KOHRA, K., MOLIERE, K., NAKANO, S. & ARIYAMA, M. (1962). *J. Phys. Soc. Jpn*, **17**, Suppl. BII, 82-87.
MAKSYM, P. A. & BEEBY, J. L. (1981). *Surface Sci.* **110**, 423-438.
MARTEN, H. & MEYER-EHMSEN, G. (1985). *Surface Sci.* **151**, 570-584.
MASUD, N. & PENDRY, J. B. (1976). *J. Phys. C*, **9**, 1833-1844.
MENADUE, J. F. (1972). *Acta Cryst.* **A28**, 1-11.
MOON, A. R. (1972). *Z. Naturforsch. Teil A*, **27**, 390-395.
MIYAKE, S., HAYAKAWA, K. & MIIDA, R. (1968). *Acta Cryst.* **A24**, 182-191.
MIYAKE, S., KOHRA, K. & TAKAGI, M. (1954). *Acta Cryst.* **7**, 393-401.
OSAKABE, N., TANISHIRO, Y., YAGI, K. & HONJO, G. (1980). *Surface Sci.* **97**, 393-408.
SHUMAN, H. (1977). *Ultramicroscopy*, **2**, 261-269.
SPENCE, J. C. H. & TAFTØ, J. (1983). *J. Microsc.* (*Oxford*), **130**, 147-154.
VAN HOVE, J. M., LENT, C. S., PUKITE, P. R. & COHEN, P. I. (1983). *J. Vac. Sci. Technol. B*, **1**, 741-746.

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Dynamical Theory of Diffraction on a Periodic System of Point Scatterers

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Abstract

Ewald's self-consistent field method is used to deduce formulae for the reflection and transmission coefficients of a crystal slab in a well arranged determinant form. No supposition concerning the magnitude of the interaction between the diffracted particles and the crystal or the number of diffracted beams is made.

1. Introduction

The diffraction of radiation on a system of scatterers is encountered in many branches of physics: let us mention the diffraction of X-rays, electrons or neutrons on a crystal or the classical diffraction of visible light on a system of small metal particles embedded in a dielectric - low-energy photodiffraction, LEPD (Ohtaka, 1980). The problem of multiple scattering is rather difficult in both classical and quantum physics. That is why different approximations are used. In the kinematical theory multiple scattering is neglected. In some dynamical theories the interaction of the radiation with the crystal is supposed to be small, the diffraction is studied in the neighbourhood of the Bragg diffraction angle, in the two-beam approximation *etc.* But the interaction is not small either in low-energy electron diffraction (LEED) or in LEPD; then computers are needed to process general formulae.

There is one case in which multiple scattering leads to relatively well arranged and simple algebraic equations - multiple scattering on point scatterers. The problem of point scatterers in quantum mechanics has been handled from the general point of view, *e.g.* by Demkov & Ostrovskij (1975). In solid-state physics the model of point scatterers is adequate in neutron diffraction, soft X-ray diffraction (Henke, Lee, Tanaka, Shimabukuro & Fujikawa, 1982), in LEED in a strong limited s approximation or in LEPD, if the diameter of the embedded particles is sufficiently small compared with the wavelength of the photon.

In our earlier papers we were engaged in Ewald's dynamical theory of X-ray diffraction on a simple periodic lattice (without basis) (Litzman, 1980; Litzman & Rózsa, 1980). The results have been used in the soft X-ray optics of thin films (Litzman & Šebelová, 1985). The aim of this paper is to deduce formulae for the reflection and transmission of radiation by a system of point scatterers forming a general lattice (with a basis). Neither a small interaction between the radiation and scatterers nor a two-beam approximation nor proximity to the Bragg diffraction angle is assumed. On the other hand we confine ourselves to scalar waves, *i.e.* to solutions of the Schrödinger equation. Vector waves (electromagnetic waves) can be handled in a similar way, the corresponding matrices being, roughly speaking, three times greater. Thus, for electromagnetic waves we confine ourselves to hints at relevant points.

2. Basic formulae

We shall study the diffraction of particles (electrons, neutrons) on a system of point scatterers, fixed at the lattice points of an ideal crystal slab with s

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basis atoms:

$$\mathbf{R}_\nu^{\mathbf{n}} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3 + \mathbf{r}_\nu, \quad (1)$$

$$n_1, n_2 = 0, \pm 1, \pm 2, \cdots, \pm\infty$$

$$n_3 = 0, 1, 2, \cdots, N$$

$$a_{3z} > 0, \quad |\mathbf{r}_{\mu z} - \mathbf{r}_{\nu z}| < a_{3z}, \mu, \nu = 1, 2, \ldots, s.$$

The origin of the orthogonal coordinate system $Oxyz$ lies at the lattice point $(0,0,0)$, the plane Oxy coincides with the 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.* $g_i a_k = 2\pi\delta_{ik}$, $i, k = 1, 2, 3$, whereas the lattice $(\mathbf{b}_1, \mathbf{b}_2)$ is reciprocal to the two-dimensional lattice $(\mathbf{a}_1, \mathbf{a}_2)$, *i.e.* $\mathbf{b}_i \perp \mathbf{e}_3$, $b_i a_k = 2\pi\delta_{ik}$, $i, k = 1, 2$. Further, $\mathbf{c}^{\parallel}$ and $\mathbf{c}^{\perp}$ denote the components of the vector $\mathbf{c} = \mathbf{c}^{\parallel} + \mathbf{c}^{\perp}$ parallel and perpendicular to the crystal surface. It holds that

$$\mathbf{g}_1^{\parallel} = \mathbf{b}_1, \quad \mathbf{g}_2^{\parallel} = \mathbf{b}_2, \quad \mathbf{g}_3^{\parallel} = 0. \quad (2)$$

Ewald's dynamical (self-consistent field) theory of diffraction leads to equations (Lax, 1951; McRae, 1966; Dederichs, 1972; our notation is the same as that of Dederichs, p. 167):

$$\varphi_i = \Psi_0 + G_0 \sum_{j \neq i}{}' T_j \varphi_j \quad (3a)$$

$$\Psi = \Psi_0 + G_0 \sum_j T_j \varphi_j \quad (3b)$$

where

$$T_j = T_\nu^{\mathbf{n}}(\mathbf{r}, \mathbf{r}') = (\hbar^2/2m) 4\pi Q_\nu \delta(\mathbf{r} - \mathbf{R}_\nu^{\mathbf{n}}) \delta(\mathbf{r}' - \mathbf{R}_\nu^{\mathbf{n}}) \quad (4)$$

is the T matrix of the scatterer on the lattice point $\mathbf{R}_\nu^{\mathbf{n}}$. Q_ν is the scattering length of scatterer ν. Its dependence on the wave vector $\mathbf{k}$ of the incident wave is given by (Dederichs, 1972)

$$Q_\nu(\mathbf{k}) = Q_\nu^0/(1 + ikQ_\nu^0). \quad (5)$$

Further

$$G_0(\mathbf{r}, \mathbf{r}') = -\frac{2m}{\hbar^2} \frac{\exp(ik|\mathbf{r} - \mathbf{r}'|)}{4\pi|\mathbf{r} - \mathbf{r}'|}, \quad (6)$$

$$\Psi_0 = f \exp(i\mathbf{k}\mathbf{r}), \quad E = \hbar^2 k^2/2m. \quad (7)$$

Equation $(3a)$ is a nonhomogeneous system of algebraic equations for $\varphi_\mu^{\mathbf{m}}(\mathbf{R}_\mu^{\mathbf{m}})$

$$\varphi_\mu^{\mathbf{m}}(\mathbf{R}_\mu^{\mathbf{m}}) = f \exp(i\mathbf{k}\mathbf{R}_\mu^{\mathbf{m}}) - \sum_{\binom{\mathbf{n}}{\nu} \neq \binom{\mathbf{m}}{\mu}}{}' Q_\nu \frac{\exp(ik|\mathbf{R}_\mu^{\mathbf{m}} - \mathbf{R}_\nu^{\mathbf{n}}|)}{|\mathbf{R}_\mu^{\mathbf{m}} - \mathbf{R}_\nu^{\mathbf{n}}|} \varphi_\nu^{\mathbf{n}}(\mathbf{R}_\nu^{\mathbf{n}}). \quad (8)$$

