

Small Oscillations, Sturm Sequences, and Orthogonal Polynomials

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The relation between small oscillations of one-dimensional mechanical n -particle systems and the theory of orthogonal polynomials is investigated. It is shown how the polynomials provide a natural tool to determine the eigenfrequencies and eigencoordinates completely, where the existence of a specific two-termed recurrence formula is essential. Physical and mathematical statements are formulated in terms of the recurrence coefficients which can directly be obtained from the corresponding secular equation. Several results on Sturm sequences and orthogonal polynomials are presented with respect to the treatment of small oscillations. The relation to the numerical treatment of the generalized eigenvalue problem is discussed and further applications to physical problems from quantum mechanics, statistical mechanics, and spin systems are briefly outlined.

1. Introduction

During the last fifteen years, an old chapter of the theory of special functions – namely that of orthogonal polynomials – has regained a remarkable amount of interest through its relation to integrable, nonlinear dynamical systems [1–3]. In the sequel, Calogero published several papers on new representations of the classical polynomials [4, 5] and on the relations between isospectral matrices and polynomials [6]. Furthermore, for some special dynamical systems (e.g., one-dimensional n -particle systems of classical mechanics), it is known that the frequencies of small oscillations coincide with the square roots of the zeros of certain classical polynomials [7–9], which to our knowledge has not been investigated systematically.

Motivated by this property of small oscillations, we will present a slightly different approach to the theory of orthogonal polynomials which will nevertheless have several points of tangency with the line mentioned above. Solving the eigenvalue problem that belongs to a one-dimensional n -particle system in the approximation of small oscillations – where it is obviously integrable – in a suitable way, one is generically led to a system of polynomials that constitute a Sturm sequence and, in the limit $n \rightarrow \infty$, a system of orthogonal polynomials. Suitable in this context means that the system is not considered as an isolated one but as

the last in a series of n systems that are defined recursively. This way, one obtains the central two-termed recurrence relation the coefficients of which carry essentially the whole physics of the system. It is therefore an interesting task to extract as many properties as possible directly from these coefficients, without calculating further intermediate quantities at all. This is precisely what we aim at.

At this point, one might apply inverse scattering methods [10] to obtain the desired results. However, we shall prefer “classical” algebraic techniques for two reasons. Firstly, the elementary presentation of the results will facilitate the understanding of the central role of the recurrence relation that also occurs in several problems of numerical analysis, quantum mechanics, and statistical mechanics. Secondly, the polynomials provide a very natural method to solve the problems completely which sometimes (e.g., for the small oscillations) is also simpler than the usual Fourier series expansion. For the same reason, we did not consider the relation to group theory where orthogonal polynomials appear as spherical functions [11], although this certainly would give interesting insight. But this is beyond the scope of the present article.

In what follows, it will be shown how oscillating systems, generalized eigenvalue problems, Sturm sequences, and orthogonal polynomials are interrelated. To this end, only elementary methods from linear algebra, analysis, and classical mechanics are necessary. Nevertheless, one can come to a unified picture with several new results, where all the physical

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and mathematical properties are extracted from the recurrence formula mentioned above, i.e., they are expressed in terms of the recurrence coefficients. These coefficients are much easier to obtain than any explicit form of the secular equation of the oscillating system, and the numerical calculation of the eigenfrequencies – which can in general not be given by a closed analytic formula – will in any case take profit from the recursion.

Since the two-termed recurrence formula that occurs in the theory of orthogonal polynomials is intimately related to the generalized eigenvalue problem $\mathbf{B}\mathbf{w} = \lambda \cdot \mathbf{A}\mathbf{w}$ with a diagonal matrix \mathbf{A} and a tridiagonal matrix \mathbf{B} , some of the results have applications to the numerical treatment of the problem, e.g., to the extrapolation to large n which is of great importance in systems where one actually is interested in the thermodynamic limit, i.e., in the limit $n \rightarrow \infty$. For example, the calculation of the spectra of quantum spin systems may profit from the corresponding numerical algorithm which is much faster than standard routines, especially if one has large matrices that are first brought to tridiagonal form by means of the popular Lanczos iteration, compare [12]. This advantage is well known [13, 14] but has to be paid for by a possible numerical instability wherefore it is usually not implemented in standard routines. Nevertheless, it is worth trying, especially in recursive systems where one can control these instabilities in a reliable way.

The article is organized as follows. In Sect. 2, the relation between small oscillations of one-dimensional n -particle systems and the theory of orthogonal polynomials is outlined by means of several examples. It is shown how the polynomials provide a natural tool to determine the eigenfrequencies and eigencoordinates completely. From the mathematical point of view, this is discussed in greater detail in Sect. 3, where the connection between Sturm sequences and the generalized eigenvalue problem is investigated. Here, the existence of a two-termed recurrence formula is essential. The notation and formulation of the statements is always adapted to the problems of small oscillations which results in a slight change w.r.t. the usual formulation

in the mathematical literature. Possible applications to tridiagonal matrices as mentioned above are also discussed, they are presented in Appendix A in the most general fashion.

