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1996 J. Phys. A: Math. Gen. 29 5103

(http://iopscience.iop.org/0305-4470/29/16/029)

J. Phys. A: Math. Gen. **29** (1996) 5103–5123. Printed in the UK

The recurrent algorithm of the rigorous solving 1-dimensional wave equations in multilayered media

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Received 11 May 1995

Abstract. The rigorous difference equations for the elements of any order of transfer matrices of coupled waves and the renormalization relations for their recursion coefficients under homogeneous and inhomogeneous rescaling are obtained. Incidentally, the generalization of Abelés theorem to arbitrary-dimensional square matrix formulae are deduced.

1. Introduction

The problems on steady states in the multilayered linear mediums are often reduced to solving a linear non-autonomous system of ordinary differential equations [1–3]

$$\frac{\mathrm{d}\mathbf{\Psi}}{\mathrm{d}x} = \mathsf{A}(x)\mathbf{\Psi} \tag{1}$$

where $\mathsf{A}(x)$ is an $N \times N$ matrix and $\mathbf{\Psi} = \mathrm{col}(\psi_1, \psi_2, \ldots, \psi_N)$ is the column of N arguments. In fact, there are the parametric resonance problems, in which the elements of the dynamical matrix $\mathsf{A}(x)$ appear as variable parameters [2]. For example, the special case of $N = 2$, when

$$\mathsf{A}(x) = \begin{pmatrix} 0 & 1 \\ k^2\epsilon(x) & 0 \end{pmatrix} \qquad \mathbf{\Psi} = \begin{pmatrix} \psi \\ \psi' \end{pmatrix} \tag{2}$$

where $\psi' = \mathrm{d}\psi/\mathrm{d}x$, corresponds to the Sturm–Liouville problem and may describe the propagation of a plane electromagnetic wave with the wavenumber $k = \omega/c$ and frequency ω in the medium with a variable dielectric permeability $\epsilon(x)$ [5], or a Schrödinger equation when $k^2\epsilon(x) = (2m/\hbar^2)(E - U(x))$, where E is the energy of the particle, $U(x)$ the potential [4] and so on.

When $N > 2$, we have a multicomponent wave equation which describes a system of coupled waves of different physical nature [3, 6]. Thus, the case of $N = 4$ may correspond to equations of polariton theory, the magnetospring, spin-photon waves [7] etc; in particular, to the Bogoliubov–de Gennes [8] equations in superconductivity when

$$\mathsf{A}(x) = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -(2m/\hbar^2)(E - U(x) + \mu) & 0 & -(2m/\hbar^2)\Delta(x) & 0 \\ 0 & 0 & 0 & 1 \\ (2m/\hbar^2)\Delta^*(x) & 0 & (2m/\hbar^2)(E + U(x) - \mu) & 0 \end{pmatrix} \quad \mathbf{\Psi} = \begin{pmatrix} u \\ u' \\ v \\ v' \end{pmatrix} \tag{3}$$

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0305-4470/96/165103+21$19.50

where μ is the Fermi energy, $U(x)$ the lattice potential, and $\Delta(x)$ the pair potential. The wave equations for particles in a magnetic field with simple orientation and also gauging may often be reduced to form (1), when we obtain a dependence on vector-potential terms in the matrix $\mathbf{A}(x)$ on and off the diagonal. The case $N = 4$ is also the one-dimensional Dirac equation, when $\boldsymbol{\Psi}$ is a bispinor and

$$\mathbf{A}(x) = -i\{\hat{\boldsymbol{\alpha}}^{-1}[(E - e\Phi(x))\mathbf{I} - \boldsymbol{\beta}m] + e\mathcal{A}(x)\mathbf{I}\}_x$$

is a matrix along the momentum component $p_x = \mathrm{i}\partial_x$, $\Phi(x)$ is a scalar, $\mathcal{A}(x)$ the vector potential, $\hat{\boldsymbol{\alpha}}$, $\boldsymbol{\beta}$ the Dirac matrices, $\mathbf{I}$ the unit matrix, and $c = \hbar = 1$ [9]. It should be remarked that the potentials are often determined from a self-consistent procedure which makes the wave problem nonlinear. This concerns particularly the potential $\Delta(x)$ in the BCS model of superconductivity or fields in quantum electrodynamics. But, so far as the procedure of self-consistency includes sums on many states, then for the one-particle spectral problems the potentials may be treated as external and pre-assigned an average.

One usually employs the Floke–Liapunov (Bloch) theorem [2] for investigation of questions concerning zones of stability, localization, and asymptotic behaviour of wavefunctions in multilayered systems with periodic $\mathbf{A}(x)$ matrices. However, in multilayered systems a rigorous periodicity is often absent, for example in systems with an accidental or non-accidental unperiodic potential profile [4, 10, 11], in multilayered systems in external fields, and in current states of superconducting superlattices where the modulus of the pair potential is periodic but not the phase [8]. The numerical analysis on the basis of the tight binding approximation is common for modelling such systems [10, 12, 13]. The transfer-matrix (dynamical mapping) technique [3, 13] is one of the formally rigorous convenient methods. Most works use this technique for the case of $N = 2$, with a binomial recurrence procedure and a peculiar role tridiagonal matrices [14]. On the other hand, it is common knowledge that for any linear differential equation of order N the equivalent rigorous difference equation which connects the values of the function in $N + 1$ discrete points (equation (5) below) is constructed. We can express the coefficients of the difference equation in terms of the one step by these point transfer-matrix elements. For example, this type of expression for the Schrödinger equation was examined in [15].

The main aim of the present paper is the construction of a rigorous analytic algorithm, generalizing this method to equations of form (1) of order higher than two, provided that the solutions of the equation for the transfer matrix are known on a sequence of x-axis intervals. The differential equation (1) is replaced by the equation for the transfer matrix and then by the rigorous difference Poincaré mapping. Constraints such as tight or weak binding are unnecessary. Our consideration accepts any boundary conditions as asymptotically free moving waves, scattered by a system, so we have immobile standing waves in the localization problems. Constructions such as a ‘segmented’ potential that has constant value regions with quasi-free motion exponential solutions [16] or other types [17] of solutions are not essential. In scattering problems, knowledge of the transfer matrix allows one to find the reflection and transmission coefficients [16] and to construct the scattering matrix [6, 18] for given potentials. An important point is that for $N > 2$ we may consider the effects of space modulation not only on the external potentials (fundamental frequencies) for different waves, but also on the coupling parameters, such as the pair potential $\Delta(x)$ in (3) (non-diagonal effects). This modulation appears in many physical effects, such as in the mixing of modes, the splitting and repulsion of different spectrum branches near degeneracy points [7], in the existence of directed wave currents in the states of a discrete spectrum (the Andreev’s states in Josephson SNS junctions [8]) and a good many others.

The elements of the transfer matrix satisfy almost the same differential and difference equations as the wavefunction. The difference equations for the elements of the transfer matrix and the renormalization relations for their coefficients of recursion under homogeneous and non-homogeneous changing of the step scale are obtained below. We have to emphasize the important role of these recurrent coefficients, because they make up the hierarchy of polynomials possessing some similarity properties. For different concrete systems and models of potentials, one may then search for the renormgroup asymptotic behaviour of the wavefunctions and spectra, especially near the fixed points of commensurability of the potentials space periodicity formation [13, 19].

The algebraic formulae for the matrix elements, being derived by a generalization of the well known two-dimensional case, are not so far evident. In this connection, we deduce some new interesting minor properties of Toeplitz $(N+1)$-diagonal band matrices in Hessenberg form [21, 23].We obtain incidentally the formulae which are a generalization of the widely used Abelés theorem [3, 5, 20] to the arbitrary power of any dimensional square matrix by using polynomials of many arguments generalizing the Chebyshev polynomials. Such a generalization of the theorem should be very helpful in the analysis of complicated processes of coupled wave propagation through multilayered periodical media.

2. The transfer matrix

The set of equations (1) is equivalent to one differential equation of Nth order with variable coefficients

$$\psi^{(N)} + a_1\psi^{(N-1)} + \ldots + a_{N-1}\psi' + a_N\psi = 0. \tag{4}$$

If $\psi_i(x)$ are the known linear independent solutions of (4), then the arbitrary solution $\psi(x)$ may be specified by its values $\psi(x_j)$ at N points, x_j, (the initial or boundary conditions) $(i, j = 1, 2, \ldots, N)$,

$$\psi(x) = \frac{1}{V(x_1, x_2, \ldots, x_N)} \sum_{j=1}^{N} V(x_1, \ldots, x_{j-1}, x, x_{j+1}, \ldots, x_N)\psi(x_j) \tag{5}$$

$$V(x_1, x_2, \ldots, x_N) = \det\{\psi_i(x_j)\} = \begin{vmatrix} \psi_1(x_1) & \psi_2(x_1) & \ldots & \psi_N(x_1) \\ \psi_1(x_2) & \psi_2(x_2) & \ldots & \psi_N(x_2) \\ \cdots & \cdots & \cdots & \cdots \\ \psi_1(x_N) & \psi_2(x_N) & \ldots & \psi_N(x_N) \end{vmatrix} \tag{6}$$

but, conveniently, to set the values of the initial conditions at one point $x_0 = 0$ using the derivatives $\mathbf{\Psi}(0) = \mathrm{col}(\psi(0), \psi'(0), \ldots, \psi^{(N-1)}(0))$, we have

$$\mathbf{\Psi}(x) = \mathsf{M}_x\mathbf{\Psi}(0) \qquad \mathbf{\Psi}(x) = \mathrm{col}(\psi(x), \psi'(x), \ldots, \psi^{(N-1)}(x)) \tag{7}$$

where $\mathsf{M}_x = \{M_{ij}(x)\}$ $(i, j = 1, 2, \ldots, N)$ is the matrix of transfer from x_0 to x. Moreover, in the representation (7) the elements of the first row M_{1j} give the required solution

$$\psi(x) = \sum_{j=1}^{N} M_{1j}(x)\psi^{(j-1)}(0) \tag{8}$$

and take the form

$$M_{1j} = \frac{W_j}{W_0} \tag{9}$$

where W_0 is the value at $x = x_0$ of the Wronskian

$$W(x) = \det\{\psi_i^{(j-1)}(x)\} = \begin{vmatrix} \psi_1(x) & \psi_2(x) & \dots & \psi_N(x) \\ \psi_1{}'(x) & \psi_2{}'(x) & \dots & \psi_N{}'(x) \\ \dots & \dots & \dots & \dots \\ \psi_1^{(N-1)}(x) & \psi_2^{(N-1)}(x) & \dots & \psi_N^{(N-1)}(x) \end{vmatrix} \tag{10}$$

and W_j is found from W_0 by replacing its j-row elements with $\psi_1(x), \psi_2(x), \dots, \psi_{(N)}$.

