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The Darwin procedure in optics of layered media and the matrix theory

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Abstract

The Darwin dynamical theory of diffraction for two beams yields a nonhomogeneous system of linear algebraic equations with a tridiagonal matrix. It is shown that different formulae of the two-beam Darwin theory can be obtained by a uniform view of the basic properties of tridiagonal matrices, their determinants (continuants) and their close relationship to continued fractions and difference equations. Some remarks concerning the relation of the Darwin theory in the three-beam case to tridiagonal block matrices are also presented.

1. Introduction

The standard problem of optics of layered media may be described as follows: a stack of layers is irradiated by an external wave; each layer is characterized by its one-dimensional scattering-length density (SLD); the reflectivity and transmissivity of the whole stack have to be computed. If the SLD of each layer is constant, the problem can be easily solved using the standard formulae for the propagation of a plane wave in a layer with a constant refraction index, and Fresnel formulae for the reflection and transmission of plane waves on the boundaries between two homogeneous layers. Sophisticated methods that simplify the algebraic manipulations when dealing with the problem can be found, for example, in the book by Knittl (1976). However, the described procedures cannot be used if the SLDs of the layers are not constant or the standard Fresnel formulae relating to the boundaries do not hold [*e.g.* for thermal neutrons or X-rays in crystals (Pinsker, 1978; Rauch & Petraschek, 1978; Sears, 1989)].

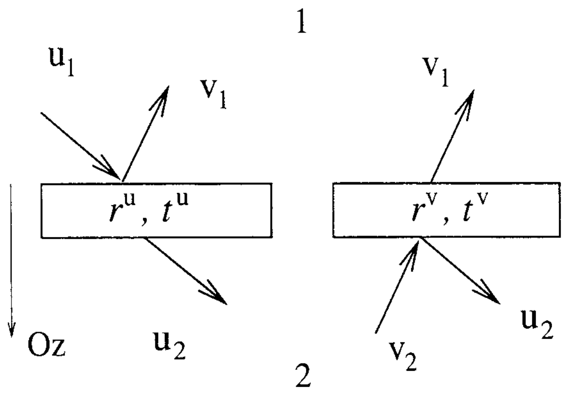
Recently, to cover such more difficult problems, the classical Darwin method (Darwin, 1914) has been generalized by many authors (Caticha, 1994; Ignatovich, 1989, 1991, 1992; Nakatani & Takahashi, 1994; Takahashi & Nakatani, 1995). In contrast to the methods developed in the above citations, we will pay attention to the fact that the two-beam Darwin theory yields a nonhomogeneous system of algebraic equations with a *tridiagonal* matrix (§3). Thus, some properties of continuants (see Appendix *A*) can be widely utilized when looking for the solution to Darwin equations.

2. The two-beam Darwin equations

First, let us consider a layer in vacuum. Whatever is its SLD, the layer can be optically characterized by its positively (u) and negatively (v) oriented coefficients of reflection (r^u, r^v) and transmission (t^u, t^v). (Positive incidence is taken to be in the direction in which the z axis increases.) Denoting the space above and below the layer by 1 or 2, respectively, for the amplitudes of the wave fields u_j and u_j, $j = 1, 2$, we have

$$\begin{aligned} u_2 &= t^u u_1, \quad v_1 = r^u u_1; \\ u_2 &= r^v v_2, \quad v_1 = t^v v_2; \end{aligned} \tag{1}$$

see Figs. 1(a) and 1(b), respectively. The coefficients r^u, r^v, t^u and t^v depend on many parameters (*e.g.* the atomic and structure factors of the layer, the surface quality, the wavelength, the angle of incidence) and can be obtained



(a) (b)

Fig. 1. The definitions of the positively (a) and negatively (b) oriented coefficients of reflection and transmission. The amplitudes of the wave fields u_j and v_j ($j = 1, 2$) are given just on the borders of the layers.

by classical optics methods in the optical region or using the dynamical theory of diffraction in the X-ray or thermal-neutron regions.

Next, let us consider a stack of N layers, each layer being characterized by the coefficients of reflection r_n^u, r_n^v and transmission t_n^u, t_n^v $(n = 1, 2, \ldots, N)$ separated by $N-1$ vacuum splits of the same width $\delta > 0$ (Fig. 2). The stack is irradiated by the external positively oriented wave $u_1 = u^{\rm inc}$. Let the wave field in the vacuum split between the $(n-1)$th and nth layers be described by one negatively oriented plane wave (v_n) and one positively oriented plane wave (u_n) only (the two-beam Darwin theory). Then the wave field in the stack is given by the equations

$$\begin{aligned}
u_1 &= u^{\rm inc},\\
v_1 &= r_1^u u_1 + t_1^v v_2 \exp(i\psi),\\
u_2 &= t_1^u u_1 + r_1^v v_2 \exp(i\psi),\\
u_n &= t_{n-1}^u u_{n-1} \exp(i\varphi) + r_{n-1}^v v_n \exp(i\psi)\\
&\qquad \text{for } n = 3, 4, \ldots, N,\\
v_n &= r_n^u u_n \exp(i\varphi) + t_n^v v_{n+1} \exp(i\psi)\\
&\qquad \text{for } n = 2, 3, \ldots, N-1,\\
v_N &= r_N^u u_N \exp(i\varphi),\\
u_{N+1} &= t_N^u u_N \exp(i\varphi),
\end{aligned} \tag{2}$$

with $\varphi = (2\pi/\lambda_o)\delta\cos\gamma_u$ and $\psi = -(2\pi/\lambda_o)\delta\cos\gamma_v$. λ_o is the wavelength of the radiation in vacuum, γ_u and γ_v are the angles (with the axis Oz) of the wave vectors $\mathbf{k}_u$ and $\mathbf{k}_v$ of the waves u_n and v_n, respectively.

