^+ - y_{rs}^+}{x_{00}^+ - y_{00}^+} = -\exp\left(-\mathrm{i}\frac{\theta_{00}^+ - \theta_{rs}^+}{2}\right)\left(\frac{K_{00z}}{K_{rsz}}\right)^{1/2} \times [Z_{rs} + \mathrm{s}(Z_{rs})(Z_{rs}^2 + 1)^{1/2} + O(h_0^{-2})] \qquad (54)$$

and

$$\frac{x_{rs}^+ - y_{rs}^+}{x_{rs}^+ - y_{00}^+} = -\exp\left(\mathrm{i}\frac{\theta_{rs}^+ - \theta_{00}^+}{2}\right)\left(\frac{K_{00z}}{K_{rsz}}\right)^{1/2} \times [Z_{rs} - \mathrm{s}(Z_{rs})(Z_{rs}^2 + 1)^{1/2} + O(h_0^{-2})] \qquad (55)$$

with Z_{rs} being defined by (33). Finally, after inserting (54) and (55) into (53*a*), (53*b*) we obtain from (18*b*) the wavefunctions of the two external waves in the Laue geometry:

$$\Psi_{00}^{>}(\mathbf{r}) = A\Big(\{\exp[\mathrm{i}(\psi_{00}^+ - \theta_{00}^+)]\}^{N+1}[Z_{rs} + \mathrm{s}(Z_{rs})(Z_{rs}^2 + 1)^{1/2}] - \{\exp[\mathrm{i}(\psi_{rs}^+ - \theta_{00}^+)]\}^{N+1}[Z_{rs} - \mathrm{s}(Z_{rs})(Z_{rs}^2 + 1)^{1/2}]\Big) \times [2\mathrm{s}(Z_{rs})(Z_{rs}^2 + 1)^{1/2}]^{-1} \exp(\mathrm{i}\mathbf{K}_{00}^+ \cdot \mathbf{r}) + O(h_0^{-2}) \qquad (56a)$$

and

$$\Psi_{rs}^{>}(\mathbf{r}) = -A\left(\frac{K_{00z}}{K_{rsz}}\right)^{1/2}\Big(\{\exp[\mathrm{i}(\psi_{00}^+ - \theta_{00}^+)]\}^{N+1} - \{\exp[\mathrm{i}(\psi_{rs}^+ - \theta_{00}^+)]\}^{N+1}\Big)[2\mathrm{s}(Z_{rs})(Z_{rs}^2 + 1)^{1/2}]^{-1} \times \{\exp[\mathrm{i}(\theta_{00}^+ - \theta_{rs}^+)]\}^{(N+1/2)} \exp(\mathrm{i}\mathbf{K}_{rs}^+ \cdot \mathbf{r}) + O(h_0^{-2}), \qquad (56b)$$

where expressions $\exp(\mathrm{i}\psi_{00}^+)$ and $\exp(\mathrm{i}\psi_{rs}^+)$ are given by (32*a*) and (32*b*), respectively. Formulae (56*a*), (56*b*) are valid for both coplanar and non-coplanar diffractions in and outside the Bragg-peak regions if all other poles of the dispersion relation are well separated from the two poles θ_{00}^+ and θ_{rs}^+.

In the Bragg-peak region where θ_{rs}^+ is near (mod 2π) to θ_{00}^+, the expressions for $\psi_{00}^+ - \theta_{00}^+$ and $\psi_{rs}^+ - \theta_{00}^+$ are given by (35*a*) and (35*b*). Then, since when changing the sign of z_{rsl} solutions ψ_{00}^+ and ψ_{rs}^+ interchange, (56*a*), (56*b*) may be expressed in the following form suitable for further discussion in §5:

$$\Psi_{00}^{>}(\mathbf{r}) = A\exp\left(-\mathrm{i}\frac{\mathbf{k}\cdot\mathbf{a}_3}{2}\right) \times \Big\{[z_{rsl} + (z_{rsl}^2 + 1)^{1/2}]\exp[\mathrm{i}(N+1)a_{3z}\tilde{\kappa}_{z-}^{\mathrm{L}}] - [z_{rsl} - (z_{rsl}^2 + 1)^{1/2}]\exp[\mathrm{i}(N+1)a_{3z}\tilde{\kappa}_{z+}^{\mathrm{L}}]\Big\} \times [2(z_{rsl}^2 + 1)^{1/2}]^{-1}\exp\left[\mathrm{i}\mathbf{K}_{00}^+\cdot\left(\mathbf{r} + \frac{\mathbf{a}_3}{2}\right)\right] \quad \text{for } z > Na_{3z} \qquad (57a)$$

and

$$\Psi_{rs}^{>}(\mathbf{r}) = (-1)^l A\exp\left(-\mathrm{i}\frac{\mathbf{k}\cdot\mathbf{a}_3}{2}\right) \times \left(\frac{K_{00z}}{K_{rsz}}\right)^{1/2}\Big\{\exp[\mathrm{i}(N+1)a_{3z}\tilde{\kappa}_{z+}^{\mathrm{L}}] - \exp[\mathrm{i}(N+1)a_{3z}\tilde{\kappa}_{z-}^{\mathrm{L}}]\Big\}[2(z_{rsl}^2 + 1)^{1/2}]^{-1} \times \exp\left[\mathrm{i}(N+1)a_{3z}\frac{\mu}{a_{3z}}\right]\exp\left[\mathrm{i}\mathbf{K}_{rs}^+\cdot\left(\mathbf{r} + \frac{\mathbf{a}_3}{2}\right)\right] \quad \text{for } z > Na_{3z}, \qquad (57b)$$

where z_{rsl} is defined by (34) and

$$\tilde{\kappa}_{z\pm}^{\mathrm{L}} = -\frac{\xi k^2}{2k_z} - \frac{\xi k^2}{2(k_z K_{rsz})^{1/2}}[z_{rsl} \pm (z_{rsl}^2 + 1)^{1/2}] \qquad (58)$$

express the differences between the z components of the wavevectors of the local field and the incident beam [see (48) and (35*a*), (35*b*)].