The elements of other transfer-matrix rows in the representation (7) are given by

$$M_{ij} = \frac{\mathrm{d}^{(i-1)} M_{1j}}{\mathrm{d}x^{(i-1)}} \qquad i = 2, \dots, N \tag{11}$$

e.g. M_{ij} is found from M_{1j} by replacing functions $\psi_k(x) \quad (k = 1, \dots, N)$ in the j-row of the W_j functions by their derivatives $\psi_k^{(i)}(x)$.

It follows from the Liouville–Jacobi theorem [1] for the systems with $\mathrm{Sp}\mathbf{A} = 0$ (that is $a_1 = 0$) that the Wronskian is x-independent, $W = W_0$, and the transfer matrix is unimodular:

$$\det \mathbf{M}_x = 1. \tag{12}$$

With the help of a non-singular linear transformation $\boldsymbol{U} = \boldsymbol{U}(x)$ we can go from (7) to any other representation

$$\widetilde{\boldsymbol{\Psi}}(x) = \boldsymbol{U}\boldsymbol{\Psi}(x) \qquad \widetilde{\mathbf{A}}(x) = \boldsymbol{U}\mathbf{A}(x)\boldsymbol{U}^{-1} - \boldsymbol{U}\frac{\mathrm{d}\boldsymbol{U}^{-1}}{\mathrm{d}x}$$

$$\widetilde{\boldsymbol{\Psi}}(x) = \mathrm{col}(\widetilde{\psi}_1(x), \dots, \widetilde{\psi}_N(x)) \tag{13}$$

$$\widetilde{\boldsymbol{\Psi}}(x) = \widetilde{\mathbf{M}}_x \widetilde{\boldsymbol{\Psi}}(0) \qquad \widetilde{\mathbf{M}}_x = \boldsymbol{U}\mathbf{M}_x\boldsymbol{U}^{-1} \tag{14}$$

where the new transfer matrix $\widetilde{\mathbf{M}_x}$ has the same determinant and eigenvalues λ_x as $\mathbf{M}_x$. One reduces the stability analysis to study the behaviour of λ_x with changing energy or other parameters.

We do not render this concrete representation any further, so by substituting (7) or (13) and (14) into (1) it is easy to see that the initial set of N equations (1) is replaced in the transfer matrix method by the set of N^2 equations for the elements of the matrix,

$$\frac{\mathrm{d}\mathbf{M}_x}{\mathrm{d}x} = \mathbf{A}(x)\mathbf{M}_x \qquad \text{or} \qquad \frac{\mathrm{d}(M_x)_{ij}}{\mathrm{d}x} = (\boldsymbol{A}(x)\boldsymbol{M}_x)_{ij} \tag{15}$$

with the initial condition

$$\mathbf{M}_0 = \mathbf{I} \qquad \text{or} \qquad (M_0)_{ij} = \delta_{ij} = \begin{cases} 1 & i = j \\ 0, & i \neq j. \end{cases} \tag{16}$$

There are certainly $N(N-1)$ relations of type (11) between the elements M_{ij}. The return to the concrete movement wavefunction is given by (7) or (14),

$$\boldsymbol{\Psi}(x) = \mathbf{M}_x \boldsymbol{\Psi}(0) \tag{17}$$

where $\boldsymbol{\Psi}(0)$ is the system of the boundary conditions. We found the spectrum from the second boundary condition at the point $x = x_L$:

$$\boldsymbol{\Psi}(x_L) = \mathbf{M}_L \boldsymbol{\Psi}(0). \tag{18}$$

The transfer matrix role resembles the role of the Green function that satisfies the non-homogeneous dynamical equation similar to the input equation but with the point source initial condition. In contrast to the Green's function equation, the equation for the transfer matrix (15) is homogeneous and does not contain a singular point source which plays the role of the diagonal initial condition (16).

In the following sections we shall show how the solutions of equations (15) may be written and analysed with the help of the determinants of $(N+1)$-diagonal matrices. Moreover, it automates the obtaining of coefficients in the recurrent formulae of type (5), which is the foundation of the roughening procedure (finding of the envelope function) for investigation of localization. The derivable formulae should be useful for the description of many other physical characteristics in parametric wave processes.

3. The recurrent procedure

Let us divide the segment $[x_0, x]$ by the points $x_1, x_2, \ldots, x_n, \ldots$; assume that the problem (15), (16) is solved on each half-interval $[x_{n-1}, x_n]$ and $\mathbf{T}_n$ is the one-step matrix of transfer from x_{n-1} to x_n derived in accordance with (9) and (11) or other formulae. Then for the transfer matrix $\mathbf{M}_n$ from x_0 to x_n evidently

$$\mathbf{M}_n = \mathbf{T}_n \mathbf{M}_{n-1} \qquad \mathbf{M}_0 = \mathbf{T}_0 = \mathbf{I} \tag{19}$$

gives the basis for the recurrence procedure for the computation of every N^2 elements $(M_n)_{ik}$ of $\mathbf{M}_n$ via the elements of the one-step matrices $\mathbf{T}_n$. Since

$$(M_n)_{ik} = (T_n)_{ii}(M_{n-1})_{ik} + \sum_{\substack{j=1\\ j\neq i}}^{N} (T_n)_{ij}(M_{n-1})_{jk} \tag{20}$$

and the element $(M_{n-1})_{ik}$ is contained under the sum in the expressions of type (20) for the other k-column $\mathbf{M}_n$ elements, by taking N of these expressions for every $n, n-1, \ldots, n-N+1$ steps under $n \geqslant N$ we get a system of N^2 equations from which $N^2 - 1$ variables $(M_n)_{jk} \quad (j \neq i)$ may be excluded. The last action is simple to perform by equating to zero an augmented determinant of the received system of N^2 equations. The linear relation thus obtained connects $N+1$ elements $(M_n)_{ik}, (M_{n-1})_{ik}, \ldots, (M_{n-N})_{ik}$ of the same type (ik) on the consecutive steps

$$(M_n)_{ik} = \sum_{l=1}^{N} (-1)^{l+1} \alpha(i)_l^{(n)} (M_{n-l})_{ik} \tag{21}$$

which is the required recurrence relation. The coefficients $\alpha(i)_l^{(n)}$ are expressed over the elements of N consecutive one-step matrices $\mathbf{T}_n$ (see the appendix, formula (A.11)). For $n < N$, i.e. the elements of the leading $N-1$ matrices $\mathbf{M}_n$, we need to compute with the help of (19) by direct matrix multiplication

$$\mathbf{M}_n = \prod_{p=1}^{n} \mathbf{T}_p. \tag{22}$$

The complete recursion is formed on the Nth step. Then we may represent result (21) via the elements of $N-1$ leading matrices $(M_l)_{ik}$ $(l = 1, 2, \ldots, N-1)$ and the previous recurrence coefficients (omitting its row index i for brevity) in a form of the determinant of the $(N+1)$-diagonal $n \times n$ matrix

$$(M_n)_{ik} = \begin{vmatrix} (M(N))_{ik} & R \\ L & \Delta \end{vmatrix} \tag{23}$$

where for $N > 2$ in the left upper corner there is a block which is the two-diagonal matrix of $(N-1)\times(N-1)$ dimensionality,

$$
(M(N))_{ik} = \begin{pmatrix}
(M_1)_{ik} & \delta_{ik} & & & & \\
 & \dfrac{(M_2)_{ik}}{(M_1)_{ik}} & 1 & & & \\
 & & \dfrac{(M_3)_{ik}}{(M_2)_{ik}} & 1 & & \\
 & & & \ddots & \ddots & \\
 & & & \dfrac{(M_{N-2})_{ik}}{(M_{N-3})_{ik}} & 1 & \\
 & & & 0 & \dfrac{(M_{N-1})_{ik}}{(M_{N-2})_{ik}} &
\end{pmatrix} \tag{24}
$$

with the rest of the elements being zero. Block $\boldsymbol{\Delta}$ is the $(N+1)$-diagonal $(n-N+1)\times(n-N+1)$ matrix

$$
\Delta = \begin{pmatrix}
\alpha_1^{(N)} & 1 & & & & & & & \\
\alpha_2^{(N+1)} & \alpha_1^{(N+1)} & 1 & & & & & & \\
\alpha_3^{(N+2)} & \alpha_2^{(N+2)} & \alpha_1^{(N+2)} & 1 & & & & & \\
\multicolumn{4}{c}{\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots} & & & & & \\
\alpha_N^{(2N-1)} & \alpha_{N-1}^{(2N-1)} & \dots & \alpha_1^{(2N-1)} & 1 & & & & \\
 & \alpha_N^{(2N)} & \alpha_{N-1}^{(2N)} & \dots & \alpha_1^{(2N)} & 1 & & & \\
 & & \ddots & \ddots & \dots & \ddots & \ddots & & \\
 & & & \alpha_N^{(n-1)} & \alpha_{N-1}^{(n-1)} & \dots & \alpha_1^{(n-1)} & 1 \\
 & & & & \alpha_N^{(n)} & \alpha_{N-1}^{(n)} & \dots & \alpha_1^{(n)}
\end{pmatrix}. \tag{24$'$}
$$

The rectangular block R with a single non-zero element equal to unity in its left lower corner and block L with non-zero elements in its right upper triangle are

$$
R = \begin{pmatrix} & & \\ 1 & & \end{pmatrix} \qquad
L = \begin{pmatrix}
\alpha_N^{(N)} & \alpha_{N-1}^{(N)} & \alpha_{N-2}^{(N)} & \dots & \alpha_2^{(N)} \\
 & \alpha_N^{(N+1)} & \alpha_{N-1}^{(N+1)} & \dots & \alpha_3^{(N+1)} \\
 & & \alpha_N^{(N+2)} & \dots & \alpha_4^{(N+2)} \\
 & & & \ddots & \dots \\
 & & & & \alpha_N^{(2N-2)} \\
0 & & & & 0 \\
\multicolumn{5}{c}{\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots}
\end{pmatrix}. \tag{24$''$}
$$

For $N = 1, (M(1))_{ik} = 1$, and for $N = 2, (M(2))_{ik} = (M_1)_{ik}$ and δ_{ik} occurs in R instead of unity.