The system of equations (2) represents a nonhomogeneous system of $2N$ linear algebraic equations for the $2N$ amplitudes $(v_1, v_2, \ldots, v_N)$ and $(u_2, u_3, \ldots, u_{N+1})$, the amplitude u_1 of the incident wave being given. Primarily, we are interested in the waves reflected (v_1) and transmitted (u_{N+1}) by the whole stack.

Note that for $\gamma_v = \pi - \gamma_u$ (symmetrical reflection) and $\delta \neq 0$ we have the original Darwin model of reflection of radiation by the atomic planes of an ideal crystal. On the other hand, putting $\delta = 0$ we have a multilayered optical system.

The system of equations (2) can be solved by different methods, leading obviously to the same results. In the most common procedure the relations

$$\begin{aligned}
\begin{pmatrix} u_n \\ v_n \end{pmatrix} &= \mathbf{A}_n \begin{pmatrix} u_{n+1} \\ v_{n+1} \end{pmatrix},\\
\begin{pmatrix} u_1 \\ v_1 \end{pmatrix} &= \mathbf{A}_1\mathbf{A}_2\ldots\mathbf{A}_N \begin{pmatrix} u_{N+1} \\ v_{N+1} \end{pmatrix},
\end{aligned} \tag{3}$$

with the boundary conditions $u_1 = u^{\rm inc}$ and $v_{N+1} = 0$, are derived from (2). Thus, the evaluation of v_1 and u_{N+1} is reduced to multiplying second-order matrices. Special attention is paid to the periodic structures where $\mathbf{A}_i = \mathbf{A}$ $\quad (i = 1, 2, \ldots, N)$. Then the evaluation of the second-order matrix $\mathbf{A}^N$ can be performed very easily using the Cayley–Hamilton theorem (Abelès, 1950; Perkins & Knight, 1984; Yeh, 1988). Another method uses the fact that, in a periodic structure, equations (2) can be considered as a system of two difference equations with boundary conditions $u_1 = u^{\rm inc}$ and $v_{N+1} = 0$. This system of difference equations can be solved by the usual ansatz $u_n = u\exp(in\alpha)$ and $v_n = v\exp(in\alpha)$, which leads to the evaluation of the eigenvectors and eigenvalues of a second-order matrix (Caticha, 1994).

In the next section (§3), we show that, when looking for the solution to Darwin's equations (2), advantage can be taken of some well known properties of the tridiagonal matrices.

3. The two-beam Darwin equations and continuants

The system of the two-beam Darwin equations (2) can be written in a matrix form as

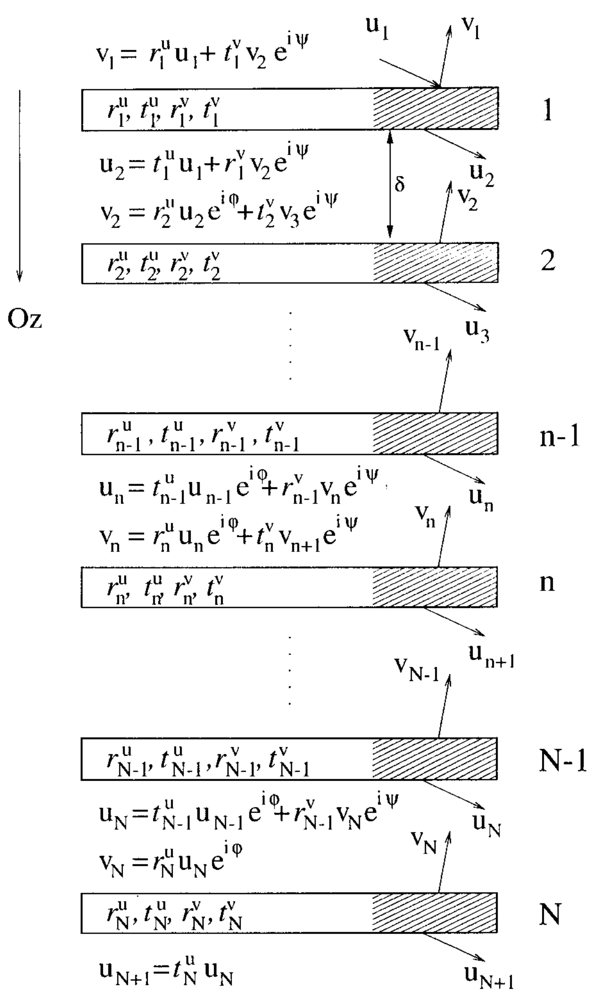


Fig. 2. The system of two-beam Darwin equations.