(ii) *Bragg geometry*

As ${}^{22}\mathbf{H} = {}^{22}\mathbf{M}^-_{rs} = {}^{22}\mathbf{M}^+_{00}$, by using (50) and (52), we get

$$\frac{\det \mathbf{M}^+_{00}}{\det \mathbf{H}} = \frac{\det^{11} \mathbf{M}^+_{00}}{\det^{11} \mathbf{H}} + O(h_0^{-2}) = \frac{\dfrac{x^+_{00} - y^-_{rs}}{x^+_{00} - y^+_{00}} - \dfrac{x^-_{rs} - y^-_{rs}}{x^-_{rs} - y^+_{00}}}{\dfrac{x^+_{00} - y^-_{rs}}{x^+_{00} - y^+_{00}} (x^+_{00})^{-(N+1)} - \dfrac{x^-_{rs} - y^-_{rs}}{x^-_{rs} - y^+_{00}} (x^-_{rs})^{-(N+1)}} + O(h_0^{-2}), \quad (59a)$$

which determines the amplitude of the external beam with $\mathbf{K}^+_{00} \equiv \mathbf{k}$, and

$$\frac{\det \mathbf{M}^-_{rs}}{\det \mathbf{H}} = \frac{\det^{11} \mathbf{M}^-_{rs}}{\det^{11} \mathbf{H}} + O(h_0^{-2}) = \frac{(x^-_{rs})^{N+1} - (x^+_{00})^{N+1}}{\dfrac{x^+_{00} - y^-_{rs}}{x^+_{00} - y^+_{00}} (x^-_{rs})^{N+1} - \dfrac{x^-_{rs} - y^-_{rs}}{x^-_{rs} - y^+_{00}} (x^+_{00})^{N+1}} + O(h_0^{-2}), \quad (59b)$$

which determines the amplitude of the external beam with $\mathbf{K}^-_{rs}$.

The fractions $(x^+_{00} - y^+_{rs})/(x^+_{00} - y^-_{00})$ and $(x^-_{rs} - y^-_{rs})/(x^-_{rs} - y^+_{00})$ in (59*a*), (59*b*) may be evaluated by using the dispersion relation (39). Using it, we obtain from (18*b*) and (18*a*) the wavefunctions of the two external waves in the Bragg geometry,

$$\Psi^>_{00}(\mathbf{r}) = A[2\mathrm{s}(Y_{rs})(Y^2_{rs} - 1)^{1/2}]\big(\{\exp[-\mathrm{i}(\psi^+_{00} - \theta^+_{00})]\}^{N+1} \times [Y_{rs} + \mathrm{s}(Y_{rs})(Y^2_{rs} - 1)^{1/2}] - \{\exp[-\mathrm{i}(\psi^-_{rs} - \theta^+_{00})]\}^{N+1} \times [Y_{rs} - \mathrm{s}(Y_{rs})(Y^2_{rs} - 1)^{1/2}]\big)^{-1} \exp(\mathrm{i}\mathbf{K}^+_{00} \cdot \mathbf{r}) + O(h_0^{-2}) \quad (60a)$$

and

$$\Psi^<_{rs}(\mathbf{r}) = A\left(\frac{K_{00z}}{K_{rsz}}\right)^{1/2} \big(\{\exp[\mathrm{i}(\psi^-_{rs} - \theta^+_{00})]\}^{N+1} - \{\exp[\mathrm{i}(\psi^+_{00} - \theta^+_{00})]\}^{N+1}\big) \times \big(\{\exp[\mathrm{i}(\psi^-_{rs} - \theta^+_{00})]\}^{N+1}[Y_{rs} + \mathrm{s}(Y_{rs})(Y^2_{rs} - 1)^{1/2}] - \{\exp[\mathrm{i}(\psi^+_{00} - \theta^+_{00})]\}^{N+1}[Y_{rs} - \mathrm{s}(Y_{rs})(Y^2_{rs} - 1)^{1/2}]\big)^{-1} \times \exp\left(\mathrm{i}\frac{\theta^-_{rs} - \theta^+_{00}}{2}\right) \exp(\mathrm{i}\mathbf{K}^-_{rs} \cdot \mathbf{r}) + O(h_0^{-2}), \quad (60b)$$

where Y_{rs} is given by (43) and expressions $\exp(\mathrm{i}\psi^+_{00})$ and $\exp(\mathrm{i}\psi^-_{rs})$ are given by (41*a*) and (41*b*), respectively. As in the Laue geometry, formulae (60*a*) and (60*b*) are valid for both coplanar and non-coplanar diffractions in and outside the Bragg-peak regions if all other poles of the dispersion relation are well separated from the two poles θ^+_{00} and θ^-_{rs}.

In the Bragg-peak region where θ^-_{rs} is near (mod 2π) to θ^+_{00}, the expressions for $\psi^+_{00} - \theta^+_{00}$ and $\psi^-_{rs} - \theta^+_{00}$ are given by (44*a*) and (44*b*). Then, (60*a*), (60*b*) may be expressed in the following form suitable for further discussion in §5:

$$\Psi^>_{00}(\mathbf{r}) = A \exp\left(-\mathrm{i}\frac{\mathbf{k} \cdot \mathbf{a}_3}{2}\right)[2(y^2_{rsl} - 1)^{1/2}] \times \big\{ \exp[-\mathrm{i}(N+1)a_{3z}\tilde{\kappa}^{\mathrm{B}}_{z-}][y_{rsl} + (y^2_{rs} - 1)^{1/2}] - \exp[-\mathrm{i}(N+1)a_{3z}\tilde{\kappa}^{\mathrm{B}}_{z+}][y_{rsl} - (y^2_{rsl} - 1)^{1/2}]\big\}^{-1} \times \exp\left[\mathrm{i}\mathbf{K}^+_{00} \cdot \left(\mathbf{r} + \frac{\mathbf{a}_3}{2}\right)\right] \quad \text{for } z > Na_{3z} \quad (61a)$$