When (8) is solved we get the wave function Ψ describing the diffracted particles from $(3b)$

$$\Psi = f \exp(i\mathbf{k}\mathbf{r}) - \sum_{\mathbf{n},\nu} Q_\nu \frac{\exp(ik|\mathbf{r} - \mathbf{R}_\nu^{\mathbf{n}}|)}{|\mathbf{r} - \mathbf{R}_\nu^{\mathbf{n}}|} \varphi_\nu^{\mathbf{n}}(\mathbf{R}_\nu^{\mathbf{n}}). \quad (9)$$

Due to the translational symmetry, we may put in (8)

$$\varphi_\mu^{m_1 m_2 m_3}(\mathbf{R}_\mu^{\mathbf{m}}) = \exp[i\mathbf{k}^{\parallel}(m_1\mathbf{a}_1 + m_2\mathbf{a}_2 + \mathbf{r}_\mu)] w_\mu^{m_3}. \quad (10)$$

The following mathematical procedure is similar to that used by Litzman (1978, 1980). We shall give here the resulting system of nonhomogeneous algebraic equations for $w_\mu^{m_3}$ in a suitable matrix form (see Appendix):

$$w - \left\{ \mathbf{I} \otimes \mathbf{C}(\mathbf{k}) + \sum_{pq}^{(n)} [\mathbf{R}(-\theta_{pq}^-) \otimes \mathbf{B}_{pq} + \mathbf{L}(\theta_{pq}^+) \otimes \mathbf{D}_{pq}] \right\} w = f \|\exp(im_3\mathbf{k}\mathbf{a}_3)\| \otimes \|\exp(i\mathbf{k}\mathbf{r}_\mu^{\perp})\|. \quad (11)$$

The following notation is used in (11):

$w = \|w_\mu^{m_3}\|$, $\quad m_3 = 0, 1, 2, \ldots, N$,
$\mu = 1, 2, \ldots, s$, is a column vector of order $(N+1)s$.

Similarly, $\|\exp(im_3\mathbf{k}\mathbf{a}_3)\|$ is a column vector of order $N+1$ and $\|\exp(i\mathbf{k}\mathbf{r}_\mu^{\perp})\|$ a column vector of order s. $\otimes$ denotes a direct matrix product. $\mathbf{R}(-\theta_{pq}^-)$ and $\mathbf{L}(\theta_{pq}^+)$ are square matrices of order $N+1$:

$$\mathbf{R}(\theta) = \begin{Vmatrix} 0 & \exp(i\theta) & \exp(i2\theta) & \ldots & \exp(iN\theta) \\ 0 & 0 & \exp(i\theta) & \ldots & \exp i(N-1)\theta \\ \vdots & & & & \vdots \\ 0 & 0 & 0 & & \exp(i\theta) \\ 0 & 0 & 0 & \ldots & 0 \end{Vmatrix}. \quad (12)$$

$\mathbf{L}(\theta) = \mathbf{R}^T(\theta)$. Matrix $\mathbf{A}^T$ is transpose to matrix $\mathbf{A}$.

$$\mathbf{D}_{pq} = \|D_{pq}^{\mu\nu}(\mathbf{k})\| = -\frac{2\pi i}{|\mathbf{a}_1 \times \mathbf{a}_2| K_{pqz}} {}^1\boldsymbol{d}_{pq} \cdot {}^2\boldsymbol{d}_{pq}^T$$

$$\mathbf{B}_{pq} = \|B_{pq}^{\mu\nu}(\mathbf{k})\| = -\frac{2\pi i}{|\mathbf{a}_1 \times \mathbf{a}_2| K_{pqz}} {}^1\boldsymbol{b}_{pq} \cdot {}^2\boldsymbol{b}_{pq}^T \quad (13)$$

are dyads of order s formed by the column vectors

$${}^1\boldsymbol{d}_{pq} = \|\exp[i\mathbf{r}_\mu(p\mathbf{b}_1 + q\mathbf{b}_2) + i\mathbf{r}_{\mu z} K_{pqz}]\|$$

$${}^2\boldsymbol{d}_{pq} = \|Q_\mu \exp[-i\mathbf{r}_\mu(p\mathbf{b}_1 + q\mathbf{b}_2) - i\mathbf{r}_{\mu z} K_{pqz}]\|$$

$${}^1\boldsymbol{b}_{pq} = \|\exp[i\mathbf{r}_\mu(p\mathbf{b}_1 + q\mathbf{b}_2) - ir_{\mu z} K_{pqz}]\|$$

$${}^2\boldsymbol{b}_{pq} = \|Q_\mu \exp[-i\mathbf{r}_\mu(p\mathbf{b}_1 + q\mathbf{b}_2) + ir_{\mu z} K_{pqz}]\|$$

$$\mu = 1, 2, \ldots, s. \quad (14)$$

$$\mathbf{C}(\mathbf{k}) = -\sum_{pq} \{(2\pi i/|\mathbf{a}_1 \times \mathbf{a}_2| K_{pqz}) \times \|Q_\nu(1 - \delta_{\mu\nu}) \exp[i(\mathbf{r}_\mu - \mathbf{r}_\nu)(p\mathbf{b}_1 + q\mathbf{b}_2) + i|\mathbf{r}_{\mu z} - \mathbf{r}_{\nu z}| K_{pqz}]\|\} - \langle Q_1, Q_2, \ldots, Q_s \rangle \mathbf{S}'(\mathbf{k}^{\parallel}). \quad (15)$$

$\langle Q_1, Q_2, \ldots, Q_s \rangle$ denotes a diagonal matrix with the elements $Q_1, Q_2, \ldots, Q_s$ on its main diagonal.