$$\mathbf{W}(2)\mathbf{X}(2) = \mathbf{U}(2) \tag{4}$$

or explicitly

$$\begin{pmatrix}
-1 & \tau_1^v & & & & & & & & & & \\
0 & \rho_1^v & -1 & & & & & & & & & \\
 & -1 & \rho_2^u & \tau_2^v & & & & & & & & \\
 & & \tau_2^u & \rho_2^v & -1 & & & & & & & \\
 & & & -1 & \rho_3^u & \tau_3^v & & & & & & \\
 & & & & \tau_3^u & & & & & & & \\
 & & & & & & \ddots & & & & & \\
 & & & & & & & & -1 & & & \\
 & & & & & & & -1 & \rho_{N-1}^u & \tau_{N-1}^v & & \\
 & & & & & & & & \tau_{N-1}^u & \rho_{N-1}^v & -1 & \\
 & & & & & & & & & -1 & \rho_N^u & 0 \\
 & & & & & & & & & & \tau_N^u & -1
\end{pmatrix}
\times \begin{pmatrix} v_1 \\ v_2 \\ u_2 \\ v_3 \\ u_3 \\ \vdots \\ u_{N-1} \\ v_N \\ u_N \\ u_{N+1} \end{pmatrix}
= \begin{pmatrix} -\rho_1\hat{u}_1 \\ -\tau_1^u\hat{u}_1 \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \tag{5}$$

where the matrix $\mathbf{W}(2)$ is a tridiagonal (continuant) matrix of order $2N$ (see Appendix A). Further, $\rho_n^u = r_n^u \exp(i\varphi)$, $\rho_n^v = r_n^v \exp(i\psi)$, $\tau_n^u = t_n^u \exp(i\varphi)$, $\tau_n^v = t_n^v \exp(i\psi)$ and $\hat{u}_1 = u_1 \exp(-i\varphi)$.

The amplitudes v_n and u_n given by (5) can be obtained using Cramer's rule. First, we evaluate the amplitudes v_1 and u_{N+1} of the waves reflected and transmitted by the stack. To proceed in this way, we have to evaluate the determinant of the matrix of the system (5), $\mathbf{W}(2)$, and the determinants of the matrices $\mathbf{W}_1(2)$ and $\mathbf{W}_{N+1}(2)$, which are constructed from $\mathbf{W}(2)$ by replacing the first and last column in $\mathbf{W}(2)$ by the column vector $\mathbf{U}(2)$, respectively. The determinant of $\mathbf{W}_{N+1}(2)$ may be evaluated easily, giving

$$\det \mathbf{W}_{N+1}(2) = (-1)^{N-1}\tau_1^u\tau_2^u \ldots \tau_N^u\hat{u}_1. \tag{6}$$

To evaluate the determinants of $\mathbf{W}(2)$ and $\mathbf{W}_1(2)$, let us introduce the submatrix $\mathbf{Q}$ of order $2N-2$ and the matrix $\mathbf{Q}_u$ of order $2N-1$,

$$\mathbf{W}(2) = \left(\begin{array}{c|c|c}
-1 & \tau_1^v\, 0 \ldots 0\;\, 0 & 0 \\ \hline
0 & & 0 \\
0 & & 0 \\
\vdots & \mathbf{Q} & \vdots \\
0 & & 0 \\ \hline
0 & 0\;\, 0 \ldots 0\; \tau_N^u & -1
\end{array}\right),$$

$$\mathbf{Q}_u = \left(\begin{array}{c|c}
\rho_1^u & \tau_1^v\;\, 0\; \ldots\; 0 \\ \hline
\tau_1^u & \\
0 & \\
\vdots & \mathbf{Q} \\
0 &
\end{array}\right), \tag{7}$$

so that

$$\mathbf{W}_1(2) = \left(\begin{array}{c|c}
 & 0 \\
 & 0 \\
\mathbf{Q}_u \cdot \mathbf{P} & 0 \\
 & \vdots \\
 & 0 \\ \hline
0\;\, 0\;\; \ldots\;\; 0\;\, \tau_N^u & -1
\end{array}\right),$$

where $\mathbf{P} = \langle -\hat{u}_1, 1, 1, \ldots, 1\rangle$ is the diagonal matrix of order $2N-1$. Then it may be seen that

$$\det \mathbf{W}(2) = \det \mathbf{Q}, \quad \det \mathbf{W}_1(2) = \hat{u}_1 \det \mathbf{Q}_u. \tag{8}$$

Using (6) and (8), we finally obtain

$$\begin{aligned} v_1 &= (\det \mathbf{Q}_u / \det \mathbf{Q})\hat{u}_1, \\ u_{N+1} &= (-1)^{N-1}[(\tau_1^u\tau_2^u \ldots \tau_N^u)/\det \mathbf{Q}]\hat{u}_1. \end{aligned} \tag{9}$$

