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Abstract. The matrix approach to the calculation of n-beam diffraction in a periodic structure is discussed. The possibility of representing N-layered transfer matrix $T_N$ through the principal minors of the matrix $T$ is investigated. The method of computing integer powers of a matrix by means of symmetric polynomials of the latter is developed. New analytic formulas for integer powers of matrices are represented. These solutions are demonstrated using examples of matrices of the sixth order.

1. Introduction

The physical properties of many natural and artificial objects are well described within the framework of one-dimensional periodic models [1, 2]. Examples of such structures that have found wide application are optical thin films [3], liquid crystals [4], superlattices [5], photonic crystals [6]. Matrix approaches have become one of the main ones in the calculations of wave propagations in such media. The problem of calculating the wave transmission through N-layered structure is reduced to finding so-called transfer matrix $T$ (or characteristic matrix [7], or scattering matrix [8], or propagator matrix [9]) of one separate layer and matrix $T^N$ for the whole structure. In this regard, of great interest are analytical solutions for integer powers of matrices. The Baker-Vandermonde formula [10] represents the solution of this problem in terms of matrix eigenvalues. A remarkable result for unimodular second-order matrices was obtained by Abelès [11] in the study of interference optical films. In his paper the elements of the characteristic matrix $M^N$ have been expressed through the trace of the matrix $M$ using the Chebyshev polynomials of the second kind. Similar formulas for the integer powers of second order matrices of general form and certain matrices of the third and fourth orders were found in [12]. In this paper, we present new analytical solutions for integer powers of nth order matrices. Their proofs are based on the properties of symmetric polynomials of nth order [13].

2. Polynomial approach to the calculation of integer powers of matrices

According to one of the corollaries of the Cayley-Hamilton theorem [14], integer power $j$ of any matrix $A$ can be expressed as a linear combination of the first $n$ powers $A_0 = I$, $A, \ldots, A^{n-1}$:

$$A^j = \sum_{h=0}^{n-1} C_{jh} A^h, \quad j \geq 0. \quad (1)$$
We use the following representation of the coordinates $C_{jh}$ [13]:

$$C_{jh} = \sum_{g=0}^{h} p_{n-h+g} B_{j-1-g}(n), \quad h = 0, 1, \ldots, n - 1, \quad j = 0, 1, 2, \ldots,$$

(2)

where $p_m, m = 1, \ldots, n$, are coefficients of characteristic equation $\lambda^n = \sum_{i=1}^{n} p_i \lambda^{n-i}$ of matrix $A = \|a_{gh}\|$ and functions $B_g(n)$ are defined by recurrence relations

$$B_g(n) = 0, \quad 0 \leq g \leq n - 2; \quad B_{n-1}(n) = 1; \quad B_{g}(n) = \sum_{j=1}^{n} p_j B_{g-j}(n), \quad g \geq n. \quad (3)$$

Two representations of the coefficients $p_m$, namely $p_1 = \sum_{g=1}^{n} \lambda_g, \quad p_2 = -\sum_{i\neq j} \lambda_i \lambda_j, \ldots, \quad p_n = (-1)^{n-1} \prod_{j=1}^{n} \lambda_j$ and $p_1 = \sum_{g=1}^{n} a_{gg}, \quad p_2 = -\sum_{j>i} a_{ji} a_{jj}, \ldots, \quad p_n = (-1)^{n-1} \det A$ give respectively two interpretation of the functions $B_g(n)$: symmetric polynomials of $n$th order [13] (symmetric with respect to the eigenvalues $\lambda_j, \quad j = 1, \ldots, n$) and polynomials of principal minors of the matrix $A$.

2.1. Expression of $A^n$ in terms of symmetric polynomials

**Theorem 1.** Symmetric polynomials of $n$th order are expressed in terms of the eigenvalues $\lambda_i, \quad i = 1, 2, \ldots, n$ of the matrix by the formulas

$$B_g(n) = \frac{\Delta_g}{\Delta_V}, \quad \Delta_V = \begin{vmatrix} 1 & \lambda_1 & \lambda_1^{n-2} & \lambda_1^{n-1} \\ 1 & \lambda_2 & \lambda_2^{n-2} & \lambda_2^{n-1} \\ \vdots & \vdots & \vdots & \vdots \\ 1 & \lambda_n & \lambda_n^{n-2} & \lambda_n^{n-1} \end{vmatrix}, \quad \Delta_g = \begin{vmatrix} 1 & \lambda_1 & \lambda_1^{n-2} & \lambda_1^g \\ 1 & \lambda_2 & \lambda_2^{n-2} & \lambda_2^g \\ \vdots & \vdots & \vdots & \vdots \\ 1 & \lambda_n & \lambda_n^{n-2} & \lambda_n^g \end{vmatrix}, \quad (4)$$

where $g$ is any integer, if all values $\lambda_i \neq 0$, and $g \geq 0$, if some eigenvalue $\lambda_i = 0$.

**Proof.** The properties of the determinants make it obvious that the formulas (4) correspond to the definition (3) of polynomials $B_g(n)$ for $g = 0, 1, \ldots, n - 1$.