Section 4 deals with the properties of orthogonal polynomials themselves, which can – in this context – be thought of as infinite Sturm sequences. This is naturally the most extensive chapter of this article where known results are reformulated for applications to small oscillations and several new results are derived by simple algebraic techniques. The aim was to extract as many properties as possible directly from the recurrence coefficients, like bounds and sum rules for the zeros and the equivalence of different recurrence relations. Here, a general formula for the coefficients of the corresponding polynomials is derived, the (elementary, but quite technical) proof of which is given in Appendix B. It is described in which sense a recurrence formula is equivalent to a system of orthogonal polynomials and how one can find a mechanical representation of precisely that system of polynomials. This is followed by some concluding remarks in Sect. 5 where we stress further physical applications of the theory of orthogonal polynomials, e.g., in quantum mechanics and statistical mechanics. As an instructive example, we present the well-known solution of the Ising quantum chain [15] in Appendix C, reformulated at the critical point in terms of Chebyshev's polynomials of the second kind.

2. Physical Examples

For an illustration of the physical context, let us first present some well-known examples from the theory of small oscillations. We restrict our analysis to 1-D n -particle systems. First, we consider the linear chain with n point masses which vibrate longitudinally under the influence of $n + 1$ springs as depicted in Figure 1. The classical Lagrange function is [16] $L_n = T_n - V_n$ with

$$T_n = \frac{1}{2} (\dot{\mathbf{x}}^T \mathbf{A} \dot{\mathbf{x}}), \quad \mathbf{A}_n = \text{diag}(m_1, \dots, m_n),$$

$$\dot{\mathbf{x}} = (\dot{x}_1, \dots, \dot{x}_n)^T \quad (1)$$

and

$$V_n = \frac{1}{2} (\mathbf{x}^T \mathbf{B}_n \mathbf{x}), \quad \mathbf{B}_n = \begin{pmatrix} k_0 + k_1 & -k_1 & & & \\ -k_1 & k_1 + k_2 & -k_2 & & 0 \\ & -k_2 & \ddots & \ddots & \\ 0 & & \ddots & \ddots & -k_{n-1} \\ & & & -k_{n-1} & k_{n-1} + k_n \end{pmatrix}. \quad (2)$$

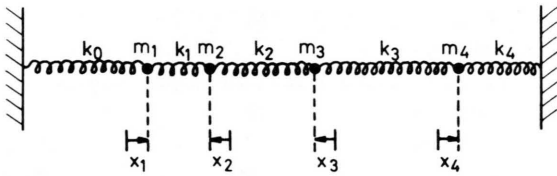


Fig. 1

The n eigenfrequencies ω of this system are given by the roots of the characteristic polynomial

$$P_n(\lambda) = \det(\mathbf{B}_n - \lambda \mathbf{A}_n) \quad (3)$$

via $\lambda = \omega^2$. By the expansion theorem of Laplace one obtains the recurrence formula

$$P_{l+1}(\lambda) = (k_l + k_{l+1} - m_{l+1} \lambda) P_l(\lambda) - k_l^2 P_{l-1}(\lambda), \\ 0 \leq l \leq n-1, \quad P_0 \equiv 1, \quad P_{-1} \equiv 0. \quad (4)$$

If $k_l > 0$ for $1 \leq l \leq n-1$ (and we will concentrate on this case) the sequence $P_n(\lambda), \dots, P_0(\lambda)$ constitutes a Sturm sequence, which is discussed in Section 3. Now, it is an obvious generalization to treat this problem recursively, i.e., to write formally L_∞ with $k_0 \geq 0$ and $k_m > 0$ for $m \in \mathbb{N}$, and to consider the recurrence formula (4) for $l \in \mathbb{N}_0$. Clearly, the roots of two consecutive polynomials mutually intersect (cf. [16]), wherefore they can easily be calculated numerically (e.g., by a bisection algorithm). In some special cases one is able to give the roots analytically, but this is, unfortunately, an exception.

Take, e.g., $m_l = 1$ for $l \in \mathbb{N}$ and $k_l = 1$ for $l \in \mathbb{N}_0$. Then, the recurrence formula reads

$$P_{n+1}(\lambda) = (2 - \lambda) \cdot P_n(\lambda) - P_{n-1}(\lambda), \quad (5)$$

resulting in

$$P_n(\lambda) = \sum_{k=0}^n (-1)^k \binom{n+k+1}{2k+1} \cdot \lambda^k, \quad (6)$$

which can easily be proved inductively. Calculating the generating function $F(t, x)$ one finds

$$F(t, x) = \sum_{n=0}^{\infty} P_n(\lambda) \cdot t^n = \frac{1}{1 + (\lambda - 2)t + t^2}. \quad (7)$$

Now, taking either the recurrence formula (5) or the generating function (7), one can directly see $P_n(\lambda)$ to be related to the Gegenbauer (or ultraspherical) polynomials $C_n^{(1)}(x)$ (see [17]) via

$$C_n^{(1)}(x) = P_n(2(1-x)). \quad (8)$$

The zeros are, ordered decreasingly, $x_l^{(n)} = \cos \frac{l\pi}{n+1}$, $1 \leq l \leq n$, which gives the eigenfrequencies $(\omega_l^{(n)})^2 = 2(1 - x_l^{(n)})$

$$\omega_l^{(n)} = 2 \cdot \sin \frac{l\pi}{2(n+1)}, \quad 1 \leq l \leq n, \quad (9)$$

usually obtained by Fourier series expansion. Hence, for $n \in \mathbb{N}$ and $1 \leq l \leq n$, we have $0 < \omega_l^{(n)} < 2$, or, reintroducing the mass m and the coupling constant k ,

$$0 < (\omega_l^{(n)})^2 < 4k/m, \quad (10)$$

where $k_l = k$, $l \geq 0$, and $m_l = m$, $l \geq 1$.