The respective coefficients of $\hat{u}_1$ in (9) yield the positively oriented coefficients of reflection (R_u^N) and transmission (T_u^N) of an N-layer stack†

$$R_u^{(N)} = \det \mathbf{Q}_u / \det \mathbf{Q}, \tag{10a}$$

$$T_u^{(N)} = (-1)^{N-1}(\tau_1^u\tau_2^u \ldots \tau_N^u)/\det \mathbf{Q}. \tag{10b}$$

Similar formulae could be obtained for the negatively oriented coefficients $R_v^{(N)}$ and $T_v^{(N)}$. The equivalence of formulae (10a) and (10b) with those yielded by the 'optical matrix method' [see equation (3)] for a system of homogeneous layers was proved by Litzman (1983) by generalizing the standard expression for the so-called split filter.

Since both matrices $\mathbf{Q}$ and $\mathbf{Q}_u$ are tridiagonal ones, the theory of Jacobian matrices and their determinants,

† The reflection and transmission coefficients in (10a) and (10b) differ from those mostly defined in the literature by the phase factor $\exp(-i\varphi)$. This modified definition is based on the fact that the amplitude u_1 of the incident wave is defined on the top boundary of the uppermost layer indexed by 1, whereas amplitudes u_n for $n = 2, 3, \ldots$ are always defined on the bottom boundary of the corresponding layer $n-1$. Without this modification, the formal simplicity of our final formulae would be destroyed.

called continuants, explained in Appendix A, may be employed when evaluating the ratios in (10a) and (10b). Using the notation introduced in (24) in Appendix A, we may write

$$\begin{aligned}\mathbf{Q}_u &= \mathbf{D}_{2N-1}(\rho_1^u, \rho_1^v, \rho_2^u, \rho_2^v, \ldots, \rho_{N-1}^u, \rho_{N-1}^v, \rho_N^u),\\ \mathbf{Q} &= \mathbf{D}_{2N-2}(\rho_1^v, \rho_2^u, \rho_2^v, \ldots, \rho_{N-1}^u, \rho_{N-1}^v, \rho_N^u).\end{aligned} \tag{11}$$

Then applying the rule given by (25) to (10a), we obtain

$$\begin{aligned}R_u^{(N)} &= \frac{D_{2N-1}(\rho_1^u, \rho_1^v, \rho_2^u, \rho_2^v, \rho_3^u, \rho_3^v, \ldots, \rho_{N-1}^u, \rho_{N-1}^v, \rho_N^u)}{D_{2N-2}(\rho_1^v, \rho_2^u, \rho_2^v, \rho_3^u, \rho_3^v, \ldots, \rho_{N-1}^u, \rho_{N-1}^v, \rho_N^u)}\\ &= \big[\rho_1^u D_{2N-2}(\rho_1^v, \rho_2^u, \rho_2^v, \rho_3^u, \ldots, \rho_N^u)\\ &\quad - \tau_1^u\tau_1^v D_{2N-3}(\rho_2^u, \rho_2^v, \rho_3^u, \rho_3^v, \ldots, \rho_N^u)\big]\\ &\quad \times \big[D_{2N-2}(\rho_1^v, \rho_2^u, \rho_2^v, \rho_3^u, \rho_3^v, \ldots, \rho_{N-1}^u, \rho_{N-1}^v, \rho_N^u)\big]^{-1}\\ &= \rho_1^u - \tau_1^u\tau_1^v\left[\frac{D_{2N-2}(\rho_1^v, \rho_2^u, \rho_2^v, \rho_3^u, \rho_3^v, \ldots, \rho_N^u)}{D_{2N-3}(\rho_2^u, \rho_2^v, \rho_3^u, \rho_3^v, \ldots, \rho_N^u)}\right]^{-1}.\end{aligned} \tag{12}$$

Using rule (25) again in the ratio of two continuants

$$\frac{D_{2N-2}(\rho_1^v, \rho_2^u, \rho_2^v, \rho_3^u, \rho_3^v, \ldots, \rho_N^u)}{D_{2N-3}(\rho_2^u, \rho_2^v, \rho_3^u, \rho_3^v, \ldots, \rho_N^u)},$$

it is clear that formula (12) for $R_u^{(N)}$ can be expressed as a continued fraction. [It is known that each continued fraction can be expressed as a ratio of two continuants (Perron, 1913)].

The coefficients of reflection $R_u^{(N)}$ and/or transmission $T_u^{(N)}$ of an N-layer stack may be expressed in other useful forms. By using (25) in (12) and/or in the respective formula for $T_u^{(N)}$ and after rearranging the results, we obtain the 'recurrence formulae'

$$\begin{aligned}R_u^{(N)} &= \rho_1^u + \tau_1^u\tau_1^v R_u^{\prime(N-1)}/[1 - \rho_1^v R_u^{\prime(N-1)}],\\ T_u^{(N)} &= \tau_1^u T_u^{\prime(N-1)}/[1 - \rho_1^v R_u^{\prime(N-1)}],\end{aligned} \tag{13}$$

where $R_R^{(N)}$ and $R_R^{\prime(N-1)}$ are the positively oriented reflection coefficients of the system formed by N layers $(12\ldots N)$ and by $N-1$ layers $(23\ldots N)$, respectively. $T_u^{(N)}$ and $T_u^{\prime(N-1)}$ have a similar meaning. Reflectivities and transmissivities of complex systems in the forms of continued fractions and the 'recurrence formulae' derived by other methods can be found, for example, in the works of Delano & Pegis (1969) and Ignatovich (1991).