Suppose that the equality (4) holds for $g = j - n + 1, \ldots, j - 1, j$, where $j \geq n - 1$. We show that then it will also true (i.e. functions (4) satisfy the definition (3)) for $g = j + 1$. Indeed, according to characteristic equation, $\lambda^{j+1} = p_1 \lambda^j + p_2 \lambda^{j-1} + \ldots + p_n \lambda^{j-n+1}$. Therefore

$$B_{j+1}(n) = \frac{1}{\Delta_V} \begin{vmatrix} 1 & \lambda_1 & \lambda_1^{n-3} & \lambda_1^{j-2} & \lambda_1^{j-1} & \lambda_1^j & \lambda_1^{j-n+1} \\ 1 & \lambda_2 & \lambda_2^{n-3} & \lambda_2^{j-2} & \lambda_2^{j-1} & \lambda_2^j & \lambda_2^{j-n+1} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & \lambda_n & \lambda_n^{n-3} & \lambda_n^{j-2} & \lambda_n^{j-1} & \lambda_n^j & \lambda_n^{j-n+1} \end{vmatrix}$$

$$= \frac{1}{\Delta_V} \sum_{h=1}^{n} p_h \Delta_{j+1-h} = \sum_{h=1}^{n} p_h B_{j+1-h}(n),$$

which agrees with the recurrence formulas (3).

Note that substitutions of the expressions (4) into the formulas (2) and (1) lead to one more proof of the Baker-Vandermonde formula.

A more explicit form of symmetric polynomials $B_g(n)$ follows from (4) if we use the value of the Vandermonde determinant $\Delta_V = \prod_{j>i}(\lambda_j - \lambda_i)$. For example, suppose that the characteristic equation of a sixth-order matrix has the form: $\lambda^6 - p_2 \lambda^4 - p_4 \lambda^2 - p_6 = 0$. In this case, the eigenvalues are pairwise equal to each other with a precision up to the sign, say
\[ \lambda_1 = -\lambda_4, \lambda_2 = -\lambda_5, \lambda_3 = -\lambda_6. \] These eigenvalues are expressed in the radicals in terms of the coefficients of the characteristic equation. In turn, the coefficients of the characteristic equation \( p_2, p_4, p_6 \) are expressed in terms of the eigenvalues \( \lambda_1, \lambda_2, \lambda_3 \) by the formulas: 
\( p_2 = \lambda_1^2 + \lambda_2^2 + \lambda_3^2, \)
\( p_4 = \lambda_1^3 \lambda_2^2 + \lambda_1^2 \lambda_3^2 + \lambda_2^2 \lambda_3^2, \)
\( p_6 = \lambda_1^3 \lambda_2^3 \lambda_3. \) In this case, the symmetric polynomials of sixth order are expressed through the matrix eigenvalues as:
\[ B_j(6) = 1 + \frac{(-1)^{j-1}}{2} \frac{A_{j-1}}{A_4}, \quad A_1 = \lambda_1^2 (\lambda_2^2 - \lambda_3^2) - \lambda_2^3 (\lambda_3^2 - \lambda_1^2) + \lambda_3^2 (\lambda_1^2 - \lambda_2^2). \] (5)

In accordance with (1)
\[ A^n = \begin{cases} 
    p_6 B_{j-2}(6) A + [p_4 B_{j-2}(6) + p_6 B_{j-4}(6)] A^3 + B_j(6) A^5, & \text{if } j = 7, 9, 11, \ldots , \\
    p_6 B_{j-1}(6) I + [p_4 B_{j-1}(6) + p_6 B_{j-3}(6)] A^2 + B_{j+1}(6) A^4, & \text{if } j = 6, 8, 10, \ldots , 
\end{cases} \] (6)

where the polynomials \( B_g(6) \) are defined by formulas (5) and \( I \) is identity matrix.

2.2. Representation of integer powers of a matrix by means of the coefficients of its characteristic equation

Theorem 2. If only two of the coefficients of the characteristic equation \( p_h \) and \( p_i, l = 2h, \) are nonzero, then the polynomials \( B_g(n) \) are expressed by the formulas:
\[ B_g(n) = \begin{cases} 
    \sqrt{(-p_l)^{n-1}} U_{j-1}(b), & \text{if } g = h(j - 1) + n - 1, \\
    0, & \text{if } g \neq h(j - 1) + n - 1, 
\end{cases} \] (7)

where 
\[ U_j(b) = \frac{\sin[(j + 1) \arccos b]}{\sqrt{1 - b^2}}, \quad b = \frac{p_h}{2\sqrt{-p_l}}. \] (8)

Proof. It’s obvious that \( h(j - 1) + n - 1 \geq n - 1. \) Therefore, it follows from (7) that \( B_g(n) = 0, \) if \( g \leq n - 2, \) which agrees with (3). If \( g = n - 1, \) then, by formulas (7) and (8), we find \( B_{n-1}(n) = U_0(b) = 1. \) This also satisfies definition (3). Finally, if \( g \geq n, \) then, according to the definition (3) and the condition of the theorem, the function (7) must be a solution of equation
\[ B_g(n) = p_h B_{g-h}(n) + p_i B_{g-1}(n), \quad g \geq n. \] (9)

It’s easy to check. Let \( g \neq h(j - 1) + n - 1. \) Then \( g - h \) and \( g - 2h \) not equal to \( h(j - 1) + n - 1. \) In this case formulas (7) give values \( B_g(n) = B_{g-h}(n) = B_{g-1}(n) = 0, \) which satisfy equation (9). At last, if \( g = h(j - 1) + n - 1, \) then substitution of (7) into (9) gives equality
\[ U_{j-1}(b) = 2b U_{j-2}(b) - U_{j-3}(b), \] (10)

whose identity is established by elementary transformations using the functions (8). Thus, the functions (7) are solutions of equations (9), which was to be proved.