and

$$\Psi^<_{rs}(\mathbf{r}) = (-1)^l A\left(\frac{K_{00z}}{K_{rsz}}\right)^{1/2} \exp\left(-\mathrm{i}\frac{\mathbf{k} \cdot \mathbf{a}_3}{2}\right) \times \big\{ \exp[\mathrm{i}(N+1)a_{3z}\tilde{\kappa}^{\mathrm{B}}_{z+}] - \exp[\mathrm{i}(N+1)a_{3z}\tilde{\kappa}^{\mathrm{B}}_{z-}]\big\} \times \big\{ \exp[\mathrm{i}(N+1)a_{3z}\tilde{\kappa}^{\mathrm{B}}_{z+}][y_{rsl} + (y^2_{rs} - 1)^{1/2}] - \exp[\mathrm{i}(N+1)a_{3z}\tilde{\kappa}^{\mathrm{B}}_{z-}][y_{rsl} - (y^2_{rsl} - 1)^{1/2}]\big\}^{-1} \times \exp\left[\mathrm{i}\mathbf{K}^-_{rs} \cdot \left(\mathbf{r} + \frac{\mathbf{a}_3}{2}\right)\right] \quad \text{for } z < 0, \quad (61b)$$

where y_{rsl} is defined by (45) and

$$\tilde{\kappa}^{\mathrm{B}}_{z\pm} = -\frac{\xi k^2}{2k_z} - \frac{\xi k^2}{2(k_z K_{rsz})^{1/2}}[y_{rsl} \pm (y^2_{rsl} - 1)^{1/2}] \quad (62)$$

express again the differences between the z components of the wavevectors of the local field and the incident beam [see equations (48) and (44*a*), (44*b*)].

To enlighten the conditions under which formulae derived for wavefunctions may be applied, let us consider *e.g.* the diffraction $\mathbf{K}^+_{11}$ in the Laue geometry. Formulae (56*a*), (56*b*) with $(r, s) = (1, 1)$ hold for all angles of incidence except those near $\gamma^{\mathrm{L}}_{02\bar{1}}$, $\gamma^{\mathrm{B}}_{100}$ and $\gamma^{\mathrm{B}}_{001}$ where beams other than $(1, 1)$ satisfy the Bragg diffraction condition, and those near grazing incidence $\gamma^{\mathrm{B}}_{000}$ and emergence $\gamma^{\mathrm{ge}}_{01}$. To find the influence of the Bragg reflection, say $\mathbf{K}^-_{10}$ on the diffraction $\mathbf{K}^+_{11}$ near $\gamma^{\mathrm{B}}_{100}$, it would be necessary to enlarge submatrices (51) of the second order ${}^{11}\mathbf{H}$, ${}^{11}\mathbf{M}^+_{11}$, ${}^{11}\mathbf{M}^+_{00}$ into matrices of the third order by including large elements $(x^+_{00} - y^-_{10})^{-1}$ and $(x^-_{10} - y^+_{00})^{-1}$ and, at the same time, to add the term with the denominator $(x - y^-_{10})$ on the left-hand side of the dispersion relation (27) (three-beam case). In the Bragg-peak region at $\gamma^{\mathrm{L}}_{11\bar{1}}$, formulae (56*a*), (56*b*) may be simplified, taking the form (57*a*), (57*b*) compatible with that yielded by the Laue theory as will be shown in the next section. Concluding, let us note that the influence of the Bragg reflections on the crystal truncation rod scattering in the case of a semi-infinite crystal was studied by Litzman & Mikulík (1999).

5. Comparison with Laue's theory

In the Laue dynamical theory of diffraction, the crystal is considered to be a continuum described by the periodic potential. If we apply this theory to neutron diffraction, the coherent wave $\psi(\mathbf{r})$, which describes neutron optical phenomena, satisfies the one-body Schrödinger equation[4]

$$\left[-\frac{\hbar^2}{2m}\Delta + v(\mathbf{r})\right]\psi(\mathbf{r}) = E\psi(\mathbf{r}). \tag{63}$$

For a finite but otherwise perfect crystal of volume V, Sears puts

$$v(\mathbf{r}) = \begin{cases} v_0 \sum_{\mathbf{h}} \exp(\mathrm{i}\mathbf{G}_{\mathbf{h}}\cdot\mathbf{r}) & \text{inside } V \\ 0 & \text{outside } V \end{cases} \tag{64}$$

with $\mathbf{G}_{\mathbf{h}}$ being the reciprocal-lattice vector and $v_0 = (2\pi\hbar^2/m)\rho b$, where m is the neutron mass, b is the bound coherent scattering length and $\rho = [\mathbf{a}_1\mathbf{a}_2\mathbf{a}_3]^{-1}$ is the number density.

Since $v(\mathbf{r})$ is discontinuous at the surface of V, one must find separate solutions of (63) inside and outside V and then match the exterior and interior solutions by requiring that $\psi(\mathbf{r})$ and $\nabla\psi(\mathbf{r})$ be continuous at the boundary. Exterior solution is expressed as a superposition of plane waves

$$\psi(\mathbf{r}) = \sum a \exp(\mathrm{i}\mathbf{k}\cdot\mathbf{r}), \tag{65}$$

in which the wavevectors $\mathbf{k}$ all have the same magnitude, which is determined by the incident-neutron energy $E = \hbar^2k^2/2m$. The interior solution is expressed as a superposition of Bloch waves

$$\psi(\mathbf{r}) = \sum A(\mathbf{r}) \exp(\mathrm{i}\mathbf{K}\cdot\mathbf{r}), \tag{66}$$

in which $A(\mathbf{r}) = \sum A_{\mathbf{h}} \exp(\mathrm{i}\mathbf{G}_{\mathbf{h}}\cdot\mathbf{r})$ is periodic. The values of $\mathbf{K}$ follow from the dispersion equation and to each value of $\mathbf{K}$ there corresponds a set of coefficients $A_{\mathbf{h}}$. The values of wave amplitudes are determined by the boundary conditions.