Finally, for completeness, let us present formulae for the amplitudes u_n and v_n of the wave fields in the vacuum splits of the stack. Using Cramer's rule and introducing continuants, we obtain from (5)

$$\begin{aligned}u_n &= (-1)^{n-1}\tau_1^u\tau_2^u\ldots\tau_{n-1}^u\\ &\quad\times\frac{D_{2(N-n)}(\rho_n^v, \rho_{n+1}^u, \ldots, \rho_N^u)}{D_{2N-2}(\rho_1^v, \rho_2^u, \rho_2^v, \ldots, \rho_{N-1}^v, \rho_N^u)}\hat{u}_1\\ &\qquad\text{for}\quad n = 2, 3, \ldots, N-1\end{aligned} \tag{14a}$$

$$u_N = (-1)^{N-1}\frac{\tau_1^u\tau_2^u\ldots\tau_{N-1}^u}{D_{2N-2}(\rho_1^v, \rho_2^u, \rho_2^v, \ldots, \rho_{N-1}^v, \rho_N^u)}\hat{u}_1, \tag{14b}$$

$$\begin{aligned}v_n &= (-1)^{n-1}\tau_1^u\tau_2^u\ldots\tau_{n-1}^u\\ &\quad\times\frac{D_{2(N-n)+1}(\rho_n^u, \rho_n^v, \rho_{n+1}^u, \ldots, \rho_{N-1}^v, \rho_N^u)}{D_{2N-2}(\rho_1^v, \rho_2^u, \rho_2^v, \ldots, \rho_{N-1}^v, \rho_N^u)}\hat{u}_1\\ &\qquad\text{for}\quad n = 2, 3, \ldots, N.\end{aligned} \tag{14c}$$

To conclude, let us mention that to find the solution of (4), the inverse of the matrix $\mathbf{W}(2)$ can be used. Then

$$\mathbf{X}(2) = \mathbf{W}(2)^{-1}\mathbf{U}(2). \tag{15}$$

How to evaluate the inverse of the tridiagonal matrix, $\mathbf{W}(2)^{-1}$, is explained in the second part of Appendix A.

4. Applications

In this section, we will apply the developed formalism to particular physical problems and demonstrate its advantages.

4.1. *Example 1*

As a simple example, let us consider a system of three layers (123) in vacuum. In this particular case,

$$\mathbf{Q} = \begin{pmatrix}\rho_1^v & -1 & 0 & 0\\ -1 & \rho_2^u & \tau_2^v & 0\\ 0 & \tau_2^u & \rho_2^v & -1\\ 0 & 0 & -1 & \rho_3^u\end{pmatrix},$$

$$\mathbf{Q}_u = \begin{pmatrix}\rho_1^u & \tau_1^v & 0 & 0 & 0\\ \tau_1^u & \rho_1^v & -1 & 0 & 0\\ 0 & -1 & \rho_2^u & \tau_2^v & 0\\ 0 & 0 & \tau_2^u & \rho_2^v & -1\\ 0 & 0 & 0 & -1 & \rho_3^u\end{pmatrix}.$$

By iteratively using (25), we obtain directly from (12) the reflectivity of the three-layer stack in the form of a continued fraction

$$R_u^{(3)} = \rho_1^u - \cfrac{\tau_1^u\tau_1^v}{\rho_1^v - \cfrac{1}{\rho_2^u - \cfrac{\tau_2^u\tau_2^v}{\rho_2^v - \cfrac{1}{\rho_3^u}}}}. \tag{16}$$

4.2. *Example 2*

As the next example let us consider an 'incomplete' periodic structure

$$(\underbrace{123}_{1}\underbrace{123}_{2}\ldots\underbrace{123}_{p}12)$$

formed by $N_p = 3p + 2$ layers where the evaluation of the determinants of $\mathbf{Q}_u$ and $\mathbf{Q}$ in (8) can be considerably simplified due to a general theorem by Rózsa (1969). For the sake of simplicity, we assume that $\rho_n^u = \rho_n^v = \rho_n$ and $\tau_n^u = \tau_n^v = \tau_n$ for $n = 1$, 2 and 3. Then the periodic continuant matrices $\mathbf{Q}$ (of order $2N_p - 2 = 6p + 2$) and $\mathbf{Q}_u$ (of order $6p + 3$) are already the symmetrical ones and thus it is possible to use directly the results summarized in the third part of Appendix *A*. Using the notation introduced in (30), we may write

$$\mathbf{Q} = \hat{\mathcal{D}}^{(1)}_{6p+2} \quad \text{and} \quad \mathbf{Q}_u = \hat{\mathcal{D}}^{(2)}_{6p+3},$$