It should be noted that the results (23) and (24) include the operation of division on the elements $(T_n)_{ij}$ which may be equal to zero. But these singularities are removable by expanding the determinants along the adjacent rows containing such elements in the denominators and in the numerators as well. Besides we may remove any zeros of $(T_n)_{ij}$ by the variation of the size of x_n steps.

In the important case of the periodic system, if the step is equal to the period of the $\mathbf{A}(x)$ matrix and $\mathbf{T}_n = \mathbf{T}$ is on a period transfer matrix (monodromy matrix [2]) then $\alpha_l^{(n)} = \alpha_l$

are identical along each diagonal and

$$\mathbf{M}_n = \mathbf{T}^n \qquad \frac{(M_l)_{ik}}{(M_{l-1})_{ik}} = \frac{(T^l)_{ik}}{(T^{l-1})_{ik}} \tag{25}$$

in accordance with the well known Sylvester formula [22] the consequence of which is the conclusion (Abelés [20]) of the fact that the integer powers of $N \times N$ matrix are representable by its matrix polynomial of $N - 1$ power (see section 6).

One can see from the derivation that the coefficients $\alpha(i)_l^{(n)}$ in the recurrence formula (21) are independent of the column index k, i.e. they are equal for all elements $(M_n)_{ik}$ in the i-row of the transfer matrix. So in accordance with (17), that is

$$\psi_i(x_n) = \sum_{k=1}^{N} (M_n)_{ik} \psi_k(0) \tag{26}$$

the same $\alpha(i)_l^{(n)}$ are the recursion coefficients in (5) for a wavefunction ψ_i from the $\mathbf{\Psi}$ column

$$\psi_i(x_n) = \sum_{l=1}^{N} (-1)^{l+1} \alpha(i)_l^{(n)} \psi_i(x_{n-l}). \tag{27}$$

We emphasize that the choice of the node points here is arbitrary and all expressions up to (27) are rigorous. In the case of non-unimodular matrices $\mathbf{T}_n$ and $\mathbf{M}_n$ we may always pass to unimodular ones $(\boldsymbol{T}_n^{(0)})_{ik}$ and $(\boldsymbol{M}_n^{(0)})_{ik}$ by the norming replacement

$$(T_n)_{ik} = (\det \mathbf{T}_n)^{1/N} (T_n^{(0)})_{ik} \qquad (M_n)_{ik} = \prod_{j=1}^{n} (\det \mathbf{T}_j)^{1/N} (M_n^{(0)})_{ik}. \tag{28}$$

4. Algebra of $(N+1)$-diagonal determinants and recurrence coefficient renormalization $(N = 1, 2, 4)$

Let us consider a question about the renormalization [13, 19] of the recurrence coefficients $\alpha(i)_l^{(n)}$ with the change of sampling of N node points, $l = 1, 2, \ldots, N$, from the set of n points, x_n, of the x-axis subdivision. The most frequent cases in the applications are $N = 2$ (Schrödinger equation, electromagnetic wave equation, elasticity equation) and $N = 4$ (two types of coupled waves, Bogoliubov, Dirac equations). So we represent their detailed results. The generalization to any arbitrary N case is evident by induction.

We denote for a clearness the leading four coefficients by

$$\alpha(i)_1^{(m)} = \alpha(i)_m \qquad \alpha(i)_2^{(m)} = \beta(i)_m \qquad \alpha(i)_3^{(m)} = \gamma(i)_m \qquad \alpha(i)_4^{(m)} = \delta(i)_m. \tag{29}$$

We note that they characterize all i-row elements of the transfer matrix, but we shall omit the i-index in the coefficients where it is convenient. It is also convenient to introduce special notations for the determinants of the $(N+1)$-diagonal matrices of $n - m + 1$ dimensiality in the right lower corner of (23), block Δ. For $N = 1, 2, 4$ they are

$$A_n^m = \begin{vmatrix} \alpha_m & 1 & & & & \\ & \alpha_{m+1} & 1 & & & \\ & & \alpha_{m+2} & 1 & & \\ & & & \ddots & \ddots & \\ & & & & \alpha_{n-1} & 1 \\ & & & & & \alpha_n \end{vmatrix}$$

$$B_n^m = \begin{vmatrix} \alpha_m & 1 & & & & \\ \beta_{m+1} & \alpha_{m+1} & 1 & & & \\ & \beta_{m+2} & \alpha_{m+2} & 1 & & \\ & & \beta_{m+3} & \alpha_{m+3} & 1 & \\ & & & \ddots & \ddots & \ddots \\ & & & & \beta_n & \alpha_n \end{vmatrix}$$

$$D_n^m = \begin{vmatrix} \alpha_m & 1 & & & & & \\ \beta_{m+1} & \alpha_{m+1} & 1 & & & & \\ \gamma_{m+2} & \beta_{m+2} & \alpha_{m+2} & 1 & & & \\ \delta_{m+3} & \gamma_{m+3} & \beta_{m+3} & \alpha_{m+3} & 1 & & \\ & \delta_{m+4} & \gamma_{m+4} & \beta_{m+4} & \alpha_{m+4} & 1 & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots \\ & & & \delta_n & \gamma_n & \beta_n & \alpha_n \end{vmatrix} \tag{30}$$

where $m < n$. By extending the definition for $m \geqslant n$ with formal properties

$$A_n^n = B_n^n = D_n^n = \alpha_n \qquad \text{for} \quad m = n \tag{31}$$

$$A_n^{n+1} = B_n^{n+1} = D_n^{n+1} = 1 \qquad \text{for} \quad m = n+1 \tag{32}$$

$$A_n^m = B_n^m = D_n^m = 0 \qquad \text{for} \quad m > n+1 \tag{33}$$

we get an $(N+1)$-diagonal determinant algebra.

4.1. *The trivial case $N = 1$*

For

$$\mathbf{M}_n = \alpha_n \mathbf{M}_{n-1} = \prod_{i=1}^{n} \alpha_i \tag{34}$$

the connection between $\mathbf{M}_n$ and $\mathbf{M}_m$ in two arbitrary points $n, m (n > m)$ is

$$\mathbf{M}_n = \alpha_{nm} \mathbf{M}_m \tag{35}$$

$$\alpha_{nm} = A_n^{m+1} = \prod_{i=m+1}^{n} \alpha_i. \tag{36}$$

4.2. *The case $N = 2$*

This is characterized by the B_n^m determinants and the matrix elements

$$(M_n)_{ik} = \begin{vmatrix} (M_1)_{ik} & \delta_{ik} & & & \\ \beta_2 & \alpha_2 & 1 & & \\ & \beta_3 & \alpha_3 & 1 & \\ & & \ddots & \ddots & \ddots \\ & & & \beta_n & \alpha_n \end{vmatrix}. \tag{37}$$

By expanding B_n^m along the row with β_{r+1} we have

$$B_n^m = B_r^m B_n^{r+1} - B_{r-1}^m \beta_{r+1} B_n^{r+2}. \tag{38}$$

In particular, along the first row $(r = m)$

$$B_n^m = \alpha_m B_n^{m+1} - \beta_{m+1} B_n^{m+2} \tag{39}$$

which increases a superscript, and along the last row $(r = n-1)$

$$B_n^m = \alpha_n B_{n-1}^m - \beta_n B_{n-2}^m \tag{40}$$

which decreases a subscript. From here with the help of (32)–(33) it is easy to verify for $r < m < n$ the following equalities,

$$\begin{vmatrix} B_m^r & B_m^{r+1} \\ B_n^r & B_n^{r+1} \end{vmatrix} = B_n^{m+2} \prod_{i=r+1}^{m+1} \beta_i \qquad \begin{vmatrix} B_{s-2}^r & B_{s-1}^r \\ B_{s-2}^l & B_{s-1}^l \end{vmatrix} = B_{l-2}^r \prod_{i=l}^{s-1} \beta_i. \tag{41}$$

That is, for $n > m > s > l > r$

$$\begin{vmatrix} B_m^r & B_m^l \\ B_n^r & B_n^l \end{vmatrix} = \begin{vmatrix} B_{s-2}^r & B_{s-1}^r \\ B_{s-2}^l & B_{s-1}^l \end{vmatrix} \cdot \begin{vmatrix} B_m^s & B_m^{s+1} \\ B_n^s & B_n^{s+1} \end{vmatrix} \cdot \beta_s = B_{l-2}^r B_n^{m+2} \prod_{i=l}^{m+1} \beta_i \tag{42}$$

and, in addition, for any B_n^m and $n, m, p > l, s, r$ the equality takes place:

$$\begin{vmatrix} B_n^s & B_n^r & B_n^l \\ B_m^s & B_m^r & B_m^l \\ B_p^s & B_p^r & B_p^l \end{vmatrix} = 0. \tag{43}$$

By acting similarly with (37) we have

$$(M_n)_{ik} = B_n^{r+1}(M_r)_{ik} - \beta_{r+1} B_n^{r+2} (M_{r-1})_{ik} \tag{44}$$

which expresses $(M_n)_{ik}$ via two arbitrary sequential terms on r and $r-1$ steps. In particular, for $r = 1$, via the leading $(M_1)_{ik}$ and $(M_0)_{ik} = \delta_{ik}$,

$$(M_n)_{ik} = B_n^2 (M_1)_{ik} - \beta_2 B_n^3 \delta_{ik} \tag{45}$$

and for $r = n - 1$ it gives (21), i.e. via two previous terms,

$$(M_n)_{ik} = \alpha_n (M_{n-1})_{ik} - \beta_n (M_{n-2})_{ik}. \tag{46}$$

We obtain the connection between $(M_n)_{ik}$ in three arbitrary points n, m, p by writing out a set of three equations (44) with fixed r and its augmented determinant, and then with the help of (39) get for any $n, m, p > l, s, r$ the equality of type (43):

$$\begin{vmatrix} (M_n)_{ik} & B_n^r & B_n^l \\ (M_m)_{ik} & B_m^r & B_m^l \\ (M_p)_{ik} & B_p^r & B_p^l \end{vmatrix} = 0. \tag{47}$$

We suppose $n > m > p$ and give to (47) a form

$$(M_n)_{ik} = \alpha_{nmp} (M_m)_{ik} - \beta_{nmp} (M_p)_{ik} \tag{48}$$

$$\alpha_{nmp} = \frac{B_n^{p+2}}{B_m^{p+2}} \qquad \beta_{nmp} = \frac{B_n^{m+2}}{B_m^{p+2}} \prod_{i=p+2}^{m+1} \beta_i. \tag{49}$$

By expanding the determinant on the left-hand side of (42), we may, if we wish, exclude the β_i product in the last formula:

$$\beta_{nmp} = \alpha_{nmp} B_m^{p+1} - B_n^{p+1}. \tag{50}$$

In particular, the recurrence formula for the transfer matrix elements across $t = 1, 2, \ldots$ steps on points x_n of the x-axis subdivision is

$$(M_{n+2t})_{ik} = \alpha_{(t)} (M_{n+t})_{ik} - \beta_{(t)} (M_n)_{ik} \tag{51}$$

$$\alpha_{(t)} = \frac{B_{n+2t}^{n+2}}{B_{n+t}^{n+2}} \qquad \beta_{(t)} = \frac{B_{n+2t}^{n+2+t}}{B_{n+t}^{n+2}} \prod_{i=n+2}^{n+1+t} \beta_i. \tag{52}$$

The last of the derived expressions is the most interesting from the physical point of view, because it describes the renormalization of the recurrent coefficients α and β with non-homogeneous (49) and homogeneous (52) rescaling.