Furthermore, for a fixed n , one can completely solve the eigenvalue problem defined by (1) and (2), which will be done in Sect. 3. For the current example (5), it is easy to verify that $U_n = (u_{ij}^{(n)})_{1 \leq i, j \leq n}$ with

$$u_{ij}^{(n)} = P_{i-1}(\lambda_j^{(n)}) \quad (11)$$

builds a matrix which columnwise consists of the eigenvectors (i.e., the eigencoordinates) of the problem.

Keeping $m_l = 1$ and $k_l = 1$, $l \in \mathbb{N}$, but taking $k_0 = 0$, one obtains a chain with mixed boundary conditions, namely free on the one side and fixed on the other. The recurrence formula now reads

$$E_{n+1} = (2 - \delta_{n,0} - \lambda) E_n - E_{n-1}, \\ n \geq 0, \quad E_0 \equiv 1, \quad E_{-1} \equiv 0, \quad (12)$$

with the solution

$$E_n(\lambda) = P_n(\lambda) - P_{n-1}(\lambda) = \sum_{l=0}^n (-1)^l \binom{n+l}{2l} \lambda^l \quad (13)$$

and the roots

$$\lambda_l^{(n)} = 4 \sin^2 \left(\frac{(2l-1)\pi}{2(2n+1)} \right), \quad 1 \leq l \leq n. \quad (14)$$

Even free boundary conditions ($k_n = 0$ for a chain with n masses) can be treated with the result

$$F_n(\lambda) = -\lambda \cdot P_{n-1}(\lambda), \quad n \geq 1. \quad (15)$$

The root $\lambda = 0$ corresponds to the translational degree of freedom, the formula for the roots of $F_n(\lambda)$ reads

$$\lambda_l^{(n)} = 4 \sin^2 \left(\frac{l\pi}{2n} \right), \quad 0 \leq l \leq n-1. \quad (16)$$

The linear chain with periodic boundary conditions ($k_{n+1} = k_0 = 1$) is more complicated because a double degeneracy of the eigenfrequencies occurs. Neverthe-

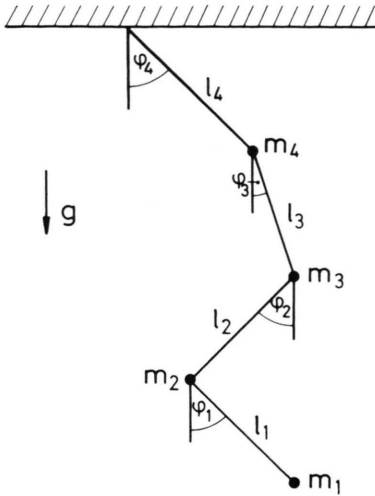


Fig. 2

less, they can be given in closed form,

$$\lambda_l^{(n)} = 4 \sin^2 \left(\frac{l\pi}{n} \right), \quad 0 \leq l \leq n-1. \quad (17)$$

It is funny to observe that the corresponding polynomials are effectively – after separating out $\lambda_0^{(n)} = 0$ and, for even n , $\lambda_{n/2}^{(n)} = 4$ – the squares of orthogonal polynomials.

Conversely, the classical polynomials can be realized by a linear chain with a suitable choice of the masses and the coupling constants. For example, $m_l = 1$, $l \in \mathbb{N}$, and $k_l = l$, $l \in \mathbb{N}_0$ leads to the well-known Laguerre polynomials (up to a normalization factor of $1/n!$), wherefore the eigenfrequencies are unbounded in the limit $n \rightarrow \infty$. Replacing the masses of the last example by $m_l = 2l - 1$, $l \in \mathbb{N}$, one is back to a system with bounded eigenfrequencies: up to a normalization factor of $1/n!$ and a shift of the interval, one obtains the Legendre polynomials with the following inequality for the eigenfrequencies

$$0 < (\omega_l^{(n)})^2 < 2, \quad n \in \mathbb{N}, \quad 1 \leq l \leq n. \quad (18)$$

Completely analogous properties can, e.g., be found in systems of n coupled pendulums in the approximation of small oscillations. This is not astonishing because the ‘nearest neighbour interaction’ directly produces the structure of (1) and (2). But it is neither essential to have a Euclidean structure in the kinetic energy, i.e., a diagonal matrix A_n , nor to have nearest neighbour interaction only, i.e., a tridiagonal matrix

B_n in the potential energy. This will be illustrated by a further example.

In the case of the n -pendulum (see Fig. 2), the Lagrangian is $L_n = T_n - V_n$ with

$$V_n = g \cdot \sum_{v=1}^n M_v l_v (1 - \cos(\varphi_v)) \quad (19)$$

and

$$T_n = \frac{1}{2} \sum_{\mu=1}^n \sum_{v=1}^n M_{\mu v} l_\mu l_v \dot{\varphi}_\mu \dot{\varphi}_v \cos(\varphi_\mu - \varphi_v), \quad (20)$$

where $M_\mu = \sum_{q=1}^\mu m_q$ and $M_{\mu v} = M_{\min\{\mu, v\}}$.