$$\begin{aligned}\mathbf{S}'(\mathbf{k}^{\|}) &= \sum_{(n_1n_2)\neq(00)}{}' \frac{\exp[ik|n_1\mathbf{a}_1+n_2\mathbf{a}_2|]}{|n_1\mathbf{a}_1+n_2\mathbf{a}_2|} \times \exp[i\mathbf{k}^{\|}(n_1\mathbf{a}_1+n_2\mathbf{a}_2)] \\ &= \frac{2\pi i}{|\mathbf{a}_1\times\mathbf{a}_2|}\sum_{pq}\frac{1}{K_{pqz}}\left[1+\Phi\left(\frac{iK_{pqz}}{2B}\right)\right] \\ &+ \sum_{(n_1n_2)\neq(00)}{}'\left(\frac{\exp[i\mathbf{k}^{\|}(n_1\mathbf{a}_1+n_2\mathbf{a}_2)]}{2|n_1\mathbf{a}_1+n_2\mathbf{a}_2|} \times\{\exp[-ik|n_1\mathbf{a}_1+n_2\mathbf{a}_2|] \times[1-\Phi(|n_1\mathbf{a}_1+n_2\mathbf{a}_2|B-ik/2B)]+\text{c.c.}\}\right) \\ &-ik-ik\Phi(ik/2B)-(2B/\sqrt{\pi})\exp(k^2/4B^2).\end{aligned} \tag{16}$$

In (16)

$$\Phi(x)=2\pi^{-1/2}\int_0^x \exp(-t^2)\,dt$$

and B is a suitable parameter which affords an equally good convergence of both sums in real and reciprocal lattices. The value $B=(\pi/|\mathbf{a}_1\times\mathbf{a}_2|)^{1/2}$ is recommended by Pendry (1974) where a more general sum is studied. The sum (16) was discussed also by Dub & Litzman (1983).

Further,

$$\begin{aligned}\mathbf{k}^{\|}_{pq}&=\mathbf{k}^{\|}+p\mathbf{b}_1+q\mathbf{b}_2,\\ K_{pqz}&=+[k^2-(\mathbf{k}^{\|}+p\mathbf{b}_1+q\mathbf{b}_2)^2]^{1/2}\\ \mathbf{K}^{\pm}_{pq}&=\mathbf{k}^{\|}_{pq}\pm\mathbf{e}_3K_{pqz},\qquad \theta^{\pm}_{pq}=\mathbf{a}_3\mathbf{K}^{\pm}_{pq},\\ &p,q=0,\pm1,\pm2,\ldots.\end{aligned} \tag{17}$$

It is always possible to find such $p_0>0$, $q_0>0$ as the elements of the matrices $\mathbf{R}(-\theta^-_{pq})$ and $\mathbf{L}(\theta^+_{pq})$ are arbitrarily small for all $|p|\geq p_0$, $|q|\geq q_0$. Thus the sum over (pq) on the left-hand side of (11) is carried out over a finite number n of different $\theta^{\pm}_{pq}$ and we denote it by $\sum^{(n)}_{pq}$.

The system (11) is very similar to that obtained in our earlier papers concerning the dynamical theory of X-ray diffraction in simple lattices. The formal difference consists in the fact that in the earlier papers (Litzman 1978, 1980) the reciprocal vectors $(\mathbf{b}_1,\mathbf{b}_2)$ were not introduced, matrices $\mathbf{B}_{pq}$, $\mathbf{D}_{pq}$ were not dyads and matrix $\mathbf{V}$ characterizing the spatial dispersion is now not introduced. But the following proposition is again valid:

Proposition

(1) Let $\psi_1, \psi_2, \ldots, \psi_{2n}$ be the roots of the equation

$$\det \mathbf{A}(\psi;\mathbf{k}^{\|})=0 \tag{18}$$

where

$$\mathbf{A}(\psi;\mathbf{k}^{\|})=\mathbf{I}-\mathbf{C}(\mathbf{k})-\sum_{pq}^{(n)}(\{\exp[i(\theta^-_{pq}-\psi)]-1\}^{-1}\mathbf{B}_{pq} +\{\exp[-i(\theta^+_{pq}-\psi)]-1\}^{-1}\mathbf{D}_{pq}). \tag{19}$$

(2) Let the s-dimensional vector $\mathbf{u}(\psi_j)$ be a solution of the homogeneous system

$$\mathbf{A}(\psi_j;\mathbf{k}^{\|})\mathbf{u}(\psi_j)=0. \tag{20}$$

(3) Let $c'_1, c'_2, \ldots, c'_{2n}$ be constants satisfying the following non-homogeneous system of linear algebraic equations:

$$\begin{aligned}&\sum_{j=1}^{2n}\frac{c'_j}{\exp[-i(\theta^+_{00}-\psi_j)]-1}\mathbf{D}_{00}\mathbf{u}(\psi_j)=f\|\exp(i\mathbf{k}\mathbf{r}^{\perp}_{\mu})\|\\ &\sum_{j=1}^{2n}\frac{c'_j}{\exp[-i(\theta^+_{pq}-\psi_j)]-1}\mathbf{D}_{pq}\mathbf{u}(\psi_j)=0\\ &\qquad (p,q)\neq(0,0)\\ &\sum_{j=1}^{2n}\frac{c'_j\exp(iN\psi_j)}{\exp[i(\theta^-_{pq}-\psi_j)]-1}\mathbf{B}_{pq}\mathbf{u}(\psi_j)=0\quad\text{for all }(p,q).\end{aligned} \tag{21}$$

Then the vector

$$\mathbf{w}=\sum_j c'_j\|\exp(im_3\psi_j)\|\otimes\mathbf{u}(\psi_j) \tag{22}$$

is the solution of (11).

Let us consider (18) in more detail. The determinant on the left-hand side of (18) can be written as a finite sum of determinants constructed from the rows of the matrices $\mathbf{I}-\mathbf{C}(\mathbf{k})$, $\mathbf{B}_{pq}$ and $\mathbf{D}_{pq}$, each of them being multiplied by some power of

$$\{\exp[i(\theta^-_{pq}-\psi)]-1\}^r\{\exp[-i(\theta^+_{pq}-\psi)]-1\}^s.$$

Because matrices $\mathbf{B}_{pq}$ and $\mathbf{D}_{pq}$ are dyads, $r, s=0, -1$ must hold. Thus supposing

$$\theta^{\pm}_{p_1q_1}\neq\theta^{\pm}_{p_2q_2}+j2\pi\quad\text{if }(p_1q_1)\neq(p_2q_2)\;j=0,\pm1,\pm2,\ldots \tag{23}$$

we can see that (18) is an algebraic equation of order $2n$ for $\exp(i\psi)$. If (23) does not hold, *i.e.* if some of the poles of the function $\det\mathbf{A}(\psi_i\mathbf{k}^{\|})$ coincide, then the solution of (18) is more complicated. Let us suppose, for example, that

$$\theta^+_{00}=\theta^{\pm}_{pq}+j2\pi,\qquad j\text{ integer}. \tag{24}$$

It is easy to show that in this case

$$\mathbf{K}^{\pm}_{pq}=\mathbf{k}+p\mathbf{g}_1+q\mathbf{g}_2-j\mathbf{g}_3,\qquad[\mathbf{K}^{\pm}_{pq}]^2=k^2 \tag{25}$$

must hold, *i.e.* the incident wave vector $\mathbf{k}$ satisfies the Bragg reflection condition.