In a periodic system, if a step is chosen which is equal to a $1/t$ part of some period, i.e. the transfer matrix on a period $\mathbf{M}_t = \mathbf{T} = \prod_{n=1}^{t} \mathbf{T}_n$, and for one-step matrices $\mathbf{T}_{n+t} = \mathbf{T}_n$, then from (A.4) and (A.6) it follows that

$$B_{n+t}^{n+2} = B_{n+2t}^{n+2+t} \qquad \prod_{i=n+2}^{n+1+t} \beta_i = \prod_{n=1}^{t} \det \mathbf{T}_n = \det \mathbf{T} \tag{53}$$

that is for a periodic system there is a transformation (52) with common coefficients for all elements M_{ik} (A.7):

$$\alpha_{(t)} = \mathrm{Sp}\mathbf{T} = \frac{B_{2t}^2}{B_t^2} \qquad \beta_{(t)} = \det \mathbf{T}. \tag{54}$$

It is possible to say that for a periodic system the renorming transformation (52) has for the values

$$\tilde{\alpha}_{(t)} = \frac{\alpha_{(t)}}{\mathrm{Sp}\mathbf{T}} \qquad \tilde{\beta}_{(t)} = \frac{\beta_{(t)}}{\det \mathbf{T}} \tag{55}$$

the fixed point $\tilde{\alpha}_{(t)} = 1, \tilde{\beta}_{(t)} = 1$. Furthermore by passing, with the help of (28), to the unimodular matrix with elements $(M_n^{(0)})_{ik} = (M_n)_{ik}/(\det \mathbf{T})^{n/2}$, in this case it is easy to see that $\beta_{(t)}^{(0)} = 1$ and the determinant B_n^m for $n \geqslant m-2$ is equal to the second-kind Chebyshev polynomial $U_{n-m+1}(y)$, where $y = \alpha_{(t)}/[2(\det \mathbf{T})^{1/2}]$ as far as such polynomials are equal [24, 25] to the determinants of tridiagonal $n \times n$ matrices,

$$U_n(y) = \begin{vmatrix} 2y & 1 & & \\ 1 & 2y & 1 & \\ & \ddots & \ddots & \ddots \\ & & 1 & 2y \end{vmatrix} \tag{56}$$

and also $U_0 = 1, U_{-1} = 0$. So, similarly to (45), we obtain from (51), for a t-step period the well known result of Abelés [3, 5, 20] for the transfer matrix $\mathbf{M}_{nt} = \mathbf{T}^n$ across n periods

$$\frac{\mathbf{T}^n}{(\det \mathbf{T})^{n/2}} = U_{n-1}\left(\frac{\alpha_{(t)}}{2(\det \mathbf{T})^{1/2}}\right) \frac{\mathbf{T}}{(\det T)^{1/2}} - U_{n-2}\left(\frac{\alpha_{(t)}}{2(\det \mathbf{T})^{1/2}}\right) \mathbf{I}. \tag{57}$$

The stability conditions require eigenvalues of $\mathbf{T}$ (multiplicators [2]) to be situated on the unit circle, i.e. $\lambda = \exp(\mathrm{i}Ka)$ where K is the quasi-momentum and a is the period along the x-axis. In the most frequently encountered case of a real potential and unimodular transfer matrices, $\beta_{(t)} = \det \mathbf{T} = 1$, from the characteristic equation one usually obtains the following quasi-momentum dispersion law:

$$2 \cos Ka = \alpha_{(t)}. \tag{58}$$

The condition of spectral stability is $|\alpha_{(t)}| \leqslant 2$. Our formula (54) allows us to find the forbidden zones in the spectrum in accordance with the potential modulation and the numbers of subperiods in the commensurate superlattices. Besides, it is convenient to chose the length of steps and the number t in accordance with the modulation character.

4.3. The case N=4

By operating in the above pattern we obtain the following results. First of all, aside from the determinants D_n^m, it is now convenient to introduce the determinants of the matrices with a shift of diagonals of D_n^m on one step and on two steps to the right:

$$\widetilde{D}_n^m = \begin{vmatrix} \beta_m & \alpha_m & 1 & & & & \\ \gamma_{m+1} & \beta_{m+1} & \alpha_{m+1} & 1 & & & \\ \delta_{m+2} & \gamma_{m+2} & \beta_{m+2} & \alpha_{m+2} & 1 & & \\ & \delta_{m+3} & \gamma_{m+3} & \beta_{m+3} & \alpha_{m+3} & 1 & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots \\ & & & \delta_{n-1} & \gamma_{n-1} & \beta_{n-1} & \alpha_{n-1} \\ & & & & \delta_n & \gamma_n & \beta_n \end{vmatrix}$$

$$\widetilde{\widetilde{D}}{}_n^m = \begin{vmatrix} \gamma_m & \beta_m & \alpha_m & 1 & & & \\ \delta_{m+1} & \gamma_{m+1} & \beta_{m+1} & \alpha_{m+1} & 1 & & \\ & \delta_{m+2} & \gamma_{m+2} & \beta_{m+2} & a_{m+2} & 1 & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots \\ & & & \delta_{n-2} & \gamma_{n-2} & \beta_{n-2} & \alpha_{n-2} \\ & & & & \delta_{n-1} & \gamma_{n-1} & \beta_{n-1} \\ & & & & & \delta_n & \gamma_n \end{vmatrix}. \tag{59}$$

By expanding D_n^m along the $r+1$ row we get

$$\begin{aligned} D_n^m &= D_r^m D_n^{r+1} + D_{r-1}^m(-\beta_{r+1} D_n^{r+2} + \gamma_{r+2} D_n^{r+3} - \delta_{r+3} D_n^{r+4}) \\ &\quad + D_{r-2}^m(\gamma_{r+1} D_n^{r+2} - \delta_{r+2} D_n^{r+3}) - D_{r-3}^m \delta_{r+1} D_n^{r+2}. \end{aligned} \tag{60}$$

In particular, along the first row ($r = m$)

$$D_n^m = \alpha_m D_n^{m+1} - \beta_{m+1} D_n^{m+2} + \gamma_{m+2} D_n^{m+3} - \delta_{m+3} D_n^{m+4} \tag{61}$$

which increases a superscript, and along the last row ($r = n-1$)

$$D_n^m = \alpha_n D_{n-1}^m - \beta_n D_{n-2}^m + \gamma_n D_{n-3}^m - \delta_n D_{n-4}^m \tag{62}$$

which decreases a subscript. From here and (31)–(33), as in the case of $N = 2$, we obtain for $r < n < m < l < s$

$$\begin{aligned} \begin{vmatrix} D_n^r & D_n^{r+1} & D_n^{r+2} & D_n^{r+3} \\ D_m^r & D_m^{r+1} & D_m^{r+2} & D_m^{r+3} \\ D_l^r & D_l^{r+1} & D_l^{r+2} & D_l^{r+3} \\ D_s^r & D_s^{r+1} & D_s^{r+2} & D_s^{r+3} \end{vmatrix} &= \begin{vmatrix} D_m^{n+2} & D_m^{n+3} & D_m^{n+4} \\ D_l^{n+2} & D_l^{n+3} & D_l^{n+4} \\ D_s^{n+2} & D_s^{n+3} & D_s^{n+4} \end{vmatrix} \prod_{j=r+3}^{n+3} \delta_j \\ &= \widetilde{\widetilde{D}}{}_{m+2}^{n+4} \begin{vmatrix} D_m^{l+2} & D_m^{l+3} \\ D_s^{l+2} & D_s^{l+3} \end{vmatrix} \prod_{j=r+3}^{n+3} \delta_j = \widetilde{\widetilde{D}}{}_{m+2}^{n+4} \widetilde{D}_{l+1}^{m+3} D_s^{l+2} \prod_{j=r+3}^{n+3} \delta_j \end{aligned} \tag{63}$$

and also the determinant of the fifth-order type of (43) is equal to zero, $\det D_n^m = 0$, the elements of which, D_n^m, have the same subscripts in each row and superscripts in each column.