In the approximation of small oscillations around the stable equilibrium position $\varphi_\mu = 0$, $1 \leq \mu \leq n$, one has $L_n = \frac{1}{2} (\dot{\varphi}^t A_n \dot{\varphi}) - \frac{1}{2} (\varphi^t B_n \varphi)$ with

$$B_n = g \cdot \text{diag}(M_1 l_1, \dots, M_n l_n), \quad (A_n)_{\mu v} = M_{\mu v} l_\mu l_v, \quad 1 \leq \mu, v \leq n. \quad (21)$$

Then, with $P_n(\lambda) = \det(B_n - \lambda A_n)$, one finds

$$P_{n+1}(\lambda) = (b_{n+1} - a_{n+1} \lambda) P_n(\lambda) - c_n^2 P_{n-1}(\lambda), \quad n \geq 0, \quad P_0 \equiv 1, \quad P_{-1} \equiv 0, \quad (22)$$

with $M_0 := 0$ and

$$a_n = m_n l_n^2, \quad b_n = g \cdot \left(\frac{M_n}{l_n} + \frac{M_{n-1}}{l_{n-1}} \right) l_n^2, \quad c_n = g M_n l_{n+1}. \quad (23)$$

Although the matrices A_n , B_n are completely different from those of the previous examples, (22) has the same structure as (4). Thus, the n -pendulum can also be used as a ‘mechanical representation’ of the classical polynomials.

For example, taking $m_k \equiv m$ and $l_k \equiv l$, $k \in \mathbb{N}$, we obtain with $x = \frac{l}{g} \lambda$ and $\tilde{P}_n(x) = P_n\left(\frac{l}{g} \lambda\right)$ the formula

$$\tilde{P}_{n+1}(x) = ((2n+1) - x) \tilde{P}_n(x) - n^2 \tilde{P}_{n-1}(x), \quad (24)$$

which again gives the Laguerre polynomials via $L_n(x) = \frac{1}{n!} \tilde{P}_n(x)$. A more detailed analysis of the n -pendulum together with the limit $n \rightarrow \infty$ has been given by Bottema [7].

All 1-D n -particle systems with a certain recursive structure can – in the approximation of small oscillations – systematically be solved by means of the theory of orthogonal polynomials and their relation to the generalized eigenvalue problem. From the above examples it should be clear how the theory of orthogonal polynomials applies to small oscillations of me-

chanical systems. In what follows, we shall investigate, in more detail, the underlying mathematical structure glueing together aspects of analysis, linear algebra, and numerical methods. This way we hope to match the problems of small oscillations adequately. Furthermore, we would like to mention similar applications to the treatment of 1-D quantum spin chains, the easiest example of which is given in Appendix C.

3. Sturm Sequencies and the Generalized Eigenvalue Problem

Let us now consider the finite sequence of real polynomials defined by

$$P_{n+1}(x) = (b_{n+1} - a_{n+1}x)P_n(x) - c_n^2 P_{n-1}(x),$$

$$0 \leq n \leq N-1, \quad P_0(x) \equiv 1, \quad P_{-1}(x) \equiv 0, \quad (25)$$

where $N \geq 2$ and $a_n > 0$ and $c_n \neq 0$ for $1 \leq n \leq N$. For convenience, we take $c_0 = 1$. If ξ is a *real* zero of $P_n(x)$ for any $1 \leq n \leq N-1$, i.e., $P_n(\xi) = 0$, we obtain $P_{n-1}(\xi)P_{n+1}(\xi) \leq 0$ from (25). But neither P_{n-1} nor P_{n+1} can vanish at $x = \xi$ because this would result in a contradiction to $P_0(x) \equiv 1$. Hence,

$$P_{n-1}(\xi) \cdot P_{n+1}(\xi) < 0. \quad (26)$$

Furthermore, if ξ is *any* zero of P_N , we have $P_{N-1}(\xi) \neq 0$ and get, by means of the recurrence formula,

$$P'_N(\xi) = \lim_{x \rightarrow \xi} \frac{P_N(x)}{x - \xi} = -a_N P_{N-1}(\xi) \neq 0. \quad (27)$$

This shows that P_N has simple roots only and, since $a_N > 0$, that for any *real* root ξ of P_N

$$\operatorname{sgn} P'_N(\xi) = -\operatorname{sgn} P_{N-1}(\xi). \quad (28)$$

So far, we have proved

Lemma 1: *The polynomials P_N, P_{N-1}, \dots, P_0 as defined by (25) build a Sturm sequence.*

For a detailed definition and the essential properties of Sturm sequences – especially the intersection properties of the zeros – the reader is referred to a standard textbook on numerical analysis (e.g. [18]).

In our context, the relevance of Sturm sequences comes out of the relation to the generalized eigenvalue problem

$$Bw = \lambda Aw \quad (29)$$

with real, symmetric matrices A and B . With the expansion theorem for determinants one can readily prove

Lemma 2: *Every finite system of polynomials as defined by (25) can be represented by the characteristic polynomials of the generalized eigenvalue problems $B_n w = \lambda A_n w$, $1 \leq n \leq N$, i.e., $P_n(\lambda) = \det(B_n - \lambda A_n)$. Here, $A_n = \operatorname{diag}(a_1, \dots, a_n)$, which is positive definite, and*

$$B_n = \begin{pmatrix} b_1 & -c_1 & & 0 \\ -c_1 & b_2 & \ddots & \\ & \ddots & \ddots & -c_{n-1} \\ 0 & & -c_{n-1} & b_n \end{pmatrix}.$$

Let us, at this point, give some comments on the relation between the generalized eigenvalue problem and the ordinary one. If the matrix A in (29) is invertible, one obtains by left multiplication with A^{-1} the equivalent equation $A^{-1}Bw = \lambda w$. However, if A is symmetric and positive definite (as in the case of small oscillations) it is advantageous to decompose A into the form $A = R^t R$ with a nonsingular, superdiagonal matrix R (i.e., $R_{ij} = 0$ if $i > j$). This way one can keep the symmetry of the eigenvalue problem which is obviously destroyed by a multiplication with A^{-1} .