In the two-beam case when $\mathbf{k}$ satisfies the condition for Bragg reflection *via* one particular reciprocal-lattice vector $\mathbf{G}_{\mathbf{h}}$, the dispersion equation yields two values of $\mathbf{K}$. If the incident wave $\psi(\mathbf{r}) = a\exp(\mathrm{i}\mathbf{k}\cdot\mathbf{r})$ enters the crystal through a plane boundary at $z = 0$, the two values of $\mathbf{K}$ are given by $\mathbf{K}_\pm = \mathbf{k} + \boldsymbol{\kappa}_\pm$ where $\boldsymbol{\kappa}_\pm = \kappa_{z\pm}\mathbf{e}_3$. The quantity $\kappa_{z\pm}$ rendering the difference between z components of the wavevectors inside and outside the crystal is given by equation (6.1.49) in Sears (1989),

$$\kappa_{z\pm} = -\frac{\xi k^2}{2k_z} - \frac{\xi k^2}{2(k_z|k_z + G_{\mathbf{h}z}|)^{1/2}}\left[\frac{\gamma}{|\delta|^{1/2}} \pm \left(\frac{\gamma^2}{|\delta|} + \mathrm{s}(\delta)\right)^{1/2}\right], \tag{67}$$

where $\mathrm{s}(\delta)$ means the sign of δ defined by (68) (+1 in Laue geometry and −1 in Bragg geometry) and $\xi = v_0/E$ is related to our parameter h_0 by (23). Parameters δ and γ are defined by equation (6.1.46) in Sears (1989). If the normalized unit-cell structure factor is equal to one,

$$\delta = \frac{k_z}{k_z + G_{\mathbf{h}z}}, \tag{68}$$

which is obviously positive or negative for the Laue and Bragg geometry, respectively, and further it can be shown that

$$\frac{\gamma}{|\delta|^{1/2}} = -\frac{1}{2}\left[\left(\frac{|k_z + G_{\mathbf{h}z}|}{k_z}\right)^{1/2} \mp \left(\frac{k_z}{|k_z + G_{\mathbf{h}z}|}\right)^{1/2} \pm \frac{2}{\xi}\left(\frac{k_z}{|k_z + G_{\mathbf{h}z}|}\right)^{1/2} \sin 2\Theta_{\mathrm{B}}\Delta\Theta\right], \tag{69}$$

where we have introduced the Bragg angle Θ_{B} and the departure $\Delta\Theta$ from Bragg's incidence of the incident wave. In (69), the sign assignment is $-+$ for the Laue geometry and $+-$ for the Bragg geometry. Note that $\gamma/|\delta|$ is equal to the y parameter defined by equation (9.23) in Rauch & Petraschek (1978), or deviation parameter η defined by equation (4.25) in Authier (2001).[5]

Finally, if reflection is neglected, the external wavefunction (65) is given in the Laue geometry by [see equation (6.2.1) in Sears (1989)]

$$\psi(\mathbf{r}) = \begin{cases} a\exp(\mathrm{i}\mathbf{k}\cdot\mathbf{r}) & z < 0 \\ a'\exp(\mathrm{i}\mathbf{k}'\cdot\mathbf{r}) + a''\exp(\mathrm{i}\mathbf{k}''\cdot\mathbf{r}) & z > d \end{cases} \tag{70}$$

and in the Bragg geometry by [see equation (6.2.2) in Sears (1989)]

$$\psi(\mathbf{r}) = \begin{cases} a\exp(\mathrm{i}\mathbf{k}\cdot\mathbf{r}) + a'\exp(\mathrm{i}\mathbf{k}'\cdot\mathbf{r}) & z < 0 \\ a''\exp(\mathrm{i}\mathbf{k}''\cdot\mathbf{r}) & z > d, \end{cases} \tag{71}$$

where amplitudes a' and a'' of reflected and forward-propagating waves, respectively, are obtained by solving the boundary-value problem. The requirement that $\psi(\mathbf{r})$ be continuous at the entrance surface at $z = 0$ and at the exit surface at $z = d$ then gives the following for the two geometries.

(i) *Laue geometry*

$$\begin{aligned}\psi'' &= a''\exp(\mathrm{i}\mathbf{k}''\cdot\mathbf{r}) \\ &= a\left\{\left[\frac{\gamma}{\delta^{1/2}} + \left(\frac{\gamma^2}{\delta} + 1\right)^{1/2}\right]\exp(\mathrm{i}\kappa_{z-}d) - \left[\frac{\gamma}{\delta^{1/2}} - \left(\frac{\gamma^2}{\delta} + 1\right)^{1/2}\right]\exp(\mathrm{i}\kappa_{z+}d)\right\}\left[2\left(\frac{\gamma^2}{\delta} + 1\right)^{1/2}\right]^{-1} \\ &\quad \times \exp(\mathrm{i}\mathbf{k}''\cdot\mathbf{r}) \qquad \text{for } z > d \end{aligned} \tag{72a}$$

and

$$\begin{aligned}\psi' &= a'\exp(\mathrm{i}\mathbf{k}'.\mathbf{r}) \\ &= a\left(\frac{k_z}{k_z + G_{\mathbf{h}z}}\right)^{1/2}\frac{1}{2(\gamma^2/\delta + 1)^{1/2}} \\ &\quad \times [\exp(\mathrm{i}\kappa_{z+}d) - \exp(\mathrm{i}\kappa_{z-}d)]\exp(\mathrm{i}q_{1z}d)\exp(\mathrm{i}\mathbf{k}'\cdot\mathbf{r}) \\ &\qquad \text{for } z > d. \end{aligned} \tag{72b}$$

[4] In this section, we follow the presentation by Sears (1989). We keep his notation with one exception, instead of $\mathbf{K}_h$, we use for the vectors of the reciprocal lattice $\mathbf{G}_h = -\mathbf{K}_h$. Further, we consider the lattice without basis thus the normalized unit-cell structure factor $F_h = 1$. Moreover, we will rearrange Sears's formulae into a form suitable for comparison with our results.