Because the matrices $\mathbf{B}^{pq}$, $\mathbf{D}^{pq}$ (13) are dyads, (21) can be written as

$$\begin{aligned}&\sum_{j=1}^{2n}\frac{c_j}{\exp(i\psi_j)-\exp(i\theta^+_{00})}\sum_{\nu=1}^{s}{}^2d^{\nu}_{00}u_{\nu}(\psi_j) =-fK_{00z}\exp(-i\theta^+_{00})\\ &\sum_{j=1}^{2n}\frac{c_j}{\exp(i\psi_j)-\exp(i\theta^+_{pq})}\sum_{\nu=1}^{s}{}^2d^{\nu}_{pq}u_{\nu}(\psi_j)=0\\ &\sum_{j=1}^{2n}\frac{c_j\exp[i(N+1)\psi_j]}{\exp(i\psi_j)-\exp(i\theta^-_{pq})}\sum_{\nu=1}^{s}{}^2b^{\nu}_{pq}u_{\nu}(\psi_j)=0\end{aligned} \tag{26}$$

with

$$c_j = (2\pi i/|\mathbf{a}_1 \times \mathbf{a}_2|)\, c'_j. \quad (27)$$

Thus we have found solution (10) of (8) as follows:

$$\varphi_\mu^{m_1 m_2 m_3}(\mathbf{R}_\mu^m) = \exp[i\mathbf{k}^\parallel(m_1\mathbf{a}_1 + m_2\mathbf{a}_2 + \mathbf{r}_\mu)] \times \sum_j c'_j \exp(im_3\psi_j) u_\mu(\psi_j) \quad (28)$$

where ψ_j, $u_\mu(\psi_j)$ and c'_j are solutions of (18), (20), and (21). By the usual analysis of the waves (28) we can deduce that one half of the solutions ψ_j, $j = n+1, \ldots, 2n$, of the dispersion equation (18) should be omitted in the semi-infinite crystal ($N \to \infty$). For these solutions IM $\psi_j < 0$ holds in a crystal with absorption. Thus in the semi-infinite crystal we put $c_j = 0$ in (26) for $j = n+1, \ldots, 2n$.

The wave function Ψ describing the diffracted particles follows immediately from (3*b*) and (28). Again using formulae for the two-dimensional lattice sums (see Appendix), we get finally:

$$\Psi(\mathbf{r}) = f \exp(i\mathbf{kr}) + \sum_{pq}^{(n)} (1/K_{pqz}) R_r(\theta_{pq}^-) \exp(i\theta_{pq}^-) \times \exp[i(\mathbf{k}_{pq}^\parallel \mathbf{r}^\parallel - zK_{pqz})], \quad z < 0 \quad (29)$$

$$\Psi(\mathbf{r}) = -\sum_{pq}^{(n)} (1/K_{pqz}) R_t(\theta_{pq}^+) \exp(-iN\theta_{pq}^+) \times \exp[i(\mathbf{k}_{pq}^\parallel \mathbf{r}^\parallel + zK_{pqz})], \quad z > Na, \quad (30)$$

$z < 0$ corresponds to the reflected particles and $z > Na$ to the transmitted particles. Further,

$$R_r(\theta_{pq}^-) = \sum_{j=1}^{2n} \frac{c_j}{\exp(i\psi_j) - \exp(i\theta_{pq}^-)} \times \sum_\nu Q_\nu \exp[-i\mathbf{r}_\nu(p\mathbf{b}_1 + q\mathbf{b}_2 - \mathbf{e}_3 K_{pqz})] u_\nu(\psi_j), \quad (31)$$

$$R_t(\theta_{pq}^+) = \sum_{j=1}^{2n} \frac{c_j \exp[i(N+1)\psi_j]}{\exp(i\psi_j) - \exp(i\theta_{pq}^+)} \times \sum_\nu Q_\nu \exp[-i\mathbf{r}_\nu(p\mathbf{b}_1 + q\mathbf{b}_2 + \mathbf{e}_3 K_{pqz})] u_\nu(\psi_j). \quad (32)$$

Because of the symmetry, the components $\mathbf{k}_{pq}^\parallel$ of the wave vectors of the reflected and transmitted waves in (29), (30) differ from the wave vector $\mathbf{k}^\parallel$ of the incident wave by the vectors of the reciprocal lattice $\mathbf{b}_1$, $\mathbf{b}_2$. In the transmitted field the incident wave $f \exp(i\mathbf{kr})$ does not appear; it is extinguished due to the first condition in (16) by the transmitted waves. This is an analogy to the Ewald extinction theorem inside the crystal.

The term $\exp(i\theta_{pq}^-) = \exp[i(\mathbf{a}_3^\parallel \mathbf{k}_{pq}^\parallel - a_{3z}K_{pqz})]$ in (29) is not included in the reflection coefficient $R_r(\theta_{pq}^-)$, by analogy with the study of X-ray reflection on a simple cubic lattice with lattice constant a (Litzman & Rózsa 1983). In that case the formulae for the reflection and transmission of a slab must coincide with classical Fresnel formulae for large wavelengths. To achieve this coincidence, it is necessary to suppose that the reflection occurs not on the 'geometrical' crystal surface $z = 0$, but on a 'physical boundary' shifted by one lattice constant over the first atomic plane of the crystal. [See below discussion of equation (59).] This may be related to the fact that Ewald (1916, p. 125) found two representations for the fields around the outermost layer.

3. Coefficients of reflection and transmission

Having obtained formulae (29)–(32) for the reflected and transmitted waves, we have essentially solved our problem. But we shall try to bring our results into more suitable algebraic form. To this end let us introduce the following notation:

$$(\exp i\theta_{00}^+, \ldots, \exp i\theta_{pq}^+, \ldots) = (y_1^+, \ldots, y_r^+, \ldots),$$
$$(\exp i\theta_{00}^-, \ldots, \exp i\theta_{pq}^-, \ldots) = (y_1^-, \ldots, y_r^-, \ldots), \quad (33a)$$

$$x_j = \exp(i\psi_j), \quad j = 1, 2, \ldots, 2n, \quad (33b)$$

$$\sum_{\nu=1}^{s} Q_\mu \exp[-i\mathbf{r}_\nu(p\mathbf{b}_1 + q\mathbf{b}_2 + \mathbf{e}_3 K_{pqz})] u_\nu(\psi_j) = \alpha_{pq}^+(j) \equiv \alpha_r^+(j)$$
$$\sum_{\nu=1}^{s} Q_\nu \exp[-i\mathbf{r}_\nu(p\mathbf{b}_1 + q\mathbf{b}_2 - \mathbf{e}_3 K_{pqz})] u_\nu(\psi_j) = \alpha_{pq}^-(j) \equiv \alpha_r^-(j). \quad (34)$$

A fundamental role will be played by the matrix $\mathbf{H}$:

$$\mathbf{H} = \left\| \begin{matrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{matrix} \right\| = \left\| \frac{h_{ij}}{x_j - y_i} \right\|$$

$$H_{11} = \left\| \frac{\alpha_i^+(j)}{x_j - y_i^+} \right\|, \quad i = 1, 2, \ldots, n; j = 1, 2, \ldots, n$$
$$H_{12} = \left\| \frac{\alpha_i^+(j)}{x_j - y_i^+} \right\|, \quad i = 1, 2, \ldots, n; j = n+1, \ldots, 2n$$
$$H_{21} = \left\| \frac{\alpha_i^-(j)}{x_j - y_i^-} \right\| \langle x_1^{N+1}, x_2^{N+1}, \ldots, x_n^{N+1} \rangle, \; i = 1, 2, \ldots, n \quad j = 1, 2, \ldots, n \quad (35)$$
$$H_{22} = \left\| \frac{\alpha_i^-(j)}{x_j - y_i^-} \right\| \langle x_{n+1}^{N+1}, x_{n+2}^{N+1}, \ldots, x_{2n}^{N+1} \rangle, \; i = 1, 2, \ldots, n \quad j = n+1, \ldots, 2n.$$