To see this, one defines $y = R w$ and obtains – by left multiplication with $(R^t)^{-1}$ – the equivalent expression

$$\tilde{B}y = \lambda y, \quad \tilde{B} = (R^t)^{-1} B R^{-1}. \quad (30)$$

The characteristic polynomial obviously fulfils

$$\det(B - \lambda A) = \det(A) \cdot \det(\tilde{B} - \lambda \mathbf{1}). \quad (31)$$

Note that \tilde{B} is symmetric iff the same is true of B . Hence, with Lemma 1 and Lemma 2, we obtain the well-known [18]

Theorem 1: *Every polynomial of the sequence $(P_k)_{0 \leq k \leq N}$ as defined by (25) has only simple, real roots.*

In numerical analysis, the relationship between the generalized eigenvalue problem (29) and the corresponding Sturm sequence P_N, P_{N-1}, \dots, P_0 is often used to determine the zeros of $P_N(\lambda)$ recursively (e.g., by means of a bisection algorithm). This can be done to an arbitrary degree of accuracy. Furthermore, the knowledge of the zeros of $P_N(\lambda)$ can be used to calculate a simple, closed formula for the corresponding eigenvectors of the problem which will now briefly be outlined.

Let $\lambda_m^{(N)}$, $1 \leq m \leq N$, be the roots of the polynomial $P_N(\lambda)$. Since A_N is positive definite, (29) may be rear-

ranged as

$$A_N^{-1} B_N \mathbf{w} = \lambda \mathbf{w}. \quad (32)$$

But $A_N^{-1} B_N$ is diagonalizable because N pairwise different eigenvalues $\lambda_m^{(N)}$, $1 \leq m \leq N$, exist. Therefore, the determination of the corresponding eigenvectors is nothing but the calculation of the matrix $U_N = (U_{i,j}^{(N)})_{1 \leq i,j \leq N}$ which fulfils

$$A_N^{-1} B_N U_N = U_N \text{diag}(\lambda_1^{(N)}, \dots, \lambda_N^{(N)}). \quad (33)$$

With $A_N^{-1} = \text{diag}(1/a_1, \dots, 1/a_N)$, $a_i > 0$ for $1 \leq i \leq N$, one obtains

$$c_i U_{i+1,j}^{(N)} = (b_i - a_i \lambda_j^{(N)}) U_{i,j}^{(N)} - c_{i-1} U_{i-1,j}^{(N)}, \quad 1 \leq i, j \leq N, \quad (34)$$

where we choose $U_{0,j}^{(N)} = U_{N+1,j}^{(N)} = 0$ for convenience (c_0 and c_N need not be specified this way). Introducing now

$$\tilde{U}_{i,j}^{(N)} = U_{i,j}^{(N)} \prod_{k=0}^{i-1} c_k, \quad c_0 := 1, \quad (35)$$

(35) reduces to the well-known recurrence formula

$$\tilde{U}_{i+1,j}^{(N)} = (b_i - a_i \lambda_j^{(N)}) \tilde{U}_{i,j}^{(N)} - (c_i)^2 \tilde{U}_{i-1,j}^{(N)}, \quad 1 \leq i, j \leq N. \quad (36)$$

But we can immediately give a solution in closed form, namely

$$\tilde{U}_{i,j}^{(N)} = P_{i-1}(\lambda_j^{(N)}), \quad (37)$$

or, reintroducing the matrix, U ,

$$U_{i,j}^{(N)} = \frac{P_{i-1}(\lambda_j^{(N)})}{\prod_{k=0}^{i-1} c_k}, \quad 1 \leq i, j \leq N, \quad c_0 := 1. \quad (38)$$

This solution automatically fulfils $U_{0,j}^{(N)} = U_{N+1,j}^{(N)} = 0$ and can be generalized to cases where not all c_j are different from zero (then (29) decomposes into independent blocks which can be treated separately). Hence we have

Theorem 2: *The j -th column of the real matrix U as defined by (38) is an eigenvector of the problem $B_N \mathbf{w} = \lambda A_N \mathbf{w}$ for the eigenvalue $\lambda_j^{(N)}$. The eigenvector is unique up to a normalization factor.*

Before we turn to infinite Sturm sequences which constitute a system of orthogonal polynomials, let us remark that the number $P_{i-1}(\lambda_j^{(N)})$ can directly be evaluated by means of the recurrence formula (25), starting from $P_{-1} \equiv 0$ and $P_0 \equiv 1$. It is not necessary to

determine the coefficients of the polynomials first. The same is true of the calculation of the roots $\lambda_j^{(N)}$ by a simple numerical procedure like the bisection algorithm.

In practice, (38) may not be suitable because numerical instabilities can occur (for the special case of $a_k = 1$, $1 \leq k \leq N$, this is discussed in detail in [13]). The execution time of a program using (38) was, however, much shorter than that of the corresponding EISPACK routine (for $N = 50$ about a factor of 20, for $N = 100$ about a factor of 30) although the accuracy for the matrices tested was the same. Therefore, at least for systems with growing N (as, e.g., occurring in spin systems), one can go beyond the limits that are dictated by the standard algorithms (and for small N , the stability can be checked by a comparison of the results). In Appendix A, a generalization to complex, not necessarily symmetric matrices is presented, which also has applications in the treatment of spin systems.