[5] For the Laue geometry, the sign of parameter η defined by Authier (2001) is opposite to the sign of $\gamma/|\delta|$ in (69).

(ii) *Bragg geometry*

$$\psi'' = a'' \exp(\mathrm{i}\mathbf{k}'' \cdot \mathbf{r}) = a[2(\gamma^2/|\delta| - 1)^{1/2}] \left\{ \exp(-\mathrm{i}\kappa_{z-}d) \left[\frac{\gamma}{|\delta|^{1/2}} + \left(\frac{\gamma^2}{|\delta|} - 1 \right)^{1/2} \right] - \exp(-\mathrm{i}\kappa_{z+}d) \left[\frac{\gamma}{|\delta|^{1/2}} - \left(\frac{\gamma^2}{|\delta|} - 1 \right)^{1/2} \right] \right\}^{-1} \exp(\mathrm{i}\mathbf{k}'' \cdot \mathbf{r}) \quad \text{for } z > d \qquad (73a)$$

and

$$\psi' = a' \exp(\mathrm{i}\mathbf{k}' \cdot \mathbf{r}) = a \left(\frac{k_z}{|k_z + G_{\mathbf{h}z}|} \right)^{1/2} [\exp(\mathrm{i}\kappa_{z+}d) - \exp(\mathrm{i}\kappa_{z-}d)] \times \left\{ \exp(\mathrm{i}\kappa_{z+}d) \left[\frac{\gamma}{|\delta|^{1/2}} + \left(\frac{\gamma^2}{|\delta|} - 1 \right)^{1/2} \right] - \exp(\mathrm{i}\kappa_{z-}d) \left[\frac{\gamma}{|\delta|^{1/2}} - \left(\frac{\gamma^2}{|\delta|} - 1 \right)^{1/2} \right] \right\}^{-1} \exp(\mathrm{i}\mathbf{k}' \cdot \mathbf{r}) \quad \text{for } z < 0 \qquad (73b)$$

with

$$\mathbf{k}' = \mathbf{k} + \mathbf{G}_\mathbf{h} - \mathbf{q}_1, \quad \mathbf{k}'' = \mathbf{k}, \qquad (74)$$

for both Laue and Bragg geometries, where $\mathbf{q}_1 = q_{1z}\mathbf{e}_3$ is given by equation (6.2.4) in Sears (1989). Introducing Bragg angle Θ_B and the departure $\Delta\Theta$ from Bragg's incidence of the incident wave, the equation for q_{1z} reads

$$q_{1z} = -\frac{k^2 \sin 2\Theta_\mathrm{B}}{k_z + G_{\mathbf{h}z}} \Delta\Theta \qquad (75)$$

so that according to (90) q_{1z} is equal to μ/a_{3z} or η/a_{3z} for the Laue or Bragg geometry, respectively.

Now we may compare wavefunctions for the Laue (72*a*), (72*b*) and Bragg (73*a*), (73*b*) geometries with our corresponding formulae (57*a*), (59*b*) and (61*a*), (61*b*). We can see that the results of both developments have the same algebraic forms but with different parameters. The thickness of the slab d is given by $(N+1)a_{3z}$, the wavevector differences $\kappa_{z\pm}$ (67) are replaced by $\tilde{\kappa}^\mathrm{L}_{z\pm}$ (58) or $\tilde{\kappa}^\mathrm{B}_{z\pm}$ (62) and the parameter $\gamma/|\delta|^{1/2}$ (69) by z_{rsl} (37) or y_{rsl} (47). The formulae by Sears are transformed into ours by replacing $|k_z + G_{\mathbf{h}z}|$, representing the z components of the diffracted beam in an infinite crystal, by K_{pqz}, defined by (4), representing the diffracted wave on a slab. This difference stems from the fact that Laue's theory is based on the expansions (64) and (66) appropriate for an infinite (unbounded) crystal whereas our development respects from the very beginning the two-dimensional translation symmetry of a crystal slab. The relation between $|k_z + G_{\mathbf{h}z}|$ and K_{rsz} is examined in detail in Appendix *B*, where it has been found that

$$\frac{K_{rsz}}{k_z} = \frac{|k_z + G_{\mathbf{h}z}|}{k_z} + \frac{\Delta\Theta \sin 2\Theta_\mathrm{B}}{\cos\gamma|\cos\gamma'|} \qquad (76)$$

with γ and γ' being the angles between $\mathbf{e}_3$ and the incident, $\mathbf{k}$, and reflected, $\mathbf{K}^\pm_{rs}$, directions, respectively. Since $\Delta\Theta$ is small, we may conclude that the differences between K_{rsz}/k_z and $|k_z + G_{\mathbf{h}z}|/k_z$ are negligible when γ and γ' are not near $\pi/2$ (grazing incidence or emergence). But the diffraction at grazing incidence or grazing emergence is not considered in the present paper.

We proceed in comparing wavevectors $\mathbf{k}'$ and $\mathbf{K}^\pm_{rs}$ of the reflected wave. Comparing (74) and (4), we can see that the component of the wavevector $\mathbf{k}'$ parallel to the crystal surface is just equal to $\mathbf{k}^{||}_{pq}$ defined by (3). On the other hand, as shown by (91), z components slightly differ, and whereas according to (4) $(\mathbf{K}^\pm_{rs})^2 = k^2$, the modulus of $\mathbf{k}'$ is not equal to k^2, $(\mathbf{k}')^2 = k^2 + q_1^2$. Furthermore, the phase factors $\exp[-\mathrm{i}(\mathbf{k}\cdot\mathbf{a}_3)/2]$, $\exp[\mathrm{i}(\mathbf{K}^+_{00}\cdot\mathbf{a}_3)/2]$, $(-1)^l \exp[\mathrm{i}(\mathbf{K}^-_{rs}\cdot\mathbf{a}_3)/2]$ and $(-1)^l \exp[\mathrm{i}(\mathbf{K}^+_{rs}\cdot\mathbf{a}_3)/2]$ in our formulae (57*a*), (57*b*) and (61*a*), (61*b*) rendering the shift of the entrance crystal surface above the first atomic plane by $\mathbf{a}_3/2$ and of the exit crystal surface below the last atomic plane by $\mathbf{a}_3/2$ appear since the thickness of the slab is considered to be $(N+1)a_{3z}$ and not Na_{3z} (see also Dub & Litzman, 2001*a*). These shifts are connected with the boundary condition problem.