By expanding (23) along the row, similarly to (44), we get the recurrence formula for the element $(M_n)_{ik}$ via four sequential terms:

$$\begin{aligned} (M_n)_{ik} &= D_n^{r+1}(M_r)_{ik} + (-\beta_{r+1} D_n^{r+2} + \gamma_{r+2} D_n^{r+3} - \delta_{r+3} D_n^{r+4})(M_{r-1})_{ik} \\ &\quad + (\gamma_{r+1} D_n^{r+2} - \delta_{r+2} D_n^{r+3})(M_{r-2})_{ik} - \delta_{r+1} D_n^{r+2}(M_{r-3})_{ik}. \end{aligned} \tag{64}$$

By setting the augmented determinant of a set of five such equations, for $l, m, n, s, p > r$, equal to zero we get

$$\begin{vmatrix} (M_n)_{ik} & D_n^r & D_n^{r+1} & D_n^{r+2} & D_n^{r+3} \\ (M_m)_{ik} & D_m^r & D_m^{r+1} & D_m^{r+2} & D_m^{r+3} \\ (M_p)_{ik} & D_p^r & D_p^{r+1} & D_p^{r+2} & D_p^{r+3} \\ (M_l)_{ik} & D_l^r & D_l^{r+1} & D_l^{r+2} & D_l^{r+3} \\ (M_s)_{ik} & D_s^r & D_s^{r+1} & D_s^{r+2} & D_s^{r+3} \end{vmatrix} = 0 \tag{65}$$

i.e. by means of (63), for $n > m > p > l > s$, we have again the recurrence relations with the renormalized coefficients

$$(M_n)_{ik} = \alpha(M_m)_{ik} - \beta(M_p)_{ik} + \gamma(M_l)_{ik} - \delta(M_s)_{ik} \tag{66}$$

$$\alpha \equiv \alpha_{nmpls} = \frac{D_n^{p+2}}{D_m^{p+2}} \qquad \beta \equiv \beta_{nmpls} = \frac{\widetilde{D}_{m+1}^{l+3} D_n^{m+2}}{\widetilde{D}_{p+1}^{l+3} D_m^{p+2}}$$
$$\gamma \equiv \gamma_{nmpls} = \frac{\widetilde{\widetilde{D}}_{p+2}^{s+4} \widetilde{D}_{m+1}^{p+3} D_n^{m+2}}{\widetilde{\widetilde{D}}_{l+2}^{s+4} \widetilde{D}_{p+1}^{l+3} D_m^{p+2}} \qquad \delta \equiv \delta_{nmpls} = \frac{\widetilde{\widetilde{D}}_{p+2}^{l+4} \widetilde{D}_{m+1}^{p+3} D_n^{m+2}}{\widetilde{\widetilde{D}}_{l+2}^{s+4} \widetilde{D}_{p+1}^{l+3} D_m^{p+2}} \prod_{j=s+4}^{l+3} \delta_j. \tag{67}$$

For $n - m = m - p = p - s = s - l = t$ this gives the recurrence formula across t steps and also, if the system is periodic across t steps, then $\mathbf{T}_{n+t} = \mathbf{T}_n$ and from (A.14) it follows that

$$D_{n+t}^{m+t} = D_n^m \qquad \widetilde{D}_{n+t}^{m+t} = \widetilde{D}_n^m \qquad \widetilde{\widetilde{D}}_{n+t}^{m+t} = \widetilde{\widetilde{D}}_n^m$$
$$\prod_{j=1}^{t} \delta_j = \prod_{j=1}^{t} \det \mathbf{T}_j = \det \mathbf{T} \tag{68}$$

where $\mathbf{T} = \prod_{j=1}^{t} \mathbf{T}_j$ is the transfer matrix on a period. Then the transformation (67) has the common coefficients (A.14) for all $(M_n)_{ik}$ elements

$$\alpha_{(t)} = \mathrm{Sp}\mathbf{T} = \frac{D_{2t}^2}{D_t^2} \qquad \beta_{(t)} = \mathrm{Sp}\widetilde{\mathbf{T}}_2 = \frac{\widetilde{D}_{2t+1}^3}{\widetilde{D}_{t+1}^3}$$
$$\gamma_{(t)} = \mathrm{Sp}\widetilde{\mathbf{T}}_3 = \frac{\widetilde{\widetilde{D}}_{2t+2}^4}{\widetilde{\widetilde{D}}_{t+2}^4} \qquad \delta_{(t)} = \det \mathbf{T}. \tag{69}$$

Here $\widetilde{\mathbf{T}}_2$ is the second and $\widetilde{\mathbf{T}}_3$ the third (of complementary minors) compound to the $\mathbf{T}$ matrices ((96)below) [21–23], i.e. the transformation (67) across t steps has a fixed point of the unit values of the parameters

$$\frac{\alpha_{(t)}}{\mathrm{Sp}\mathbf{T}} \qquad \frac{\beta_{(t)}}{\mathrm{Sp}\widetilde{\mathbf{T}}_2} \qquad \frac{\gamma_{(t)}}{\mathrm{Sp}\widetilde{\mathbf{T}}_3} \qquad \frac{\delta_{(t)}}{\det \mathbf{T}}. \tag{70}$$

Furthermore, with the help of (28), in this case (64) gives for $r = 3$ the following generalization to $N = 4$ of Abelés formula (57) for a transfer matrix $\mathbf{M}_{nt} = \mathbf{M}_t^n = \mathbf{T}^n$ across $n \geqslant 3$ periods,

$$\begin{aligned} \frac{\mathbf{T}^n}{(\det \mathbf{T})^{n/4}} &= U_{n-3}(\tilde{\alpha}, \tilde{\beta}, \tilde{\gamma}) \frac{\mathbf{T}^3}{(\det \mathbf{T})^{3/4}} + \\ &(-\tilde{\beta} U_{n-4}(\tilde{\alpha}, \tilde{\beta}, \tilde{\gamma}) + \tilde{\gamma} U_{n-5}(\tilde{\alpha}, \tilde{\beta}, \tilde{\gamma}) - U_{n-6}(\tilde{\alpha}, \tilde{\beta}, \tilde{\gamma})) \frac{\mathbf{T}^2}{(\det \mathbf{T})^{1/2}} + \\ &(\tilde{\gamma} U_{n-4}(\tilde{\alpha}, \tilde{\beta}, \tilde{\gamma}) - U_{n-5}(\tilde{\alpha}, \tilde{\beta}, \tilde{\gamma})) \frac{\mathbf{T}}{(\det \mathbf{T})^{1/4}} - U_{n-4}(\tilde{\alpha}, \tilde{\beta}, \tilde{\gamma}) \mathbf{I} \end{aligned} \tag{71}$$

in which

$$\tilde{\alpha} = \mathrm{Sp}\mathbf{T}^{(0)} = \frac{\alpha_{(t)}}{(\det \mathbf{T})^{1/4}}$$
$$\tilde{\beta} = \mathrm{Sp}\widetilde{\mathbf{T}}_2^{(0)} = \frac{\beta_{(t)}}{(\det \mathbf{T})^{1/2}} \qquad \tilde{\gamma} = \mathrm{Sp}\widetilde{\mathbf{T}}_3^{(0)} = \frac{\gamma_{(t)}}{(\det \mathbf{T})^{3/4}} \tag{72}$$

and $\alpha_{(t)}$ and $\beta_{(t)}$ are also expressed with the help of (69) via the elements of the transfer matrix on a period. Instead of Chebyshev polynomials in (71) we have polynomials of three arguments $U_n(x, y, z)$ defined by means of the determinants of five-diagonal $n \times n$ matrices

$$U_n(x,y,z) = \begin{vmatrix} x & 1 & & & & & \\ y & x & 1 & & & & \\ z & y & x & 1 & & & \\ 1 & z & y & x & 1 & & \\ & 1 & z & y & x & 1 & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots \\ & & & 1 & z & y & x \end{vmatrix} \tag{73}$$

and also $U_0 = 1, U_n = 0$ for $n < 0$. Formula (71) is simplified in the periodic system with the unimodular one-step transfer matrix

$$\begin{aligned}\mathbf{T}^n = {} & U_{n-3}(\alpha,\beta,\gamma)\mathbf{T}^3 + (-\beta U_{n-4}(\alpha,\beta,\gamma) + \gamma U_{n-5}(\alpha,\beta,\gamma) - U_{n-6}(\alpha,\beta,\gamma))\mathbf{T}^2 \\ & + (\gamma U_{n-4}(\alpha,\beta,\gamma) - U_{n-5}(\alpha,\beta,\gamma))\mathbf{T} - U_{n-4}(\alpha,\beta,\gamma)\mathbf{I}.\end{aligned} \tag{74}$$

It should be underlined that in (71) and (74) it is not required to solve preliminarily the characteristic equation of the fourth order for the determination of the eigenvalues of $\mathbf{T}$, unlike the results [3, 5, 20] established on the Sylvester interpolation formula.

When we analyse the stability conditions and find allowed zones in the coupled wave spectrum we may come across more possible combinations. The eigenvalues λ of matrix $\mathbf{T}$ are not necessarily pairwise complex conjugative and some pairs of them may leave the unit circle after mutual collision. In the simplest and widespread case of the unimodular transfer matrix $\delta_{(t)} = \det \mathbf{T} = 1$ with four roots of the form $\lambda = \exp(\mathrm{i}Ka)$, from the characteristic equations ((94) and (96) below) it is not hard to write out the universal equation analogous to (58) for the quasi-momentum dispersion law

$$2\cos 2Ka - (\alpha_{(t)} + \gamma_{(t)})\cos Ka - i(\alpha_{(t)} - \gamma_{(t)})\sin Ka + \beta_{(t)} = 0 \tag{75}$$

where it is convenient to find the coefficients from (69), and also $\alpha_{(t)} = \gamma_{(t)}^*$ and $\beta_{(t)}$ is real as a consequence of the Viète theorem. Equation (75) describes the magnification of zone quantity, their possible intersection and repulsion near the degeneracy points in accordance with the potential and coupling parameter space modulation.