In (35) the index 1 in $\alpha_1^\mp$, $y_1^\mp$ always corresponds to $\alpha_{00}^\mp$, $y_{00}^\mp = \exp(i\theta_{00}^\mp)$ and $\langle \ldots \rangle$ again denotes a diagonal matrix. Further, introducing column vectors $\mathbf{c}$, $\mathbf{f}$ of order $2n$,

$$\mathbf{c} = \|c_1, c_2, \ldots, c_{2n}\|^T,$$
$$\mathbf{f} = \|-fk_z \exp(-i\mathbf{k}\mathbf{a}_3), 0, 0, \ldots, 0\|^T, \quad (36)$$

we can write (26) as

$$\mathbf{H}c = f, \quad \text{i.e. } c = \mathbf{H}^{-1}f = (1/\det \mathbf{H}) \operatorname{adj} \mathbf{H}f. \tag{37}$$

Using this notation we get from (31)

$$R_r(\theta_{pq}^-) = \left\| \frac{\alpha_{pq}^-(1)}{x_1 - y_{pq}^-}, \frac{\alpha_{pq}^-(2)}{x_2 - y_{pq}^-}, \ldots, \frac{\alpha_{pq}^-(2n)}{x_{2n} - y_{pq}^-} \right\| c$$
$$= -fk_z \exp(-i\mathbf{k}\mathbf{a}_3) \det \mathbf{M}^-(pq)/\det \mathbf{H} \tag{38}$$

and similarly from (32)

$$R_t(\theta_{pq}^+) = -fk_z \exp(-i\mathbf{k}\mathbf{a}_3) \det \mathbf{M}^+(pq)/\det \mathbf{H}. \tag{39}$$

The matrices $\mathbf{M}^-(pq)$ and $\mathbf{M}^+(pq)$ in (38) and (39) differ from the matrix $\mathbf{H}$ (35) in the first row only. Their first rows read

$$\|M^-(pq)_{1,j}\| = \left\| \frac{\alpha_{pq}^-(1)}{x_1 - y_{pq}^-}, \frac{\alpha_{pq}^-(2)}{x_2 - y_{pq}^-}, \ldots, \frac{\alpha_{pq}^-(2n)}{x_{2n} - y_{pq}^-} \right\| \tag{40}$$

$$\|M^+(pq)_{1,j}\| = \left\| \frac{x_1^{N+1}\alpha_{pq}^+(1)}{x_1 - y_{pq}^+}, \frac{x_2^{N+1}\alpha_{pq}^+(2)}{x_2 - y_{pq}^+}, \ldots, \frac{x_{2n}^{N+1}\alpha_{pq}^+(2n)}{x_{2n} - y_{pq}^+} \right\|. \tag{41}$$

Otherwise

$$M^+(pq)_{ij} = M^-(pq)_{ij} = H_{ij}, \quad \begin{matrix} i = 2, 3, \ldots, 2n \\ j = 1, 2, \ldots, 2n \end{matrix}. \tag{42}$$

The numerical evaluation of the determinants of the matrices $\|a_{ij}(x_j - y_i)^{-1})\|$ appearing in (38) and (39) make difficult those solutions $x_j = \exp(i\psi_j)$ which are close to the poles $y_j = \exp(i\theta_j^\pm)$ for which the terms $(x_j - y_i^\pm)^{-1}$ diverge. To get rid of this difficulty we shall change the determinants in (38) and (39) to another algebraic form in which these divergences in numerator and denominator cancel one another. To this end we shall introduce the Lagrange polynomials $L_i(y)$, $i = 1, 2, \ldots, 2n$, on supporting points (33a)

$$y_1 = y_1^+ = \exp(i\theta_{00}^+), \qquad y_2 = y_2^+, \ldots, y_n = y_n^+,$$
$$y_{n+1} = y_1^- = \exp(i\theta_{00}^-), \qquad y_{n+2} = y_2^-, \ldots, y_{2n} = y_n^- \tag{43}$$

in the usual way:

$$\omega(y) = (y - y_1)(y - y_2)\ldots(y - y_{2n}),$$
$$L_i(y) = \omega(y)/(y - y_i)\omega'(y_i); \qquad L_i(y_j) = \delta_{ij}. \tag{44}$$

Thus

$$1/(x_j - y_i) = [L_i(x_j)/\omega(x_j)]\, \omega'(y_i) \tag{45}$$

and we can write

$$\det \left\| \frac{a_{ij}}{x_j - y_i} \right\| = \frac{\omega'(y_1)\omega'(y_2)\ldots\omega'(y_{2n})}{\omega(x_1)\omega(x_2)\ldots\omega(x_{2n})} \times \det \|a_{ij}L_i(x_j)\|. \tag{46}$$

Further let us write the matrices $\mathbf{M}^+(pq)$ and $\mathbf{M}^-(pq)$[(40), (41)] in a form which is more similar to that of $\mathbf{H}$ (35):

$$\mathbf{M}^+(pq) = \left\| \frac{m^+(pq)_{ij}}{x_j - y_i} \right\| \qquad \mathbf{M}^-(pq) = \left\| \frac{m^-(pq)_{ij}}{x_j - y_i} \right\| \tag{47}$$

with

$$m^+(pq)_{1j} = \frac{x_j^{N+1}\alpha_{pq}^+(j)}{x_j - y_{pq}^+}(x_j - y_1^+), \qquad j = 1, 2, \ldots, 2n$$
$$m^-(pq)_{1j} = \frac{\alpha_{pq}^-(j)}{x_j - y_{pq}^-}(x_j - y_1^+) \tag{48}$$
$$m^+(pq)_{ij} = m^-(pq)_{ij} = h_{ij} \quad \text{for } i = 2, 3, \ldots 2n;$$
$$j = 1, 2, \ldots 2n.$$

Then we can write (38) and (39) as

$$R_r(\theta_{pq}^-) = -fk_z \exp(-i\mathbf{k}\mathbf{a}_3) \frac{\det\|m^-(pq)_{ij}L_i(x_j)\|}{\det\|h_{ij}L_i(x_j)\|} \qquad i, j = 1, 2, \ldots, 2n \tag{49}$$

$$R_t(\theta_{pq}^+) = -fk_z \exp(-i\mathbf{k}\mathbf{a}_3) \frac{\det\|m^+(pq)_{ij}L_i(x_j)\|}{\det\|h_{ij}L_i(x_j)\|} \qquad i, j = 1, 2, \ldots, 2n. \tag{50}$$

As the Lagrange polynomials are regular, singularities in quotients (49), (50) can appear in the terms $m^+(pq)_{1j}$, $m^-(pq)_{1j}$ only. Moreover, these formulae give some view of the influence of the different solutions ψ_j of the dispersion equation (18) on R_r and R_t. Let us consider first the reflectivity of a semi-infinite crystal. As $N \to \infty$, $j = n+1, \ldots, 2n$, $x_j^{N+1} \to \infty$, we get for the reflectivity of a semi-infinite crystal

$$R_r^\infty(\theta_{pq}^-) = -fk_z \exp(-i\mathbf{k}\mathbf{a}_3) \frac{\det\|m^-(pq)_{ij}L_i(x_j)\|}{\det\|h_{ij}L_i(x_j)\|} \qquad i, j = 1, 2, \ldots, n. \tag{51}$$

Now let us suppose that for some solutions x_j (33b) of the dispersion equation (18)

$$x_j \doteq y_j \quad \text{for } j = s, s+1, \ldots, n, \quad s > 1$$

holds. Then, following (44),

$$L_i(x_j) \doteq \delta_{ij} \quad \text{for } j = s, s+1, \ldots, n.$$

Thus

$$\det\|h_{ij}L_i(x_j)\|_{i,j=1,2,\ldots,n}$$
$$= \det\|h_{ij}L_i(x_j)\|_{i,j=1,2,\ldots s-1} \times \prod_{j=s}^{n} h_{jj} \tag{52}$$

and a similar relation holds for $\det\|m^-(pq)_{ij}L_i(x_j)\|$.