4. Orthogonal Polynomials

Consider a real valued, a.e. (almost everywhere) positive function $w(x)$ with the property that $\int_a^b w(x) x^k dx$ exists in the Lebesgue sense for every $k \in \mathbb{N}_0$, i.e., $w(x) x^k \in L_1(a, b)$. Then we define: A system of real polynomials P_k , $k \in \mathbb{N}_0$, is called *orthogonal* on the finite or infinite interval (a, b) with respect to the weight function $w(x)$ if the following conditions are satisfied.

- (1) P_k , $k \in \mathbb{N}_0$, is a polynomial of degree k , i.e., we have $P_k(x) = \sum_{l=0}^k \alpha_l^{(k)} x^l$, with $\text{sgn}(\alpha_l^{(k)}) = (-1)^k$.
- (2) For $k, l \in \mathbb{N}_0$, the polynomials fulfil the orthogonality condition $\int_a^b w(x) P_k(x) P_l(x) dx = h_k \delta_{kl}$ with positive constants h_k .

An orthogonal system is called *orthonormal* if $h_k = 1$ for $k \in \mathbb{N}_0$.

Obviously, this is only one of several possibilities for a unique determination of the polynomials, which has been chosen to match the problems of small oscillations as presented in Section 2. For a general mathematical discussion, the reader is referred to the books of Szegő [19] and Freud [20]. Sometimes it is advantageous to generalize the Lebesgue measure $w(x) dx$ to the Lebesgue–Stieltjes measure $d\alpha(x)$ obtained from a

realvalued, non decreasing, bounded function $\alpha(x)$ which is defined on the entire interval (a, b) and assumes there infinitely many different values (for details, see [20]). If $\alpha(x)$ is absolutely continuous, one can define $w(x) = \alpha'(x)$ and is back to the case of the above definition.

From the various properties of orthogonal polynomials, the recurrence formula will be essential in the sequel. In fact, as shown in Sect. 2, it is this very recurrence property that joins orthogonal polynomials with the theory of small oscillations. To simplify the notation, we define

$$\alpha_k^{(n)} = 0, \text{ if } k < 0 \text{ or } k > n. \quad (39)$$

Now, we can formulate

Theorem 3: Every system of orthogonal polynomials fulfils the recurrence formula $P_{n+1}(x) = (b_{n+1} - a_{n+1}x)P_n(x) - (c_n)^2 P_{n-1}(x)$ for $n \geq 0$ with $P_{-1}(x) \equiv 0$, $P_0(x) \equiv \alpha_0^{(0)} > 0$, and the recurrence coefficients

$$a_{n+1} = -\frac{\alpha_{n+1}^{(n+1)}}{\alpha_n^{(n)}} > 0, \quad n \geq 0,$$

$$b_{n+1} = a_{n+1} \left(\frac{\alpha_n^{(n+1)}}{\alpha_{n+1}^{(n+1)}} - \frac{\alpha_{n-1}^{(n)}}{\alpha_n^{(n)}} \right), \quad n \geq 0,$$

$$(c_n)^2 = \frac{a_{n+1}}{a_n} \cdot \frac{h_n}{h_{n-1}} > 0, \quad n \geq 1.$$

For a proof, see [19] or [21]. Our notation has again been adapted to the problems of small oscillations.

Before we proceed to a more detailed investigation of the polynomials let us pause for some remarks on a converse of Theorem 3 which is a straightforward generalization of known results [22] on the so-called moment problem and justifies the central role of the two-termed recurrence formula.

Theorem 4: Given a recurrence formula like that of Theorem 3 with real numbers $b_n, n \in \mathbb{N}$, nonvanishing real numbers $c_n, n \in \mathbb{N}$, and positive numbers $a_n, n \in \mathbb{N}$, one can find a Lebesgue–Stieltjes measure $d\alpha(x)$ with respect to which the polynomials $P_n, n \in \mathbb{N}_0$, build an orthogonal system. If $d\alpha(x)$ effectively is a measure on a finite interval $[a, b]$, it is uniquely determined.

The proof of this theorem can easily be reduced to several theorems in [20] which are based on the Stieltjes–Hamburger theory of the classical moment

problem [22]. The uniqueness statement concerning $d\alpha(x)$ is more complicated for infinite intervals (a, b) , but some sufficient criteria are known [20]. The uniqueness of $d\alpha(x)$ is of some interest because it guarantees the polynomials $P_n, n \in \mathbb{N}_0$, to be complete in the space $L^2_{d\alpha}$! Theorems 3 and 4 clarify in which sense a certain type of recurrence relation is equivalent to a system of orthogonal polynomials.

One can give a formal expression for $d\alpha(x)$ in terms of an infinite series. Let us illustrate this for the case of a finite interval $[a, b]$. Defining Gram's matrices

$$G_n = (G_{ij}^{(n)})_{0 \leq i, j \leq n} = \int_a^b P_i(x) P_j(x) dx \quad (40)$$

and their inverses, $F_n = G_n^{-1} = (F_{ij}^{(n)})_{0 \leq i, j \leq n}$, one obtains

$$d\alpha(x) = \lim_{n \rightarrow \infty} h_0 \sum_{k=0}^n F_{0,k}^{(n)} P_k(x) dx. \quad (41)$$

In the case of infinite intervals $-(a, \infty)$, $(-\infty, b)$, $(-\infty, \infty)$ – one can start from a certain weight function $-e^{a-x}$, e^{x-b} , e^{-x^2} – so that the elements of Gram's matrices are finite.