where respective generating submatrices $\mathbf{D}^{(i)}_{123456}$ and matrix elements $b_6^{(i)}$ $(i = 1, 2)$ are given by

$$\mathbf{D}^{(1)}_{123456} = \begin{pmatrix} \rho_1 & -1 & 0 & 0 & 0 & 0 \\ -1 & \rho_2 & \tau_2 & 0 & 0 & 0 \\ 0 & \tau_2 & \rho_2 & -1 & 0 & 0 \\ 0 & 0 & -1 & \rho_3 & \tau_3 & 0 \\ 0 & 0 & 0 & \tau_3 & \rho_3 & -1 \\ 0 & 0 & 0 & 0 & -1 & \rho_1 \end{pmatrix}$$

and

$$b_6^{(1)} = -\tau_1,$$

and

$$\mathbf{D}^{(2)}_{123456} = \begin{pmatrix} \rho_1 & \tau_1 & 0 & 0 & 0 & 0 \\ \tau_1 & \rho_1 & -1 & 0 & 0 & 0 \\ 0 & -1 & \rho_2 & \tau_2 & 0 & 0 \\ 0 & 0 & \tau_2 & \rho_2 & -1 & 0 \\ 0 & 0 & 0 & -1 & \rho_3 & \tau_3 \\ 0 & 0 & 0 & 0 & \tau_3 & \rho_3 \end{pmatrix}$$

and

$$b_6^{(2)} = 1.$$

The determinants of matrices $\mathbf{Q}$ and $\mathbf{Q}_u$ can be evaluated by (35). Finally, we obtain the coefficient of reflection of the 'incomplete' periodic structure (Litzman, 1983),

$$R_u^{(Np)} = \frac{\tau_3[\rho_2(\rho_1^2 - \tau_1^2) - \rho_1]U_p(x) - \tau_1\tau_2\rho_3 U_{p-1}(x)}{\tau_3(\rho_1\rho_2 - 1)U_p(x) - \tau_1\tau_2(\rho_3^2 - \tau_3^2)U_{p-1}(x)}, \tag{17}$$

where $U_k(x)$ are Chebyshev polynomials [see (32)].

In most cases, thin-film optics deals with 'complete' periodic structures (1212 ... 12), each film being characterized by a constant refraction index (Born & Wolf, 1968; Knittl, 1976; Yeh, 1988). Adopting our approach employing the theory of periodic continuants, we may handle more general cases by a uniform view: the number of films in each period is arbitrary, the scattering-length density of a film is not constant, the last period need not be full [see submatrix $\mathbf{D}_{12\ldots r}$ of (30)].

4.3. *Example 3*

Finally, let us mention that the determinants of $\mathbf{Q}$ and/or $\mathbf{Q}_u$ given in (7) are polynomials in ρ_i,

$$\det \mathbf{Q} = A_0 + \sum_i A_i\rho_i + \sum_{i,j} A_{ij}\rho_i\rho_j + \sum_{i,j,k} A_{ijk}\rho_i\rho_j\rho_k + \ldots \tag{18}$$

and similarly for $\det \mathbf{Q}_u$. When, for example, evaluating the coefficient A_{24}, we first put $\rho_i = 0$ in the matrix $\mathbf{Q}$ for all *i* except 2 and 4, and then use theorems for evaluation of the continuants. Proceeding in this way, we obtain (Litzman & Rózsa, 1984)

$$\begin{aligned} \det \mathbf{Q} &= (-1)^{N-1} + Q^{(2)} + Q^{(4)} + \ldots \\ \det \mathbf{Q}_u &= Q_u^{(1)} + Q_u^{(3)} + \ldots, \end{aligned} \tag{19}$$

where

$$\begin{aligned} Q_u^{(1)} &= \sum_i B_i\rho_i \\ &= (-1)^{N-1}(\rho_1 + \tau_1^2\rho_2 + \tau_1^2\tau_2^2\rho_3 + \ldots \\ &\quad + \tau_1^2\tau_2^2\ldots\tau_{N-1}^2\rho_N), \\ Q^{(2)} &= \sum_{i,j} A_{ij}\rho_i\rho_j \\ &= (-1)^N(\rho_1\rho_2 + \rho_1\tau_2^2\rho_3 + \rho_1\tau_2^2\tau_3^2\rho_4 + \ldots \\ &\quad + \rho_1\tau_2^2\tau_3^2\ldots\tau_{N-1}^2\rho_N + \rho_2\rho_3 + \rho_2\tau_3^2\rho_4 \\ &\quad + \rho_2\tau_3^2\tau_4^2\rho_5 + \ldots + \rho_2\tau_3^2\tau_4^2\ldots\tau_{N-1}^2\rho_N \\ &\quad + \rho_{N-2}\rho_{N-1} + \rho_{N-2}\tau_{N-1}^2\rho_N + \rho_{N-1}\rho_N), \\ Q_u^{(3)} &= \sum_{i,j,k} B_{ijk}\rho_i\rho_j\rho_k \quad \textit{etc.} \end{aligned} \tag{20}$$

It is worth noting that by using (19) a perturbative approach may be developed, revealing directly the influence of the reflection coefficient ρ_i of a particular layer on the reflection coefficient of the whole stack.