Having found wavefunctions, we may evaluate reflectivities. Using (57*b*) and (61*b*), we get respective reflectivity of the Bragg reflected wave in the Laue and Bragg geometries,

$$I^>_{rs} = \frac{\sin^2[(N+1)a_{3z}(\pi/\Delta)(z^2_{rsl}+1)^{1/2}]}{z^2_{rsl}+1} \quad \text{(Laue geometry)} \qquad (77)$$

$$I^<_{rs} = \frac{1 - \cos^2[(N+1)a_{3z}(\pi/\Delta)(y^2_{rsl}-1)^{1/2}]}{y^2_{rsl} - \cos^2[(N+1)a_{3z}(\pi/\Delta)(y^2_{rsl}-1)^{1/2}]} \quad \text{(Bragg geometry),} \qquad (78)$$

where

$$\Delta = \frac{|\mathbf{a}_1 \times \mathbf{a}_2|a_{3z}}{2Q_0} k(\cos\gamma|\cos\gamma'|)^{1/2}. \qquad (79)$$

Naturally, (77) and (78) conform to the results of the standard Laue theory [see equations (9.30) and (9.35) in Rauch & Petraschek (1978)] if the thickness of the slab is $(N+1)a_{3z}$ and Δ is considered to be the *Pendellösung* distance [see *e.g.* equation (9.22) in Rauch & Petraschek (1978)].

6. Summary and concluding remarks

In this paper, we have treated the diffraction on a crystalline slab as a multiple scattering problem based upon the Ewald equations (10*a*), (10*b*). This approach overcomes the limitations of Laue's method (Sears, 1989).

We have considered from the very beginning the two-dimensional symmetry of a crystalline slab. Thus, (i) the wavevectors $\mathbf{K}^\pm_{pq}(\mathbf{k})$ of the diffracted waves in the Laue (+) and Bragg (−) geometries are given by (4), and (ii) the two-dimensional interplanar and intraplanar lattice sums have been calculated, the latter given by (14*a*), expressing rigorously the local-field effects. The multiple-beam wavefunctions above and below the slab are then given by (18*a*) and (18*b*), respectively, which are valid for any angle of incidence. Amplitudes of the wavefunctions are determined by determinants of fundamental matrices $\mathbf{H}$ (16) and $\mathbf{M}_{pq}^{\pm}$ (19*a*), (19*b*), the elements of which are simple functions of $\theta_{pq}^{\pm} = \mathbf{a}_3 \cdot \mathbf{K}_{pq}^{\pm}(\mathbf{k})$, being given by the geometry and the wavelength only, and of solutions $\psi_{pq}^{\pm}$ of the dispersion equation (13). We have found that the dispersion relation is represented for both coplanar and non-coplanar diffractions by a 'dispersion plot' (20) with poles $\theta_{pq}^{\pm}$, which are of crucial importance since, as indicated by (7*a*), (7*b*), the confluence of two poles means that Bragg reflection occurs. Thus the Ewald sphere is replaced by 'the Γ diagram' (Fig. 1) and no three-dimensional dispersion surface or approximate dispersion hyperbolae are introduced. With 'the Γ diagram', it is possible to find Bragg diffraction positions and also to predict the mutual influence of diffractions in different directions. Furthermore, no boundary conditions needed in Laue's theory are to be applied. Thus, the question of the nature of boundary surfaces does not appear.

Next we have shown that to handle particular cases it is necessary to rearrange matrices $\mathbf{H}$ and $\mathbf{M}_{pq}^{\pm}$ into the forms proper to evaluate quotients $\det \mathbf{M}_{pq}^{-} / \det \mathbf{H}$ and $\det \mathbf{M}_{pq}^{+} / \det \mathbf{H}$ by using formula (50) for evaluating the determinant of a symmetrically partitioned square matrix. In particular, considering that only two poles θ_{00}^{+} and θ_{rs}^{+} in the Laue geometry or θ_{00}^{+} and θ_{rs}^{-} in the Bragg geometry may coincide, the other ones being well separated from both θ_{00}^{+} and $\theta_{rs}^{\pm}$, the problem can be reduced to a two-beam one. The corresponding wavefunctions of the forward-propagating wave and the diffracted one, given by (56*a*), (56*b*) or (60*a*), (60*b*) for the Laue or Bragg geometry, respectively, are valid for both coplanar and non-coplanar diffractions in and outside the Bragg-peak region and thus should not be confused with the two-beam approximation in the standard Laue theory. Then, the solution in the Bragg-peak region is a special case of the general solution. We have shown that in the Bragg-peak region formulae (56*a*), (56*b*) and (60*a*), (60*b*) result in (57*a*), (57*b*) and (61*a*), (61*b*), respectively, which have the same algebraic forms as wavefunctions (72*a*), (72*b*) and (73*a*), (73*b*) derived in the frame of Laue's theory, but the parameters differ, and the 'mathematical' boundary planes are shifted from the corresponding surface atomic layers. The differences in parameters could be understood if we take into account that our development considers from the very beginning the two-dimensional translation symmetry of a crystal slab, whereas in the Laue theory the Schrödinger equation with the optical potential possessing the full translation symmetry of the unbounded crystal is to be solved and after that the interior solution is matched to the exterior one.