Given the recurrence relation, the normalization constants h_n are not longer arbitrary. From Theorem 3 one can derive

$$h_n = (c_n)^2 \frac{a_n}{a_{n+1}} h_{n-1} \quad (42)$$

and, consequently, one obtains.

Corollary 1: Let $n \geq m \geq 0$. Then

$$h_n = h_m \frac{a_{m+1}}{a_{n+1}} \prod_{v=m+1}^n (c_v)^2 = h_0 \frac{a_1}{a_{n+1}} \prod_{v=1}^n (c_v)^2.$$

The constant $h_0 > 0$ therefore reflects the only degree of freedom one has to change the normalization without changing the recurrence relation. Obviously, a positive factor can be absorbed in the weight function $w(x)$, so that one can always choose $h_0 = 1$ without loss of generality.

Furthermore, one can define a new set of polynomials, \bar{P}_n , by

$$\bar{P}_n = \frac{1}{q_n} P_n, \quad n \geq 0, \quad q_n \neq 0, \quad \bar{P}_{-1} = P_{-1} \equiv 0. \quad (43)$$

These new polynomials are – up to normalization and perhaps up to a sign – identical to the old ones (and hence equivalent as an orthogonal function system), but now they satisfy a recurrence formula with the

new coefficients

$$\begin{aligned}\bar{a}_{n+1} &= \frac{\varrho_n}{\varrho_{n+1}} a_{n+1}, & n \geq 0, \\ \bar{b}_{n+1} &= \frac{\varrho_n}{\varrho_{n+1}} b_{n+1}, & n \geq 0, \\ (\bar{c}_n)^2 &= \frac{\varrho_{n-1}}{\varrho_{n+1}} (c_n)^2, & n \geq 1, \\ \bar{h}_n &= \frac{1}{\varrho_n^2} h_n, & n \geq 0.\end{aligned}\quad (44)$$

Taking now $\varrho_n = \sqrt{h_n}$, one obtains $\bar{h}_n = 1$ for $n \geq 0$ and, from Theorem 3, $(\bar{c}_n)^2 = \frac{\bar{a}_{n+1}}{\bar{a}_n}$. Hence, in case of orthonormal polynomials, the coefficients are functions of \bar{a}_n and \bar{b}_n , $n \geq 0$, only.

Let us now focus on the question how to express the coefficients $\alpha_i^{(n)}$ by the numbers a_i , b_j , and c_k . Without loss of generality, we take in what follows $\alpha_0^{(0)} = 1$, i.e., $P_0 \equiv 1$. Please note that $P_0 \equiv p \neq 1$ simply would mean to multiply all polynomials – and hence their coefficients – by the same constant p , which is a direct consequence of the recurrence formula. In order to get a closed formula for the coefficients $\alpha_i^{(n)}$, $n \geq 1$, we define

$$d_i^j = (c_i)^2 \delta_{i+1}^j, \quad (45)$$

where δ_i^j is the Kronecker symbol. This proves useful for

Theorem 5: *The coefficients $\alpha_i^{(n)}$ of $P_n(x)$, $n \geq 1$, are given by the formula*

$$\alpha_i^{(n)} = \sum_{k=0}^{\lfloor \frac{n-l}{2} \rfloor} \frac{(-1)^{l+k}}{l! k! (n-l-2k)!} \cdot \sum_{\pi \in S_n} \left\{ \prod_{\mu=1}^l a_{\pi(\mu)} \prod_{v=1}^k d_{\pi(l+2v-1)}^{\pi(l+2v)} \prod_{q=l+2k+1}^n b_{\pi(q)} \right\},$$

where $[y] = \max \{n \in \mathbb{Z} | n \leq y\}$ denotes the Gauß bracket and the empty product is taken to be unity. From the definition of d_i^j in Eq. (45), we have no contribution to $\alpha_i^{(n)}$ by permutations with $\pi(l+2v-1) + 1 \neq \pi(l+2v)$ for $1 \leq v \leq k$.

This formula can be proved inductively by carefully rearranging the summation indices and using the following recurrence relation for the coefficients $\alpha_i^{(n)}$:

$$\alpha_i^{(n+1)} = b_{n+1} \alpha_i^{(n)} - a_{n+1} \alpha_{i-1}^{(n)} - d_n^{n+1} \alpha_i^{(n-1)}. \quad (46)$$

This is a direct consequence of Theorem 3. As an explicit proof of Theorem 5 is quite technical, it is deferred to Appendix B. Some special cases of Theorem 5 are evident.