If \( -1 \leq b \leq 1, \) the functions \( U_j(b) \) with indexes \( j \geq 0 \) are orthogonal Chebyshev polynomials of the second kind.

For instance for sixth order matrix \( A \) with \( p_1 = p_2 = 0, p_3 \neq 0, p_4 = p_5 = 0, p_6 \neq 0, \) we find from (1), (2) and (7)
\[ A^{6+i+3k} = p_6 B_{5+3k}(6) A^i + B_{8+3k}(6) A^{i+3}, \quad i = 0, 1, 2, \quad k = 0, 1, \ldots \] (11)

where \( B_g(6) = (\det A)^{\frac{g}{3}} \sin \left(\frac{(g - 2) \arccos b}{3}\right) / \sqrt{1 - b^2}, \quad b = p_3/(2\sqrt{\det A}) \) for \( g = 5, 8, 11, \ldots \) and \( B_g(6) = 0 \) for \( g \neq 5, 8, 11, \ldots \)
Example. Transfer matrix $T$ of elastic waves in a crystalline layer of thickness $d$ is expressed by the formula $T = \exp(Wd)$, where sixth-order matrix $W = \|w_{ij}\|$ is determined [15] from the system of equations of motion and Hooke’s law. For many geometries of elastic waves scattering by a cubic crystal, the symmetric polynomials $\mathcal{B}_g(6)$ of the matrix $W$ and matrices $W^j$ satisfy relations (5) and (6) respectively. For these cases, the analytical solution for the transfer matrix system of equations of motion and Hooke’s law. For many geometries of elastic waves scattering by the formula

$$
\Delta \lambda_1^3 \lambda_2^3 (\lambda_1^2 - \lambda_2^2), \quad \tau_{20} = \lambda_1^2 \lambda_3^2 (\lambda_1^2 - \lambda_3^2), \quad \tau_{30} = \lambda_1^2 \lambda_2^2 (\lambda_1^2 - \lambda_2^2), \quad c_{g1} = \tau_{g1}/\lambda_g, \quad \tau_{12} = \lambda_2^4 - \lambda_3^4, \\
\tau_{23} = \lambda_4^2 - \lambda_1^2, \quad \tau_{32} = \lambda_1^2 - \lambda_2^2, \quad \tau_{33} = \tau_{22}/\lambda_2, \quad \tau_{34} = \lambda_3^2 - \lambda_2^2, \quad \tau_{24} = \lambda_1^2 - \lambda_2^2, \quad \tau_{35} = \tau_{44}/\lambda_g.
$$

In the case when the matrix $W$ has the form (11), an analytic solution for the elastic wave transfer matrix can be found in a similar way.

For sufficiently small thickness $d$ the series $\sum_{j=1}^{\infty} (Wd)^j/(j!)$ is well approximated by the sum of the first two or three terms, i.e. $T = I + Wd + W^2d^2/2$. Such definition of the matrix $T$, if $\|w_{ij}\|d \ll 1$, provides calculation of matrix $T$ elements with a relative error of less than $6 (\max |w_{ij}|d)^3$. This allows us to consider a homogeneous layer of thickness $Nd$ as $N$-layered periodic structure and calculate its transfer matrix $T_N$ in accordance with the formulas (1), (2), (3). It is easy to show that in this case the coefficients $p_m$ and the polynomials of principal minors up to terms of the second order of smallness in $\max |w_{ij}|d$ are expressed by the formulas

$$
p_m = (-1)^{m-1} 6! (1 + mx)/|m! (6 - m)!|, \quad m = 1, \ldots, 6; \quad \mathcal{B}_g(6) = c_g [1 + (g - 5)x], \quad g \geq 5,
$$

where $x = \sum_{j=1}^{6} w_{ij}d/6$ and the coefficients $c_g$ are determined from the recurrence relations: $c_0 = 0, g \leq 4; c_5 = 1; c_g = \sum_{j=1}^{6} c_{g-j} 6!/|j! (6 - j)!|, g \geq 5$.

3. Conclusion

As the examples of two- and four-beam scattering of electromagnetic waves in layered media show, analytical formulas for transfer matrices facilitate a theoretical study of the features of the corresponding diffraction spectra. Such formulas as (6), (11), (12) play no less important role in the verification of numerical algorithms for calculating matrices $T_N$ with large $N$, since round-off errors during matrix calculations depend strongly on the number of matrix multiplications.

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