Let us apply formulae (20) to the study of the reflectivity of a stack of thin films in the soft X-ray region (Litzman, Dub & Ševčík, 1984;† Litzman & Rózsa, 1984; Litzman & Sebelová, 1985). In the soft X-ray region, the reflection coefficient ρ of a thin film evaluated in the frame of the dynamical diffraction theory is related to ρ^o following from the classical Fresnel theory (being of the order of 10^{-3}) by the relation (Litzman, Dub & Ševčík, 1984)

$$\rho/\rho^o = (2\pi a/\lambda_o)\cos\gamma_o/\sin[(2\pi a/\lambda_o)\cos\gamma_o]. \tag{21}$$

† Note that captions to Figs. 2 and 3 have been interchanged in this paper.

The right-hand side of (21) depends on the ratio of the wave length λ_o and the lattice parameter of the film, a, and on the incidence angle γ_o only, but not on the refraction index of the film. On the other hand, for the corresponding transmission coefficients, it approximately holds that $\tau = \tau^o$. Then, expressing determinants of matrices $\mathbf{Q}$ and $\mathbf{Q}_u$ as polynomials in ρ_i, we have found (Litzman & Rózsa, 1984) that to a good approximation the same relation as (21) holds for the reflection coefficients of the whole stack of thin films. The same conclusion may be drawn for the optics of thermal neutrons.

5. Conclusions and further perspectives

The Darwin procedure is, together with the approach developed by Ewald (1916, 1917), the first formulation of the dynamical theory of diffraction. Nevertheless, it attracts attention even 80 years after its origin. We have shown that formulae of the two-beam Darwin theory, in particular the reflectivity and transmissivity of the stack of layers, can be obtained by a uniform view of basic properties of tridiagonal matrices, their determinants (called continuants), and their close relationship to continued fractions and difference equations. A comparison of the Bethe–Laue dynamical theory of diffraction in a periodic system of homogeneous multilayers with the 'optical matrix method' [see equation (3)] has been discussed recently by Sears (1997).

Recently, the diffraction from a set of atomic layers in the three-beam Bragg case has been studied (Takahashi & Nakatani, 1995). In this three-beam case, we have, instead of (3),

$$\begin{pmatrix} u_n \\ v_n \\ w_n \end{pmatrix} = \mathbf{A}(n) \begin{pmatrix} u_{n+1} \\ v_{n+1} \\ w_{n+1} \end{pmatrix} \tag{22}$$

with boundary conditions $u_1 = u^{\rm inc}$ and $v_{N+1} = w_{N+1} = 0$, and, consequently, equation (4) assumes the form

$$\mathbf{W}(3)\mathbf{X}(3) = \mathbf{U}(3), \tag{23}$$

where the matrix $\mathbf{W}(3)$ is a *tridiagonal block* matrix. Whereas the properties of the tridiagonal matrices have been studied for a long time, interest in the tridiagonal block matrices arose only in the past decade (Rózsa *et al.*, 1989). We intend to use these recent results for the Darwin multibeam theory in a forthcoming paper.

APPENDIX *A*
Jacobian matrices and continuants

*A*1. *Jacobian matrix*

The quadratic matrix of the form

$$\mathbf{D}_n(a_1a_2\ldots a_n) = \begin{pmatrix} a_1 & -b_1 & 0 & \ldots & 0 & 0 \\ -c_1 & a_2 & -b_2 & \ldots & 0 & 0 \\ 0 & -c_2 & a_3 & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \ldots & a_{n-1} & -b_{n-1} \\ 0 & 0 & 0 & \ldots & -c_{n-1} & a_n \end{pmatrix} \tag{24}$$

is called a *Jacobian matrix* or a *continuant matrix*. The determinant of $\mathbf{D}_n(a_1a_2\ldots a_n)$ is called the *continuant* and will be denoted by $D_n(a_1a_2\ldots a_n)$. The principal minor of the continuant $D_n(a_1a_2\ldots a_n)$ constructed from its $i_1, i_2, \ldots, i_p$ rows and columns will be denoted by $D_{i_1i_2\ldots i_p}$ or $D_p(a_{i_1}a_{i_2}\ldots a_{i_p})$. Clearly,

$$D_n(a_1a_2\ldots a_n) = a_1D_{n-1}(a_2\ldots a_n) - b_1c_1D_{n-2}(a_3a_4\ldots a_n) \tag{25}$$

holds. Another useful formula for the calculation of a continuant,

$$\begin{aligned} D_n(a_1a_2\ldots a_n) &= D_k(a_1a_2\ldots a_k)D_{n-k}(a_{k+1}a_{k+2}\ldots a_n) \\ &\quad - b_kc_kD_{k-1}(a_1a_2\ldots a_{k-1})D_{n-k-1}(a_{k+2}a_{k+3}\ldots a_n), \end{aligned} \tag{26}$$

can be easily derived by a famous relation due to Jacobi [see equation (1.3) in the paper by Rózsa (1969)].