5. The arbitrary N case

We generalize the above results by introducing under consideration, as in (30), from m to n steps the determinants Δ_n^m of the $(N+1)$-diagonal $(n-m+1)$-order matrices, standing in the right lower corner block Δ of (23), where $m \geqslant N$, with the notation (21) for the recursion coefficients. Then the generalization of (60) for these determinants is $(m \leqslant r < n)$

$$\Delta_n^m = \sum_{p=0}^{N-1} \Delta_{r-p}^m \left(\sum_{l=1}^{N-p} (-1)^{l+p+1} \alpha_{l+p}^{(r+l)} \Delta_n^{r+l+1} \right) \tag{76}$$

with

$$\Delta_n^n = \alpha_1^{(n)} \qquad \Delta_n^{n+1} = 1 \qquad \Delta_n^m = 0 \qquad \text{for} \quad m > n+1.$$

We may derive from here the formulae of reduction of minor order of type (63) and also prove equality to zero of the $(N+1)$-order determinant, composed of the elements Δ_n^m by rule (43), i.e. they have the same subscripts n_i in rows and superscript m_j in columns $(i, j = 1, \ldots, N+1)$:

$$\det \Delta_{n_i}^{m_j} = 0. \tag{77}$$

The transfer matrix via N sequential terms is

$$(M_n)_{ik} = \sum_{p=0}^{N-1} \left(\sum_{l=1}^{N-p} (-1)^{l+p+1} \alpha_{l+p}^{(r+l)} \Delta_n^{r+l+1} \right) (M_{r-p})_{ik}. \tag{78}$$

In the case of a periodic system with the one-step transfer matrix $\mathbf{T}$ on a period the coefficients are common for all elements M_{ik}, so we have the generalization of formula (71) $(n \geqslant N-1)$

$$\frac{\mathbf{T}^n}{(\det \mathbf{T})^{n/N}} = \sum_{p=0}^{N-1} \left(\sum_{l=1}^{N-p} (-1)^{l+p+1} \tilde{\alpha}_{l+p} U_{n-N-l+1}^{(N)}(\tilde{\alpha}_j) \right) \frac{\mathbf{T}^{N-p-1}}{(\det \mathbf{T})^{(N-p-1)/N}} \tag{79}$$

$$\tilde{\alpha}_{l+p} = \frac{\alpha_{l+p}}{(\det \mathbf{T})^{(l+p)/N}} \qquad \alpha_{l+p} \equiv \alpha_{l+p}^{(N+l-1)} = s_{l+p} = \mathrm{Sp}\widetilde{\mathbf{T}}_{l+p}$$

where s_j are the coefficients of the $\mathbf{T}$ matrix characteristic polynomial (94), $\mathrm{Sp}\widetilde{\mathbf{T}}_j$ are the sums of the jth order principal minors of $\mathbf{T}$ (96) which are equal to traces of the jth compound to $\mathbf{T}$ matrices $\widetilde{\mathbf{T}}_j$, in particular $\mathrm{Sp}\widetilde{\mathbf{T}}_N = \widetilde{\mathbf{T}}_N = \det \mathbf{T}$ [21–23]; furthermore, $U_n^{(N)} = U_n^{(N)}(\tilde{\alpha}_1, \ldots, \tilde{\alpha}_{N-1})$ is the polynomial of $N-1$ variables generalizing (73), i.e. it is equal to the determinant of the $(N+1)$-diagonal $n \times n$ matrix of $N-1$ arguments $\tilde{\alpha}_j$, each of which stands on its own diagonal downwards from the main diagonal between two identity diagonals:

$$U_n^{(N)}(\alpha_1, \ldots, \alpha_{N-1}) = \begin{vmatrix} \alpha_1 & 1 & & & & & & & \\ \alpha_2 & \alpha_1 & 1 & & & & & & \\ \alpha_3 & \alpha_2 & \alpha_1 & 1 & & & & & \\ \multicolumn{4}{c}{\dots\dots\dots\dots\dots\dots} & & & & & \\ \alpha_{N-1} & \alpha_{N-2} & \ldots & \alpha_1 & 1 & & & & \\ 1 & \alpha_{N-1} & \alpha_{N-2} & \ldots & \alpha_1 & 1 & & & \\ & 1 & \alpha_{N-1} & \alpha_{N-2} & \ldots & \alpha_1 & 1 & & \\ & & \ddots & \ddots & \ddots & \ldots & \ddots & \ddots & \\ & & & 1 & \alpha_{N-1} & \alpha_{N-2} & \ldots & \alpha_1 & 1 \\ & & & & 1 & \alpha_{N-1} & \alpha_{N-2} & \ldots & \alpha_1 \end{vmatrix}$$

$$\text{and} \quad U_0^{(N)} = 1 \qquad U_n^{(N)} = 0 \quad \text{for} \quad n < 0. \tag{80}$$

The last result (79) looks simpler in the case of the unimodular $\mathbf{T}$ matrix

$$\mathbf{T}^n = \sum_{p=0}^{N-1} \left(\sum_{l=1}^{N-p} (-1)^{l+p+1} \alpha_{l+p} U_{n-N-l+1}^{(N)} \right) \mathbf{T}^{N-p-1}. \tag{81}$$

The polynomials $U_n^{(N)} = U_n^{(N)}(\alpha_1, \ldots, \alpha_{N-1})$ obey the recurrent relations resembling expression (21),

$$U_n^{(N)} = \sum_{l=1}^{N} (-1)^{l+1} \alpha_l U_{n-l}^{(N)} \qquad \alpha_N = 1$$
$$U_0^{(N)} = 1 \qquad U_n^{(N)} = 0 \quad \text{for} \quad n < 0 \tag{82}$$

and satisfy the admissible differential equations

$$\frac{\partial U_n^{(N)}}{\partial \alpha_1} = (-1)^l \frac{\partial U_{n+l}^{(N)}}{\partial \alpha_{1+l}} \qquad l = 1, 2, \ldots, N-2 \tag{83}$$

$$\sum_{l=0}^{N} \alpha_l \frac{\partial^N U_n^{(N)}}{\partial \alpha_1^{N-l} \partial \alpha_2^l} + N \frac{\partial^{N-1} U_n^{(N)}}{\partial \alpha_1^{N-2} \partial \alpha_2} = 0 \tag{84}$$

where $\alpha_0 = \alpha_N = 1$. By differentiation of (83) with respect to different α_l we may get the relations between the higher derivations of polynomials $U_n^{(N)}$ and from (84) the differential equations of lower power that we shall not write down here.

We shall now find the renormalization of the coefficients α_l under changing of the step. Corresponding relations will have, similarly to (67) and (69), the form of the ratio of products of the determinants, received from Δ_n^m by shifting diagonals to the right.

Let us introduce the notation $(\Delta_l)_n^m$ for the determinant of the matrix received from the matrix of the determinant $\Delta_n^m \equiv (\Delta_1)_n^m$ by shifting of the diagonals on $l-1$ to the right; for example, for $N = 4$ in (59) this will be $(D_1)_n^m = D_n^m$, $(D_2)_n^m = \widetilde{D}_n^m$, $(D_3)_n^m = \widetilde{\widetilde{D}}_n^m$ and so on. It is easy to notice that for $l = N$ such a matrix is an upper triangular and in its j-row on the main diagonal is $\alpha_N^{(j)}$, hence

$$(\Delta_N)_n^m = \prod_{j=m}^{n} \alpha_N^{(j)}. \tag{85}$$

In this notation for an arbitrary N the generalization of (66) is

$$(M_{n_{(N+1)}})_{ik} = \sum_{l=1}^{N} (-1)^{l+1} \alpha_l (M_{n_{(N-l+1)}})_{ik} \tag{86}$$

and the generalization of (67) is the following renormalizing relation

$$\alpha_l = \frac{(\Delta_l)_{n_{(N-l+2)}+l-1}^{n_{(N-l)}+l+1}}{(\Delta_l)_{n_{(N-l+1)}+l-1}^{n_{(N-l)}+l+1}} \cdot F_l \tag{87}$$

where $F_l = 1$ for $l = 1$, and for $N \geqslant l > 1$

$$F_l = \prod_{p=1}^{l-1} \frac{(\Delta_p)_{n_{(N-p+2)}+p-1}^{n_{(N-p+1)}+p+1}}{(\Delta_p)_{n_{(N-p+1)}+p-1}^{n_{(N-p)}+p+1}}. \tag{88}$$

For $l = N$ in (87) the fraction, standing before F_l, is equal to

$$\frac{(\Delta_N)_{n_2+N-1}^{n_{(0)}+N+1}}{(\Delta_N)_{n_1+N-1}^{n_{(0)}+N+1}} = \frac{\prod_{j=n_{(0)}+N+1}^{n_2+N-1} \alpha_N^{(j)}}{\prod_{j=n_{(0)}+N+1}^{n_1+N-1} \alpha_N^{(j)}} = \prod_{j=n_1+N}^{n_2+N-1} \alpha_N^{(j)} \tag{89}$$

where $n_{(0)}$ is the number of any initial node $n_{(0)} < n_{(N-l+1)}$; one can see that its dependence in (89) is cancelled.

In a periodic system across t steps by generalization of (68) we have

$$\begin{aligned} &(\Delta_p)^{n_{(l)}}_{n_{(m)}} = (\Delta_p)^{n_{(l+1)}}_{n_{(m+1)}} \qquad F_l = 1 \\ &n_{(N-l+1)} - n_{(N-l)} = t \qquad n_{(N-l+2)} - n_{(N-l)} = 2t \end{aligned} \tag{90}$$

and so on. The generalization of formulae (69) in this case will be that for all matrix elements the common coefficients are

$$\alpha_{l(t)} = \frac{(\Delta_l)^{l+1}_{2t+l-1}}{(\Delta_l)^{l+1}_{t+l-1}}. \tag{91}$$

In particular, for the last coefficient at $l = N$ from (85) it follows, obviously, that

$$\alpha_{N(t)} = \prod_{j=1}^{t} \alpha_N^{(j)} = \prod_{j=1}^{t} \det \mathbf{T}_j = \det \mathbf{T} \tag{92}$$

where $\mathbf{T}$ is the transfer matrix across the period. In such a periodic system the transformation (87) across t steps has a fixed point in which all the parameters $\alpha_{l(t)}/\mathrm{Sp}\widetilde{\mathbf{T}}_l$ are equal to unit, where $\mathrm{Sp}\widetilde{\mathbf{T}}_l$ is the trace of the lth compound to the $\mathbf{T}$ matrix.

6. Recurrence coefficients in a periodical system

In the periodic multilayered systems there exists at hand the Sylvester (Abelés [20]) formula of the polynomial interpolation for the transfer matrix $\mathbf{T}^n$ on n periods via the lowest $N-1$ powers of the one-step $\mathbf{T}$ matrix on a period

$$\mathbf{T}^n = \sum_{r=1}^{N} (\lambda_r)^n \frac{\prod_{s\neq r}(\lambda_s \mathbf{I} - \mathbf{T})}{\prod_{s\neq r}(\lambda_s - \lambda_r)} \tag{93}$$

where λ_s are the eigenvalues of the one-step matrix $\mathbf{T}$ which are the solutions of the characteristic equation

$$\det(\lambda \mathbf{I} - \mathbf{T}) = \sum_{l=0}^{N} (-1)^l s_l \lambda^{N-l} = 0 \qquad s_0 = 1 \tag{94}$$

that is unsolvable analytically, in general, as the N-order algebraic equation. For $N = 2$ the solution of the quadratic equation (94) permitted Abelés to derive formula (57) i.e. to express the coefficients before $\mathbf{T}$ and $\mathbf{I}$ in (93) via the Chebyshev polynomials of the second kind. In the case of coupled waves, when $N > 2$, the solution of equation (94) sometimes is considered as an obstruction to be overcome [3], which demands one, for the employment of (93), to develop approximate methods of finding λ_s or to also explore approximate methods of the perturbation theory by weak coupling of waves.