Because of (48) the terms

$$\prod_{j=s}^{n} h_{jj} = \prod_{j=s}^{n} m^-(pq)_{jj}$$

cancel one another in $R_r^\infty(\theta_{pq}^-)$ (51). We can see that those beams for which $\psi_j \doteq \theta_j^+$ have only a small influence on R_r^∞. A similar consideration can be applied to (49), (50).

Generally we can say that those solutions ψ_j of the dispersion equation (18) which are near the poles have only a small influence on the reflectivity and transmittivity of the slab.

4. Semi-infinite crystal

Formulae (49) and (50) express the reflection and transmission coefficients R_r, R_t of the slab by the solutions ψ_j and $\mathbf{u}(\psi_j)$ of equations (18) and (20). To get an idea of the properties of our formulae let us consider the case of a simple lattice, *i.e.* $s=1$. Using (19), (15), (16) and (5), (18) reads

$$\begin{aligned}\frac{2\pi}{|\mathbf{a}_1\times\mathbf{a}_2|}\sum_{pq}^{(n)}\Bigg[&\frac{1}{K_{pqz}}\frac{\sin(a_{3z}K_{pqz})}{\cos(\psi-\mathbf{a}_3^{\parallel}\mathbf{k}_{pq}^{\parallel})-\cos(a_{3z}K_{pqz})}\\&-\frac{1}{K_{pqz}}\Phi\left(\frac{iK_{pqz}}{2B}\right)\Bigg]\\&+ik\Phi(ik/2B)+(2/\sqrt{\pi})B\exp(k^2/4B^2)\\&-\sum_{n_1n_2\neq(00)}{}'\Bigg(\frac{\exp[i\mathbf{k}^{\parallel}(n_1\mathbf{a}_1+n_2\mathbf{a}_2)]}{2|n_1\mathbf{a}_1+n_2\mathbf{a}_2|}\\&\times\{\exp(-ik|n_1\mathbf{a}_1+n_2\mathbf{a}_2|)\\&\times[1-\Phi(|n_1\mathbf{a}_1+n_2\mathbf{a}_2|B-ik/2B)]+\text{c.c.}\}\Bigg)\\&=1/Q_0.\end{aligned}\tag{53}$$

The function on the left-hand side of (53) is real (for real ψ) for all (pq) and has poles for

$$\psi=\mathbf{a}_3^{\parallel}\mathbf{k}_{pq}^{\parallel}\pm a_{3z}K_{pqz}+j2\pi=\theta_{pq}^{\pm}+j2\pi.\tag{54}$$

If the interaction of the incident particles with the scatterers is small, *i.e.* $|\mathbf{a}_1\times\mathbf{a}_2|\gg|Q_0|^2$, then the solutions of (53) should be near the poles (54).

The coefficient $\alpha_{pq}^{\mp}(j)$ in the matrices $\mathbf{H}$, $\mathbf{M}^{\mp}(pq)$ [(35), (40), (41)] can be put equal to 1 for $s=1$. Employing a useful formula for the evaluation of $\det\|(x_j-y_i)^{-1}\|$, we can handle (38) and (39) without introducing Lagrange polynomials into them. For the reflectivity of a semi-infinite crystal we can write in this case (Litzman & Rózsa, 1980; Avron, Grossman & Høegh-Krohn, 1983)

$$\begin{aligned}R_r^\infty(\theta_{pq}^-)=-fk_z\exp(-i\mathbf{k}\mathbf{a}_3)&\frac{\exp(i\psi_1)-\exp(i\theta_{00}^+)}{\exp(i\psi_1)-\exp(i\theta_{pq}^-)}\\&\times\prod_{j=2}^{(n)}\frac{\exp(i\psi_j)-\exp(i\theta_{00}^+)}{\exp(i\psi_j)-\exp(i\theta_{pq}^-)}\\&\times\frac{\exp(i\theta_j^+)-\exp(i\theta_{pq}^-)}{\exp(i\theta_j^+)-\exp(i\theta_{00}^+)}.\end{aligned}\tag{55}$$

Let us emphasize that (55) is exact: no supposition has been made about the magnitude of the interaction between the incident particles and the crystal, the proximity to the Bragg reflection angle or the number of diffracted waves. From (55) it is evident that those beams for which $\psi_j\to\theta_j^+$ have only a small influence on $R^\infty(\theta_{pq}^-)$, as mentioned at the end of § 3.

A more detailed analysis of formula (55) for the soft X-ray region, leading to 'generalized' Fresnel formulae, has been performed by Litzman & Rózsa (1983).

Let us consider now the Bragg reflection (24), *i.e.* we suppose

$$\theta_{00}^+=\theta_{rs}^-+j2\pi+\varepsilon,\qquad|\varepsilon|\ll1.\tag{56}$$

In this case we shall write the dispersion equation (18) as

$$\begin{aligned}1+QS'(\mathbf{k}^{\parallel})-b_{00}&\frac{\exp(i\theta_{00}^+)}{\exp(i\psi)-\exp(i\theta_{00}^+)}\\-b_{rs}&\frac{\exp(-i\theta_{rs}^-)}{\exp(-i\psi)-\exp(-i\theta_{rs}^-)}\\-\sum_{pq}{}'b_{pq}&\Bigg[\frac{\exp(i\theta_{pq}^+)}{\exp(i\psi)-\exp(i\theta_{pq}^+)}\\&+\frac{\exp(-i\theta_{pq}^-)}{\exp(-i\psi)-\exp(-i\theta_{pq}^-)}\Bigg]=0.\end{aligned}\tag{57}$$

Multiplying (57) by

$$[\exp(i\psi)-\exp(i\theta_{00}^+)][\exp(-i\psi)-\exp(-i\theta_{rs}^-)]$$

we find

$$\left.\begin{aligned}&\exp(i\psi_1)\to\exp(i\theta_{00}^+)\\&\frac{\exp(i\psi_1)-\exp(i\theta_{00}^+)}{\exp(i\psi_1)-\exp(i\theta_{rs}^-)}\to\frac{b_{00}}{b_{rs}}=\frac{K_{rsz}}{K_{00z}}\end{aligned}\right\}\quad\text{if }\varepsilon\to0.$$

Thus, following (55)

$$\left.\begin{aligned}&\lim R_r^\infty(\theta_{rs}^-)=-fK_{rsz}\exp(-i\mathbf{k}\mathbf{a}_3)\\&\lim R_r^\infty(\theta_{pq}^-)=0\quad\text{for }(pq)\neq(rs)\end{aligned}\right\}\quad\text{if }\varepsilon\to0\tag{58}$$

whereby we have supposed that the Bragg condition is satisfied for one pair, (00), (rs), only.