By the similarity transformation with the diagonal matrix

$$\mathbf{A} = \left\langle 1, \left(\frac{b_1}{c_1}\right)^{1/2}, \left(\frac{b_1b_2}{c_1c_2}\right)^{1/2}, \ldots, \left(\frac{b_1b_2\ldots b_{n-1}}{c_1c_2\ldots c_{n-1}}\right)^{1/2} \right\rangle, \tag{27}$$

the matrix (24) can be transformed into a *symmetrical* Jacobian matrix

$$\mathbf{A}\mathbf{D}_n\mathbf{A}^{-1} = \begin{pmatrix} a_1 & (b_1c_1)^{1/2} & & & \\ (b_1c_1)^{1/2} & a_2 & (b_2c_2)^{1/2} & & \\ & (b_2c_2)^{1/2} & a_3 & & \\ & & & \ddots & \\ & & & & (b_{n-1}c_{n-1})^{1/2} \\ & & & (b_{n-1}c_{n-1})^{1/2} & a_n \end{pmatrix}. \tag{28}$$

Thus in the following we shall be concerned with symmetrical continuant matrices only.

A2. Inverse of a symmetrical Jacobian matrix

The inverse of a symmetrical Jacobian matrix (24) where $b_i = c_i \neq 0$ is given as (Gantmacher & Krein, 1960)

$$\mathbf{D}_n^{-1} = \mathbf{R} = (r_{ij})$$

with

$$r_{ij} = \begin{cases} u_i v_j & \text{if } i \leq j \\ v_i u_j & \text{if } i \geq j \end{cases}. \tag{29}$$

The factors u_i and v_j can easily be calculated using a simple recurrence relation (Brevilacqua *et al.*, 1988).

A3. Symmetrical continuant

A *symmetrical continuant* in which $a_{k+m} = a_k$ and $b_{k+m} = b_k$ is called a *periodic continuant*. Let us consider the periodic continuant matrix

$$\hat{\mathcal{D}}_{mp+r} = \begin{pmatrix} \boxed{\mathbf{D}_{12\ldots m}} & \overset{1)}{} 0 & & 0 \\ & -b_m & \overset{2)}{} & \\ -b_m & & & \\ 0 & \boxed{\mathbf{D}_{12\ldots m}} & & \\ & & -b_m & \\ & -b_m & & \\ & & \ddots & \overset{p)}{} \\ & & \boxed{\mathbf{D}_{12\ldots m}} & 0 \\ & & & -b_m \\ & & -b_m & \\ 0 & & 0 & \boxed{\mathbf{D}_{12\ldots r}} \end{pmatrix} \tag{30}$$

where $\mathbf{D}_{12\ldots m}$ and $\mathbf{D}_{12\ldots r}$ with $r < m \leq n$ are submatrices of the same symmetrical continuant matrix.

Following equation (1.6) in the work of Rózsa (1969), $\det \hat{\mathcal{D}}_{mp+r} = \mathcal{D}_{mp+r}$ can be evaluated as follows. We denote

$$x = (D_{12\ldots m} - b_m^2 D_{2\ldots m-1})/b_1 b_2 \ldots b_m. \tag{31}$$

Further, we introduce Chebyshev polynomials of the second kind in the form of a continuant

$$U_n(x) = \begin{array}{c} \begin{array}{cccccc} 1) & 2) & & & & n) \end{array} \\ \begin{vmatrix} x & -1 & & & & \\ -1 & x & -1 & & & \\ & -1 & & & & \\ & & & \ddots & & \\ & & & & & -1 \\ & & & & -1 & x \end{vmatrix} \end{array}$$

$$= \sum_{k=0}^{(n/2)} (-1)^k \binom{n-k}{k} x^{n-2k}$$

$$= \prod_{p=1}^{n} [x - 2\cos(p\pi/n+1)] \tag{32}$$

and the polynomials

$$Y_n(x) = (b_1 b_2 \ldots b_m)^n U_n(x). \tag{33}$$

Then,

$$\mathcal{D}_{mp} = Y_p(x) + b_m^2 D_{2\ldots m-1} Y_{p-1}(x), \tag{34}$$

$$\mathcal{D}_{mp+r} = D_{1\ldots r} Y_p(x) + b_m^2 b_1^2 \ldots b_r^2 D_{r+2\ldots m-1} Y_{p-1}(x) \quad \text{for} \quad 1 \leq r \leq m-3, \tag{35}$$

$$\mathcal{D}_{mp+m-2} = D_{1\ldots m-2} Y_p(x) + b_m^2 b_1^2 \ldots b_{m-2}^2 Y_{p-1}(x), \tag{36}$$

$$\mathcal{D}_{mp+m-1} = D_{1m-1} Y_p(x). \tag{37}$$

Formulae (31), (34) and (37) are valid for $m > 2$. For $m = 2$,

$$x = (D_{12} - b_2^2)/b_1 b_2 \tag{38}$$

and

$$\mathcal{D}_{2p} = Y_p(x) + b_2^2 Y_{p-1}(x), \quad \mathcal{D}_{2p+1} = D_1 Y_p(x) \tag{39}$$

hold.

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