Formulae (71) and (79), deduced above, and generalizing the Abelés formula (57), show that the computation of the eigenvalues of $\mathbf{T}$ is unnecessary. The point is that the coefficients s_l of the characteristic equation (94) are equal to the symmetric functions of its roots (the Viète theorem) and, on the other hand, they may be determined if we know the traces of the powers to $N-1$ of the $\mathbf{T}$ matrix [22] over which the coefficients before any powers of $\mathbf{T}$ in (93) are expressed. Really, according to the known Cayley–Hamilton theorem [21–23], every square matrix satisfies its own characteristic equation, so we have

$$\mathbf{T}^N = \sum_{l=1}^{N} (-1)^{l+1} s_l \mathbf{T}^{N-l} \tag{95}$$

where the coefficients s_l are equal [21-23] to the sums of the principal minors of $\mathbf{T}$ of lth order, that are the traces of the lth compound to the $\mathbf{T}$ matrices, $\widetilde{\mathbf{T}}_l$:

$$s_1 = \mathrm{Sp}\mathbf{T} = \sum_{i=1}^{N} T_{ii} \qquad s_2 = \mathrm{Sp}\widetilde{\mathbf{T}}_2 = \sum_{i,j=1}^{N} T_{jj}^{ii} \qquad \dots \qquad s_N = \mathrm{Sp}\widetilde{\mathbf{T}}_N = \det \mathbf{T}. \tag{96}$$

By comparing (95) and (21) we see that $s_l = \alpha_l$. Then we pass over from (95) to (93) by successive recurrence multiplying by $\mathbf{T}$ and make sure that the renormalized recursion coefficients in formulae (79) are determined by the traces (96) of the compound to the $\mathbf{T}$ matrices forming the polynomials $U_n^{(N)} = U_n^{(N)}(\alpha_1, \dots, \alpha_{N-1})$ that generalize the second-kind Chebyshev polynomials.

The amount and order of the minors in the sums (96) extend abruptly with increasing N. In order to determine the coefficients $\alpha_l = s_l$ instead of an explicit summarizing (96), as a matter of convenience we introduce, in addition, the polynomials $T_n^{(N)} = T_n^{(N)}(\alpha_1, \dots, \alpha_{N-1})$, generalizing the first-kind Chebyshev polynomials [24], as the determinants of $(N+1)$-diagonal $n \times n$ matrices of the form

$$T_n^{(N)}(\alpha_1, \dots, \alpha_{N-1}) \\ = \begin{vmatrix} \frac{1}{N}\alpha_1 & 1 & & & & & & & \\ \frac{2\alpha_2}{N} & \alpha_1 & 1 & & & & & & \\ \frac{3\alpha_3}{N} & \alpha_2 & \alpha_1 & 1 & & & & & \\ \cdots & \cdots & \cdots & \cdots & & & & & \\ \frac{(N-1)\alpha_{N-1}}{N} & \alpha_{N-2} & \dots & \alpha_1 & 1 & & & & \\ 1 & \alpha_{N-1} & \alpha_{N-2} & \dots & \alpha_1 & 1 & & & \\ & 1 & \alpha_{N-1} & \alpha_{N-2} & \dots & \alpha_1 & 1 & & \\ & & \ddots & \ddots & \ddots & \dots & \ddots & \ddots & \\ & & & 1 & \alpha_{N-1} & \alpha_{N-2} & \dots & \alpha_1 & 1 \\ & & & & 1 & \alpha_{N-1} & \alpha_{N-2} & \dots & \alpha_1 \end{vmatrix}. \tag{97}$$

We see by expanding (97) along the last row that, as $U_n^{(N)}$ in (82), the polynomials $T_n^{(N)}$ obey the recurrent relations

$$T_n^{(N)} = \sum_{l=1}^{N} (-1)^{l+1} \alpha_l T_{n-l}^{(N)} \tag{98}$$

where $\alpha_N = 1$ and the leading $N-1$ term we found explicitly by (97). By expanding (97) along the first column we see for ourselves the validity of the relations

$$T_n^{(N)} = \frac{1}{N} \sum_{l=1}^{N} (-1)^{l+1} l \alpha_l U_{n-l}^{(N)}. \tag{99}$$

For $N = 2$ this gives the known formulae [24] for the Chebyshev $T_n(y) \equiv T_n^{(2)}, U_n(y) \equiv U_n^{(2)}$ polynomials with $y = \alpha_1/2$:

$$T_n(y) = 2yT_{n-1}(y) - T_{n-2}(y) \qquad T_0(y) = 1 \qquad T_1(y) = y \\ T_n(y) = yU_{n-1}(y) - U_{n-2}(y). \tag{100}$$

By evaluation of trace (79) we verify the satisfiability of the equality

$$\mathrm{Sp}(\mathbf{T}^n) = N T_n^{(N)} \tag{101}$$

and then we found the coefficients $\alpha_l = s_l$ from the chain of equations (101) taken successively for $n = 1, 2, \dots, N-1$. For example, with the help of (97), the leading three terms give

$$\begin{aligned}
\alpha_1 &= \mathrm{Sp}\mathbf{T} \\
\alpha_2 &= \tfrac{1}{2}[(\alpha_1)^2 - \mathrm{Sp}(\mathbf{T}^2)] \\
\alpha_3 &= \tfrac{1}{3}[\mathrm{Sp}(\mathbf{T}^3) - (\alpha_1)^3 + 3\alpha_1\alpha_2]
\end{aligned} \tag{102}$$

and so on.

7. Conclusion

We emphasize that the recursion scheme examined in this work does not require periodicity of the system in any way. It is sufficient to know how to solve the one-step problem for the initial set of differential equations (1) or (15) for the transfer matrix. Such a problem may often be found to be simple enough, for example, with piecewise constant potentials like Kronig–Penny or with delta-function potentials. The arbitrary smooth potential may always be replaced by the piecewise constant one with a rather small step and pre-assigned accuracy.

Obtained rigorous analytical relations permit us, as usual, to compose the programs of numerical algorithms [23] more rationally and to understand their results more deeply.

It should be noted in conclusion that from the physical and mathematical points of view the applicability of many of the derived formulae is not restricted to the linear equation with variable coefficients (1) or (4). It is wider, as far as the dynamical mapping method and therefore, based on (19), the algebraic recurrence scheme is applicable to some other classes of differential and difference equations. First of all, we can apply them to the set of linear equations that describes an important case of a given system of N coupled plane waves $u_j = A_j \exp(\mathrm{i}k_j x)$, $j = 1, \dots, N$, which pass through the piecewise constant multilayered medium with strong space dispersion in layers (Bloch electrons, short wave phonons, magnons and so on),

$$L_j\left(E, \frac{\mathrm{d}}{\mathrm{d}x}\right)u_j + \sum_{l\neq j} \Delta_{lj}(E)u_l = 0 \tag{103}$$

where E is the spectral parameter, Δ_{lj} the piecewise constant parameters of wave coupling and the linear operators L_j in layers are not the rational algebraic functions of $\mathrm{d}/\mathrm{d}x$ as in (4) and so forth.

Moreover, even for some nonlinear equations, in the composition of numerical algorithms for their solution, we may formally use one part of our results (formulae for the elements of matrix products, powers, etc), but may not use the other part (in particular, the recurrence coefficients α on the interval of $N+1$ recursion points, will be dependent on the function values in all the previous steps). These questions require further investigation.

Acknowledgments

I am very thankful to Yu I Kuznetsov for discussion of the results and to E D Krupnikov and V Yu Peisakhovich for help in preparation of this manuscript.

Appendix. Computation of the recursion coefficients

Here we shall derive the formulae expressing the recursion coefficients $\alpha(i)_l^{(n)}$ for the elements $(M_n)_{ik}$ of the transfer matrix in (21), (27) and (28) via the elements of the one-step matrix $(T_n)_{jl}$ on the recursion interval from $n-N+1$ to n steps. First, we examine the simplest case of $N=2$ and carry out the operations described between formulae (20) and (21) directly. The transfer matrices $\mathbf{M}_n$ and $\mathbf{T}_n$ have four elements $(M_n)_{ik}$ and $(T_n)_{ik}$ $(i,k=1,2)$. We write out relations (20) for both elements $(M_n)_{ik}$ and $(M_n)_{jk}$ $(j\neq i)$ of the k-column,

$$\begin{aligned}(M_n)_{ik} &= (T_n)_{ii}(M_{n-1})_{ik} + (T_n)_{ij}(M_{n-1})_{jk}\\ (M_n)_{jk} &= (T_n)_{jj}(M_{n-1})_{jk} + (T_n)_{ji}(M_{n-1})_{ik}\end{aligned} \tag{A.1}$$

and add two analogous equations for the previous step, i.e. with the exchange $n \longrightarrow n-1$, so we get four equations on three unknowns $(M_n)_{jk}, (M_{n-1})_{jk}, (M_{n-2})_{jk}$. Their elimination is equivalent to equating the augmented determinant to zero:

$$\begin{vmatrix} (T_n)_{ii}(M_{n-1})_{ik} - (M_n)_{ik} & 0 & (T_n)_{ij} & 0\\ (T_n)_{ji}(M_{n-1})_{ik} & 0 & (T_n)_{jj} & -1\\ (T_{n-1})_{ii}(M_{n-2})_{ik} - (M_{n-1})_{ik} & (T_{n-1})_{ij} & 0 & 0\\ (T_{n-1})_{ji}(M_{n-2})_{ik} & (T_{n-1})_{jj} & -1 & 0\end{vmatrix} = 0. \tag{A.2}$$

By expanding along the first column, we get the binomial recurrence relations for the elements $(M_n)_{ik}$ whose coefficients are independent of the k-column index, i.e. they are identical for the elements $(M_n)_{11}$ and $(M_n)_{12}$ of the first row and for the elements $(M_n)_{21}$ and $(M_n)_{22}$ of the second row of the transfer matrix. We write them in the form of (21) with the proposition that $(T_{n-1})_{ij}\neq 0$ (see the text concerning the possibility of $\mathbf{T}_n$ elements vanishing) in notation (29)

$$(M_n)_{1k} = \alpha(1)_n(M_{n-1})_{1k} - \beta(1)_n(M_{n-2})_{1k} \qquad k=1,2 \tag{A.3}$$

$$\alpha(1)_n = (T_n)_{11} + (T_{n-1})_{22}\frac{(T_n)_{12}}{(T_{n-1})_{12}} \qquad \beta(1)_n = \frac{(T_n)_{12}}{(T_{n-1})_{12}}\det\mathbf{T}_{n-1} \tag{A.4}$$

$$(M_n)_{2k} = \alpha(2)_n(M_{n-1})_{2k} - \beta(2)_n(M_{n-2})_{2k} \qquad k=1,2 \tag{A.5}$$

$$\alpha(2)_n = (T_n)_{22} + (T_{n-1})_{11}\frac{(T_n)_{21}}{(T_{n-1})_{21}} \qquad \beta(2)_n = \frac{(T_n)_{21}}{(T_{n-1})_{21}}\det\mathbf{T}_{n-1}. \tag{A.6}$$

For the periodic system if a step is equal to the period then $(T_n)_{lj} = (T_{n-1})_{lj} \equiv T_{lj}$ and the coefficients are also independent of the i-row index:

$$\alpha = \alpha(1)_n = \alpha(2)_n = \mathrm{Sp}\,\mathbf{T} \qquad \beta = \beta(1)_n = \beta(2)_n = \det\mathbf{T}. \tag{A.7}$$

Relations (A.4), (A.6) and (A.7) are of wide use in the theory of wave propagation in disordered media and in superlattices [10, 12–15].