Inserting (58) into (29) we find

$$\begin{aligned}\Psi(r)=f\exp(i\mathbf{k}\mathbf{r})&-f\exp(-i\mathbf{k}\mathbf{a}_3)\\&\times\exp[i\mathbf{k}_{rs}^{\parallel}(\mathbf{r}^{\parallel}+\mathbf{a}_3^{\parallel})-iK_{rsz}(z+a_{3z})]\end{aligned}\tag{59}$$

if

$$\theta_{00}^+=\theta_{rs}^-+j2\pi.$$

The last equation proves that total reflection occurs if the Bragg condition is satisfied. In the standard dynamical theory of Ewald or von Laue total reflection is proved by the analysis of the dispersion equation in the two-beam approximation and by supposing that the interaction between the incident particles and the crystal is small (*i.e.* the refractive index is very near to 1). Our results (58) and (59) based on n-beam strong interaction formulae [(55), (57)] are more general. In Laue's theory total reflection does not occur exactly for the classical Bragg reflection angle but is shifted proportionally to the mean polarizability of the crystal. In our case this shift is zero because the scatterers are in vacuum. To get the intensity of the reflected wave in the neighbourhood of the Bragg angle ('rocking curve') a numerical analysis of (55) would be necessary.

As has been pointed out by James (1963) there is a problem of how to introduce in Laue's dynamical theory the boundary conditions 'when the electromagnetic waves concerned have lengths comparable with the interatomic distances. In this respect Ewald's method is logically superior.' By this is meant that in Ewald's theory no boundary conditions are needed. The solution (59) gives a partial answer to James's note. The second term on the right-hand side of (59) shows that the reflection of the incident wave does not occur on the 'geometrical crystal surface' $z=0$ but on a 'physical boundary' shifted by $-\mathbf{a}_3$ over the first plane of scatterers. Let us mention that Ewald's method can also be used to obtain a better understanding of so-called additional boundary conditions for dielectrics with spatial dispersion (Litzman, 1981).

Let us consider briefly the more general case of a lattice with basis, *i.e.* $s\geq 2$. In this case $\mathbf{B}_{pq}$ and $\mathbf{D}_{pq}$ in (19) and (21) are dyads, *i.e.* matrices of order s but of rank one. Thus, using standard rules of determinant theory, the dispersion equation (18) can again be written in a form

$$\sum_{pq}\left[a^-_{pq}\frac{\exp(-i\theta^-_{pq})}{\exp(-i\psi)-\exp(-i\theta^-_{pq})}+a^+_{pq}\frac{\exp(i\theta^+_{pq})}{\exp(i\psi)-\exp(i\theta^+_{pq})}\right]=b. \qquad (60)$$

As in (57), (60) is an algebraic equation of order $2n$ for $\exp(i\psi)$ and (54) are poles. But the coefficients a^+_{pq}, a^-_{pq} depend now on θ^+_{rs}, θ^-_{rs} and can diverge for $\varepsilon\to 0$. This circumstance makes the general analysis of (60) difficult.

In the study of the diffraction of electromagnetic waves, the matrices $\mathbf{B}_{pq}$ and $\mathbf{D}_{pq}$ are no longer dyads, which complicates formally the scattering problem.

5. Summary

Ewald's self-consistent field method (Ewald, 1916, 1917) in quantum-mechanical formulation is used for the study of diffraction of particles on a system of point scatterers fixed on lattice points of a periodic crystal slab with s basis atoms. The problem is of course trivial if the slab consists of one layer only. Then we can put in (10) $w_\mu=1$. Difficulties arise in satisfying the boundary conditions if the slab contains more layers.

The use of matrix algebra enables us to express the coefficients of reflection R_r and transmission R_t in well arranged algebraic forms (49) and (50) in terms of Lagrange polynomials $L(x)$. To use these formulae it is necessary to solve an algebraic equation (18), which in the n-beam approximation is of order $2n$. This order is independent of the number $N+1$ of layers and of the number s of atoms in the elementary cell of the crystal. The solution of (18) is facilitated by the occurrence of the poles (54) in the matrix $\mathbf{A}$ (19). Further, solution of the algebraic system (20) of order s is needed.

To derive formulae (49) and (50), no supposition is made concerning the magnitude of interaction between the particles and the crystal, the number n of diffracted beams or the proximity to the Bragg diffraction angle. To get an idea about the general solution the diffraction on a semi-infinite crystal for $s=1$ is discussed in more detail. The expression for the reflection coefficient has in this case a very simple form, (55), in which the parameters $\exp(i\theta_{pq})$ are known and $\exp(i\psi_j)$ are solutions of the dispersion equation (57). (55) gives the reflection coefficients for all wavelengths at any angle of incidence. If our theory is applied to a system of oscillating dipoles it is possible to deduce from (55) a correction to the classical Fresnel formulae in the soft X-ray region (Litzman & Rózsa, 1983). Dielectrics with spatial dispersion can be handled in a similar way (Litzman, 1978, 1980, 1981).

APPENDIX

1. Lattice sums

To deduce some formulae in our paper we have to evaluate two-dimensional lattice sums of two kinds:

$$S(\mathbf{k}^{\parallel},\mathbf{R}^{\parallel},\mathbf{u})=\sum_{n_1n_2}\left\{\frac{\exp(ik|n_1\mathbf{a}_1+n_2\mathbf{a}_2-\mathbf{R}^{\parallel}+\mathbf{u}|)}{|n_1\mathbf{a}_1+n_2\mathbf{a}_2-\mathbf{R}^{\parallel}+\mathbf{u}|}\times\exp[i\mathbf{k}^{\parallel}(n_1\mathbf{a}_1+n_2\mathbf{a}_2-\mathbf{R}^{\parallel})]\right\} \qquad (A.1)$$

$$S'(\mathbf{k}^{\parallel})=\sum_{(n_1n_2)\neq(00)}{}'\left\{\frac{\exp(ik|n_1\mathbf{a}_1+n_2\mathbf{a}_2|)}{|n_1\mathbf{a}_1+n_2\mathbf{a}_2|}\times\exp[i\mathbf{k}^{\parallel}(n_1\mathbf{a}_1+n_2\mathbf{a}_2)]\right\}. \qquad (A.2)$$