Summarizing, let us point out that our approach based upon the Ewald method yields the solution to the diffraction problem that is valid generally and thus, in principle, it may be applied to extreme cases outside the scope of the standard dynamical theory of diffraction. In particular, we already treated the diffraction at the Bragg angle near $\pi/2$ (Litzman *et al.*, 1996) or the influence of Bragg diffractions on the coplanar and non-coplanar crystal truncation rod scattering (Litzman & Mikulík, 1999). Our approach enables us to study other extreme cases, such as the diffraction at grazing incidence or grazing emergence (Authier, 2001, ch. 8), where three poles in our dispersion relation (13) coincide. Then submatrices (51) or (52) of the second order would have to be replaced by submatrices of the third order, which contain all relevant large elements, the dispersion relation becoming now an equation of the third order too.

Concluding, let us mention that we have considered a crystal with a cell containing one atom only. The general solution of the diffraction problem found in Litzman (1986) may be applied to a lattice with general basis but resulting formulae for diffracted waves in such a transparent form as derived in the present paper have hitherto been obtained for a single atomic plane only (Dub & Litzman, 2001*b*). The case with distributed cell content would be challenging also because of the question of where to locate the boundary and the question posed by Ignatovich *et al.* (1996) on forbidden reflections.

APPENDIX *A*
Parameters μ and η

The parameters μ and η are defined by (26) and (38) for the Laue and Bragg geometry, respectively. After inserting the Bragg condition for the Laue geometry (7*a*) into (26), we obtain

$$\begin{aligned}\mu &= \theta_{00}^{+}(\mathbf{k}) - \theta_{pq}^{+}(\mathbf{k}) - [\theta_{00}^{+}(\mathbf{k}_B) - \theta_{pq}^{+}(\mathbf{k}_B)]\\ &= \mathbf{a}_3 \cdot \mathbf{k} - \mathbf{a}_3 \cdot \mathbf{K}_{pq}^{+}(\mathbf{k}) - [\mathbf{a}_3 \cdot \mathbf{k}_\mathrm{B} - \mathbf{a}_3 \cdot \mathbf{K}_{pq}^{+}(\mathbf{k}_\mathrm{B})]\\ &= a_{3z}[K_{pqz}(\mathbf{k}_\mathrm{B}) - K_{pqz}(\mathbf{k}) + k_z - k_{\mathrm{B}z}].\end{aligned}$$

Analogously in the Bragg geometry,

$$\begin{aligned}\eta &= \theta_{00}^{+}(\mathbf{k}) - \theta_{pq}^{-}(\mathbf{k}) - [\theta_{00}^{+}(\mathbf{k}_B) - \theta_{pq}^{-}(\mathbf{k}_B)]\\ &= \mathbf{a}_3 \cdot \mathbf{k} - \mathbf{a}_3 \cdot \mathbf{K}_{pq}^{-}(\mathbf{k}) - [\mathbf{a}_3 \cdot \mathbf{k}_\mathrm{B} - \mathbf{a}_3 \cdot \mathbf{K}_{pq}^{-}(\mathbf{k}_\mathrm{B})]\\ &= a_{3z}[-K_{pqz}(\mathbf{k}_\mathrm{B}) + K_{pqz}(\mathbf{k}) + k_z - k_{\mathrm{B}z}].\end{aligned}$$

If all the wavevectors $\mathbf{k}$, $\mathbf{k}_\mathrm{B}$, $\mathbf{K}_{pq}^{+}(\mathbf{k})$, $\mathbf{K}_{pq}^{+}(\mathbf{k}_\mathrm{B})$ or $\mathbf{k}$, $\mathbf{k}_\mathrm{B}$, $\mathbf{K}_{pq}^{-}(\mathbf{k})$, $\mathbf{K}_{pq}^{-}(\mathbf{k}_\mathrm{B})$ in the Laue or Bragg geometry, respectively, and the normal to the crystal surface, $\mathbf{e}_3$, oriented towards the inside of the crystal lie in the same plane (the case of coplanar diffraction), we can write $k_{\mathrm{B}z} = k\cos\gamma_\mathrm{B}$, $k_z = k\cos(\gamma_\mathrm{B} + \Delta\gamma)$ and $K_{pqz}(\mathbf{k}_\mathrm{B}) = \pm k \cos\gamma'_\mathrm{B}$, with the sign + and − for the Laue and Bragg geometry, respectively, where γ_B and γ'_B are the angles between $\mathbf{e}_3$ and the incident and reflected directions at Bragg's incidence, respectively. Then for small $\Delta\gamma$, we find after lengthy but easy algebra that

$$\mu = -a_{3z}k^2 \frac{1}{K_{pqz}} \sin(\gamma_\mathrm{B} - \gamma'_\mathrm{B})\Delta\gamma + O[(\Delta\gamma)^2] \qquad (80)$$

and

$$\eta = a_{3z}k^2 \frac{1}{K_{pqz}} \sin(\gamma_\mathrm{B} - \gamma'_\mathrm{B})\Delta\gamma + O[(\Delta\gamma)^2]. \qquad (81)$$

Next we introduce the Bragg angle $\Theta_\mathrm{B} = |\gamma_\mathrm{B} - \gamma'_\mathrm{B}|/2$ and the departure from Bragg incidence of the incident wave $\Delta\Theta$. In both the Bragg and Laue geometries, two different situations may occur.

(i) Laue geometry: (i1) if $\gamma_B > \gamma'_B$ then $\Delta\gamma = \Delta\Theta$; (i2) if $\gamma_B < \gamma'_B$ then $\Delta\gamma = -\Delta\Theta$.

(ii) Bragg geometry: (ii1) if $\gamma_B > \gamma'_B$ then $\Delta\gamma = -\Delta\Theta$; (ii2) if $\gamma_B < \gamma'_B$ then $\Delta\gamma = \Delta\Theta$.