With a rise of matrix order N the order of the set of equations (20) containing the element $(M_n)_{ik}$ on recursion steps increases abruptly as N^2. The expanding of the augmented determinant of N^2-1 order for these systems is a good exercise in computer algebra. It is possible to show that the result may be expressed in terms of the elements of all the compounds to the $\mathbf{T}_n$ matrices on the recursion steps. But we may proceed more simply. The point is that as far as the recursion coefficients $\alpha(i)^n_l$ in (21) only depend on the i index of the transfer matrix row and are common for all columns k, we may find them as the solutions of an appropriate system of N linear non-homogeneous equations. To derive them we substitute the expressions

$$\mathbf{M}_j = \left(\prod_{l=n-N+1}^{j}\mathbf{T}_l\right)\mathbf{M}_{n-N} \qquad j=n-N+1,\ldots,n \tag{A.8}$$

into (21), that is all matrices $\mathbf{M}_j$ included in (21) we express with the help of (19) via the matrix farthest on the right, $\mathbf{M}_{n-N}$. Then we replace this initial matrix $\mathbf{M}_{n-N}$ by the unit matrix $\mathbf{I}$ since the coefficients $\alpha(i)_l^{(n)}$ are independent of the initial matrix in the recursion interval. So (21) gives the equations

$$\left(\prod_{j=n-N+1}^{n} \boldsymbol{T}_j\right)_{ik} = \sum_{l=1}^{N-1}(-1)^{l+1}\alpha(i)_l^n\left(\prod_{j=n-N+1}^{n-l} \mathbf{T}_j\right)_{ik} + (-1)^{N+1}\alpha(i)_N^{(n)}\delta_{ik}. \tag{A.9}$$

Under the fixed row index i we take from (A.9) the equations, $k = 1, 2, \ldots, N$, which give us the closed set of required N linear non-homogeneous equations for coefficients $\alpha(i)_l^{(n)}$ which we find by the Cramer's rule as the ratio of known determinants. For example, when $N = 3$ we have from (A.9) in notation (29) the following set of equations,

$$\begin{aligned}
(\boldsymbol{T}_n\boldsymbol{T}_{n-1}\boldsymbol{T}_{n-2})_{i1} &= \alpha(i)_n(\boldsymbol{T}_{n-1}\boldsymbol{T}_{n-2})_{i1} - \beta(i)_n(T_{n-2})_{i1} + \gamma(i)_n\delta_{i1}\\
(\boldsymbol{T}_n\boldsymbol{T}_{n-1}\boldsymbol{T}_{n-2})_{i2} &= \alpha(i)_n(\boldsymbol{T}_{n-1}\boldsymbol{T}_{n-2})_{i2} - \beta(i)_n(T_{n-2})_{i2} + \gamma(i)_n\delta_{i2}\\
(\boldsymbol{T}_n\boldsymbol{T}_{n-1}\boldsymbol{T}_{n-2})_{i3} &= \alpha(i)_n(\boldsymbol{T}_{n-1}\boldsymbol{T}_{n-2})_{i3} - \beta(i)_n(T_{n-2})_{i3} + \gamma(i)_n\delta_{i3}
\end{aligned} \tag{A.10}$$

and so on. Hence we may use for the computation of the recursion coefficients from $n - N + 1$ to n steps the following general formula,

$$\alpha(i)_l^n = (-1)^{l+1}\frac{D_l(i)}{D_0(i)} \tag{A.11}$$

where the determinant of system (A.9) is

$$D_0(i) = \begin{vmatrix}
\delta_{i1} & \delta_{i2} & \ldots & \delta_{iN}\\
(T_{n-N+1})_{i1} & (T_{n-N+1})_{i2} & \ldots & (T_{n-N+1})_{iN}\\
(\boldsymbol{T}_{n-N+2}\boldsymbol{T}_{n-N+1})_{i1} & (\boldsymbol{T}_{n-N+2}\boldsymbol{T}_{n-N+1})_{i2} & \ldots & (\boldsymbol{T}_{n-N+2}\boldsymbol{T}_{n-N+1})_{iN}\\
\cdots & \cdots & \cdots & \cdots\\
(\prod_{j=n-N+1}^{n-1}\boldsymbol{T}_j)_{i1} & (\prod_{j=n-N+1}^{n-1}\boldsymbol{T}_j)_{i2} & \ldots & (\prod_{j=n-N+1}^{n-1}\boldsymbol{T}_j)_{iN}
\end{vmatrix} \tag{A.12}$$

and $D_l(i)$ is found from $D_0(i)$ by replacing its $(N - l + 1)$-row elements by the elements

$$\left(\prod_{j=n-N+1}^{n}\boldsymbol{T}_j\right)_{ik} \qquad k = 1, 2, \ldots, N. \tag{A.13}$$

For the periodic system with step equal to the period the one-step transfer matrices are identical, $\mathbf{T}_j = \mathbf{T}$, so from (A.11) and the Cayley–Hamilton theorem it immediately follows that, independently of the i-row index,

$$\alpha_l = s_l \tag{A.14}$$

where s_l are the coefficients of the $\mathbf{T}$ matrix characteristic polynomial (94) and are given by formulae (96), i.e. they are equal to the traces of the lth compound to the $\mathbf{T}$ matrices.

References

[1] Arnold V I 1975 *Ordinary Differential Equations* (Moscow: Nauka) in Russian

[2] Yakubovich Y A and Starzhinskii V M 1972 *Linear Differential Equations with Periodic Coefficients* (Moscow: Nauka) in Russian; 1975 (New York: Wiley); 1987 *Parametric Resonance in Linear Systems* (Moscow: Nauka) in Russian

[3] Bass F G, Bulgakov A A and Tetervov A P 1989 *High-Frequency Properties of Semiconductors with Superlattices* (Moscow: Nauka) in Russian

[4] Cycon H L, Froese R G, Kirch W and Simon B 1987 *Schrödinger Operators* (Berlin: Springer)
Levitan B M and Sargsian I S 1988 *Sturm-Liouville and Dirac Operators (Moscow: Nauka)* in Russian

[5] Born M and Wolf E 1980 *Principles of Optics* (New York: Pergamon)
Yariv A and Yeh P 1983 *Optical Waves in Crystals* (New York: Wiley)

[6] Nagano S 1994 *Phys. Rev.* B **50** 10 531

[7] Kittel C 1963 *Quantum Theory of Solids* (New York: Wiley)

[8] Svidzhinskii A V 1982 *Non-Homogeneous Space Problems of Superconductivity* (Moscow: Nauka) in Russian
Kulik I O 1970 *Sov.Phys.–JETP* **30** 944
Bagwell P 1992 *Phys. Rev.* B **46** 12 537
Plehn H, Wacker O-J and Kümmel R 1994 *Phys. Rev.* B **49** 12 140
[9] Berestetskii V R, Lifshitz E M and Pitaevskii L P 1974 *Quantum Electrodynamics (Landau and Lifshitz, Course of Theoretical Physics, v IV)* (Moscow: Nauka) in Russian; 1989 (New York: Pergamon)
[10] Lifshitz I M, Gredeskul S A and Pastur L A 1982 *Introduction to the Theory of Disordered Systems* (Moscow: Nauka) in Russian; 1988 (New York: Wiley)
[11] Pastur L A 1987 Spectral properties of random and almost-periodic operators *Math. Phys. Rev.* **6** 1 (New York: Harwood Academic)
[12] Lieb E and Mattis D E (eds) 1966 *Mathematical Physics in One Dimension* (New York: Academic)
[13] Sokoloff J B 1985 *Phys. Rep.* **126** 189
[14] Iliin V P and Kuznetsov Yu I 1985 *Tridiagonal Matrices* (Moscow: Nauka) in Russian
[15] Sanchez A, Macia E and Dominguez-Adame F 1994 *Phys. Rev.* B **49** 147
[16] Rozman M G, Reineker R and Tehver R 1994 *Phys. Rev.* A **49** 3310
[17] Peres A 1983 *J. Math. Phys.* **24** 1110
[18] Anderson P W, Thouless D J, Abrahams E and Fisher D S 1980 *Phys. Rev.* B **22** 3519
[19] Jose J V 1983 *J. Phys. A: Math. Gen.* **16** L205
[20] Abelés F 1950 *Ann. Phys., Paris* **5** 596,706
[21] Horn R A and Johnson C R 1986 *Matrix Analysis* (Cambridge: Cambridge University Press)
[22] Gantmacher F R 1988 *Theory of Matrices* (Moscow: Nauka) in Russian; 1977 (New York: Chelsea)
[23] Voevodin V V and Kuznetsov Yu A 1984 *Matrices and Computations* (Moscow: Nauka) in Russian
[24] Paszkowski S 1975 *Computational Applications of Chebyshev Polynomials and Series* (Warszawa: Nauka) in Polish; 1983 (Moscow: Nauka) in Russian
[25] Brillouin L and Parodi M 1959 *Wave Propagation in Periodic Structures* (Moscow: ILP) in Russian