The main difference between (A.1) and (A.2) is that in (A.2) the origin (0, 0) is excluded from the summation. Both sums converge slowly. But because (A.1) is a periodic function of $\mathbf{R}^{\parallel}(x,y)$, it can be transformed into a sum over the reciprocal lattice which, as we shall see, converges rapidly. By standard Fourier procedure we write

$$S(\mathbf{k}^{\parallel},\mathbf{R}^{\parallel},\mathbf{u})=\sum_{m_1m_2}f(m_1m_2)\exp[i(m_1\mathbf{b}_1+m_2\mathbf{b}_2)\mathbf{R}^{\parallel}]$$

where

$$f(m_1m_2)=\frac{1}{|\mathbf{a}_1\times\mathbf{a}_2|}\iint\limits_{(a_1a_2)} S(\mathbf{k}^{\|},\mathbf{R}^{\|},\mathbf{u})\times\exp[-i(m_1\mathbf{b}_1+m_2\mathbf{b}_2)\mathbf{R}^{\|}]\,d\mathbf{R}^{\|}$$

$$=\frac{1}{|\mathbf{a}_1\times\mathbf{a}_2|}\int_{-\infty}^{\infty}\int\frac{\exp(ik|\mathbf{R}^{\|}-\mathbf{u}|)}{|\mathbf{R}^{\|}-\mathbf{u}|}\times\exp[-i(\mathbf{k}^{\|}+m_1\mathbf{b}_1+m_2\mathbf{b}_2)\mathbf{R}^{\|}]\,d\mathbf{R}^{\|}$$

$$=\frac{1}{|\mathbf{a}_1\times\mathbf{a}_2|}\exp(-i\mathbf{u}^{\|}\mathbf{k}^{\|}_{m_1m_2})\times\int_{-\infty}^{\infty}\int\frac{\exp[ik(x^2+y^2+u_z^2)^{1/2}]}{(x^2+y^2+u_z^2)^{1/2}}\times\exp(-i\mathbf{R}^{\|}\mathbf{k}^{\|}_{m_1m_2})\,dx\,dy$$

$$=\frac{1}{|\mathbf{a}_1\times\mathbf{a}_2|}2\pi i\exp(-i\mathbf{u}^{\|}\mathbf{k}^{\|}_{m_1m_2})\times\frac{\exp(i|u_z|K_{m_1m_2z})}{K_{m_1m_2z}}.$$

We get finally

$$S(\mathbf{k}^{\|},\mathbf{R}^{\|},\mathbf{u})=\frac{2\pi i}{|\mathbf{a}_1\times\mathbf{a}_2|}\sum_{m_1m_2}\exp(-i\mathbf{u}^{\|}\mathbf{k}^{\|}_{m_1m_2})\times\frac{\exp(i|u_z|K_{m_1m_2z})}{K_{m_1m_2z}}\exp[i(m_1\mathbf{b}_1+m_2\mathbf{b}_2)\mathbf{R}^{\|}].$$

The meaning of $\mathbf{k}^{\|}_{m_1m_2}$ and $K_{m_1m_2z}$ is explained in formula (17) of the main text.

The transformation of the sum (A.2) into a rapidly convergent one is much more difficult. Ewald (1932) studied a three-dimensional lattice sum of the type (A.2) and his procedure can be applied to the two-dimensional one as well (Dub & Litzman, 1983). We thus get (16) which is in agreement with the more general result given by Pendry (1974).

2. Formula (11)

Introducing (10) into (8) we get the following system of algebraic equations for $w_\nu^{n_3}$:

$$w_\mu^{m_3}=f\exp[i\mathbf{k}(m_3\mathbf{a}_3+\mathbf{r}_\mu^{\perp})]-\sum_{(\mathbf{n}\nu)\neq(\mathbf{m}\mu)}{}' Q_\nu\frac{\exp(ik|\mathbf{R}_\mu^{\mathbf{m}}-\mathbf{R}_\nu^{\mathbf{n}}|)}{|\mathbf{R}_\mu^{\mathbf{m}}-\mathbf{R}_\nu^{\mathbf{n}}|}\times\exp(i\mathbf{k}^{\|}[(n_1-m_1)\mathbf{a}_1+(n_2-m_2)\mathbf{a}_2+\mathbf{r}_\nu-\mathbf{r}_\mu])w_\nu^{n_3}. \quad (A.3)$$

Using (A.1) and (A.2) for the two-dimensional sums over (n_1n_2) on the right-hand side of (A.3), we get, quite similarly to Litzman (1978, 1980), equation (11) of the main text.

3. Formula (53)

For $s=1$ dispersion equation (18) reads

$$1+QS'(\mathbf{k}^{\|})-\sum_{pq}^{(n)}b_{pq}\left[\frac{\exp(-i\theta_{pq}^{-})}{\exp(-i\psi)-\exp(-i\theta_{pq}^{-})}+\frac{\exp(i\theta_{pq}^{+})}{\exp(i\psi)-\exp(i\theta_{pq}^{+})}\right]=0$$

with

$$b_{pq}=-\frac{2\pi iQ}{|\mathbf{a}_1\times\mathbf{a}_2|K_{pqz}} \quad (13)$$

$$ik=(1/Q)-(1/Q_0). \quad (5)$$

Using equation (16) for $S'(\mathbf{k}^{\|})$, we get after some easy algebra formula (53) of the main text.

References

AVRON, J. E., GROSSMAN, A. & HØEGH-KROHN, R. (1983). *Phys. Lett. A*, **94**, 42–44.

DEDERICHS, P. H. (1972). *Dynamical Diffraction Theory by Optical Potential Method. Solid State Physics*, Vol. 27, edited by H. EHRENREICH, F. SEITZ & D. TURNBULL, pp. 135–236. New York: Academic Press.

DEMKOV, JU. N. & OSTROVSKIJ, V. N. (1975). *Metod Potencialov Nulevogo Radiusa v Atomnoj Fizike.* Leningrad: Izd. Leningradskogo Universiteta.

DUB, P. & LITZMAN, O. (1983) *Scr. Fac. Sci. Nat. Univ. Purkynianae Brun.* Vol. **13**, No 6-7 (*Physica*), pp. 283–290.

EWALD, P. P. (1916). *Ann. Phys. (Leipzig)*, **49**, 1–38, 117–143.

EWALD, P. P. (1917). *Ann. Phys. (Leipzig)*, **54**, 519–597.

EWALD, P. P. (1932). *Ann. Inst. H. Poincaré*, Tom. VIII, Fasc. II, pp. 79–110.

HENKE, B. L., LEE, P., TANAKA, T. J., SHIMABUKURO, R. L. & FUJIKAWA, B. K. (1982). *At. Data Nucl. Data Tables*, **27**, 1–144.

JAMES, R. W. (1963). *The Dynamical Theory of X-ray Diffraction. Solid State Physics*, Vol. 15, edited by F. SEITZ & D. TURNBULL, p. 61. New York: Academic Press.

LAX, M. (1951). *Rev. Mod. Phys.* **23**, 287–310.

LITZMAN, O. (1978). *Optica Acta*, **25**, 509–526.

LITZMAN, O. (1980). *Optica Acta*, **27**, 231–240.

LITZMAN, O. (1981) *Phys. Status Solidi B*, **104**, K109–K111.

LITZMAN, O. & RÓZSA, P. (1980). *Czech. J. Phys. B*, **30**, 816–826.

LITZMAN, O. & RÓZSA, P. (1983). *Czech. J. Phys. B*, **33**, 1303–1314.

LITZMAN, O. & ŠEBELOVÁ, I. (1985). *Optica Acta*, **32**, 839–844.

MCRAE, E. G. (1966). *J. Chem. Phys.* **45**, 3258–3276.

OHTAKA, K. (1980). *J. Phys. C*, **13**, 667–680.

PENDRY, J. B. (1974). *Low Energy Electron Diffraction*, p. 137. London: Academic Press.