Considering all above possibilities, from (80) and (81) we obtain finally

$$\mu = -a_{3z}k^2 \frac{1}{K_{pqz}} \sin 2\Theta_B \Delta\Theta + O[(\Delta\Theta)^2] \qquad (82)$$

and

$$\eta = a_{3z}k^2 \frac{1}{K_{pqz}} \sin 2\Theta_B \Delta\Theta + O[(\Delta\Theta)^2]. \qquad (83)$$

APPENDIX *B*
Relation between $|k_z + G_{\mathbf{h}z}|$ and K_{rsz}

The vectors $\mathbf{K}^{\pm}_{pq}(\mathbf{k})$ defined by (4) can be expressed in two coordinate systems ($\mathbf{b}_1$, $\mathbf{b}_2$, $\mathbf{e}_3$) and ($\mathbf{g}_1$, $\mathbf{g}_2$, $\mathbf{g}_3$):

$$\begin{aligned}\mathbf{K}^{\pm}_{pq}(\mathbf{k}) &= \mathbf{k}^{||} + p\mathbf{b}_1 + q\mathbf{b}_2 \pm \mathbf{e}_3 K_{pqz}(\mathbf{k}) \\ &= \mathbf{k} + y_1\mathbf{g}_1 + y_2\mathbf{g}_2 + y_3\mathbf{g}_3.\end{aligned}$$

As $\mathbf{g}^{||}_1 = \mathbf{b}_1$, $\mathbf{g}^{||}_2 = \mathbf{b}_2$, we get $y_1 = p$ and $y_2 = q$. Thus,

$$\mathbf{K}^{\pm}_{pq}(\mathbf{k}) = \mathbf{k} + p\mathbf{g}_1 + q\mathbf{g}_2 + y_3\mathbf{g}_3. \qquad (84)$$

Multiplying the last equation by $\mathbf{a}_3$, we obtain $\theta^{\pm}_{pq} = \theta^{+}_{00} + 2\pi y_3$ [*cf*. definition (6)], so that

$$y_3 = \frac{\theta^{\pm}_{pq} - \theta^{+}_{00}}{2\pi}. \qquad (85)$$

Using (84), we get

$$\begin{aligned}K_{rsz}(\mathbf{k}) &= \mathbf{e}_3 \cdot \mathbf{K}^{\pm}_{rs}(\mathbf{k}) \\ &= \pm(\mathbf{k} + r\mathbf{g}_1 + s\mathbf{g}_2 + y_3\mathbf{g}_3) \cdot \mathbf{e}_3 \\ &= \pm(\mathbf{k} + r\mathbf{g}_1 + s\mathbf{g}_2 - l\mathbf{g}_3) \cdot \mathbf{e}_3 \pm (y_3 + l)\mathbf{g}_3 \cdot \mathbf{e}_3,\end{aligned}$$

where the signs + and − correspond to the Laue and Bragg geometries, respectively. Considering that $\mathbf{G_h} = r\mathbf{g}_1 + s\mathbf{g}_2 - l\mathbf{g}_3$ and y_3 is given by (85), we find that the term K_{rsz} is related to the following terms as given below.

(i) *In the Laue geometry*

K_{rsz} is related to $k_z + G_{\mathbf{h}z} > 0$ by

$$\begin{aligned}K_{rsz}(\mathbf{k}) &= k_z + G_{\mathbf{h}z} + (\theta^{+}_{rs} - \theta^{+}_{00} + 2\pi l)\frac{\mathbf{g}_3 \cdot \mathbf{e}_3}{2\pi} \\ &= k_z + G_{\mathbf{h}z} - \mu \frac{1}{a_{3z}},\end{aligned} \qquad (86)$$

where the parameter μ, defined by (26), is, in the case of coplanar diffraction, given by (82).

(ii) *In the Bragg geometry*

K_{rsz} is related to $|k_z + G_{\mathbf{h}z}|$, $k_z + G_{\mathbf{h}z} < 0$, by

$$\begin{aligned}K_{rsz}(\mathbf{k}) &= |k_z + G_{\mathbf{h}z}| - (\theta^{-}_{rs} - \theta^{+}_{00} + 2\pi l)\frac{\mathbf{g}_3 \cdot \mathbf{e}_3}{2\pi} \\ &= |k_z + G_{\mathbf{h}z}| + \eta \frac{1}{a_{3z}},\end{aligned} \qquad (87)$$

where the parameter η, defined by (38), is, in the case of coplanar diffraction, given by (83).

Finally, introducing (82) into (86) and (83) into (87), we get for either geometry

$$K_{rsz} = |k_z + G_{\mathbf{h}z}| + \frac{k}{|\cos\gamma'|}\Delta\Theta \sin 2\Theta_B + O[(\Delta\Theta)^2] \qquad (88)$$

and consequently

$$\frac{K_{rsz}}{k_z} = \frac{|k_z + G_{\mathbf{h}z}|}{k_z} + \frac{\Delta\Theta \sin 2\Theta_B}{\cos\gamma|\cos\gamma'|} + O[(\Delta\Theta)^2], \qquad (89)$$

where γ and γ' are the angles between $\mathbf{e}_3$ and the incident, $\mathbf{k}$, and reflected, $\mathbf{K}^{\pm}_{rs}$, directions, respectively. Since $\Delta\Theta$ is small, we may conclude that the difference between K_{rsz}/k_z and $|k_z + G_{\mathbf{h}z}|/k_z$ is negligible when γ and γ' are not near $\pi/2$.

Finally, inserting (88) into (75) under the assumption that γ and γ' are not near $\pi/2$, we get

$$q_{1z}a_{3z} = \mu + O[(\Delta\Theta)^2] \quad \text{or} \quad \eta + O[(\Delta\Theta)^2] \qquad (90)$$

for the Laue and Bragg geometry, respectively. Then after inserting (90) into (74) and considering (88), (82) and (83), we get that

$$k'_z = K_{rsz} + O[(\Delta\Theta)^2]. \qquad (91)$$

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