Corollary 2: *The coefficients of the polynomials fulfil*

$$\begin{aligned}\alpha_n^{(n)} &= (-1)^n \prod_{\mu=1}^n a_{\mu}, \\ \alpha_n^{(n+1)} &= (-1)^n \prod_{\mu=1}^{n+1} a_{\mu} \sum_{v=1}^{n+1} \frac{b_v}{a_v}.\end{aligned}$$

This is, of course, in agreement with Theorem 3. Furthermore, we find the following simplification:

Corollary 3: *If $c_k = 0$ for all k , i.e., $P_{n+1}(x) = (b_{n+1} - a_{n+1}x)P_n(x)$ with $P_0 \equiv 1$, the polynomials read $P_n(x) = \sum_{l=0}^n \beta_l^{(n)} x^l$ with $\beta_0^{(0)} = 1$ and*

$$\beta_l^{(n)} = \frac{(-1)^l}{l!(n-l)!} \sum_{\pi \in S_n} \left\{ \prod_{\mu=1}^l a_{\pi(\mu)} \prod_{q=l+1}^n b_{\pi(q)} \right\}, \quad n \geq 1.$$

Occasionally, especially for several of the so-called classical polynomials, the coefficients of the recurrence relation take the simple form $a_k = a$, $b_k = b$, $c_k = c$ for $k \in \mathbb{N}$. In order to obtain an appropriate simplification of Theorem 5, we need the ensuing combinatoric identity.

Lemma 3: *Let $k \in \mathbb{N}_0$ and $n \geq \max \{1, 2k\}$. Then holds*

$$\sum_{\pi \in S_n} \left\{ \prod_{v=1}^k \delta_{1+\pi(2v-1)}^{\pi(2v)} \right\} = (n-k)!$$

Proof:

A counting procedure from elementary combinatoric analysis shall be used. First, take the number of possibilities you have to distribute k indistinguishable dumb-bells to n boxes which turns out to be $\binom{n-k}{k}$. Then, distinguish these k pairs which results in an additional faktor $k!$ Now, take all permutations of the remaining free boxes, which gives the factor $(n-2k)!$ But $\binom{n-k}{k} k! (n-2k)! = (n-k)!$ ■

A direct application of this Lemma yields the desired simplification of Theorem 5.

Corollary 4: If $a_k = a$, $b_k = b$, $c_k = c$ for all $n \in \mathbb{N}$, we simply have

$$\alpha_i^{(n)} = \sum_{k=0}^{\lfloor \frac{n-l}{2} \rfloor} (-1)^{l+k} \binom{n-k}{k} \binom{n-2k}{l} a^l b^{n-l-2k} c^{2k}$$

and $h_n = c^{2n} h_0$.

The importance of orthogonal polynomials for the theory of small oscillations is shown by Lemma 2 of the preceding Section, now replacing the finite sequence, $(P_k)_{0 \leq k \leq N}$, by the infinite one, $(P_k)_{k \in \mathbb{N}_0}$. Remember that

$$\det(B_n - \lambda A_n) = \det(A_n) \cdot \det(\tilde{B}_n - \lambda \mathbf{1}) \quad (47)$$

with

$$\begin{aligned} \tilde{B}_n &= (R_n^t)^{-1} B_n (R_n)^{-1}, \\ R_n &= \text{diag}(\sqrt{a_1}, \dots, \sqrt{a_n}). \end{aligned} \quad (48)$$

Consequently,

$$(\tilde{B}_n)_{ij} = \frac{b_i}{a_i} \delta_{ij} - \frac{c_i}{\sqrt{a_i a_{i+1}}} (\delta_{i+1}^j + \delta_{i-1}^j). \quad (49)$$

Let us now introduce the roots $\lambda_m^{(n)}$, $1 \leq m \leq n$, of the polynomials $P_n(\lambda)$ by

$$\det(\tilde{B}_n - \lambda \mathbf{1}) = \prod_{m=1}^n (\lambda_m^{(n)} - \lambda). \quad (50)$$

Evaluating both sides of (47) one gets, by a simple comparison of coefficients, an interesting relation between the zeros of orthogonal polynomials and the recurrence coefficients, namely

Theorem 6: The roots $\lambda_m^{(n)}$, $1 \leq m \leq n$, of $P_n(\lambda)$ satisfy the following equations for $1 \leq l \leq n$.

$$\begin{aligned} \sum_{\pi \in S_n} \left\{ \prod_{\varrho=l+1}^n \lambda_{\pi(\varrho)}^{(n)} \right\} &= \sum_{k=0}^{\lfloor \frac{n-l}{2} \rfloor} \frac{(-1)^k (n-l)!}{k! (n-l-2k)!} \\ &\cdot \sum_{\pi \in S_n} \left\{ \prod_{v=1}^k \frac{d_{\pi(2v-1)}^{\pi(2v)}}{a_{\pi(2v-1)} a_{\pi(2v)}} \prod_{\varrho=l+2k+1}^n \frac{b_{\pi(\varrho)}}{a_{\pi(\varrho)}} \right\}. \end{aligned}$$

If $a_k = a$, $b_k = b$, $c_k = c$, for $k \in \mathbb{N}$, this reduces to

$$\begin{aligned} \sum_{\pi \in S_n} \left\{ \prod_{\varrho=l+1}^n \lambda_{\pi(\varrho)}^{(n)} \right\} \\ = \sum_{k=0}^{\lfloor \frac{n-l}{2} \rfloor} (-1)^k \frac{(n-k)! (n-l)!}{k! (n-l-2k)!} \left(\frac{b}{a} \right)^{n-l} \left(\frac{c}{b} \right)^{2k}. \end{aligned}$$

For $l = n-1$, $l = n-2$, and $l = 0$ we state the relations of Theorem 6 explicitly.

Corollary 5: The roots of $P_n(\lambda)$ obey

$$\begin{aligned} \text{(I)} \quad \sum_{m=1}^n \lambda_m^{(n)} &= \sum_{i=1}^n \frac{b_i}{a_i}, \\ \text{(II)} \quad \sum_{m=1}^n (\lambda_m^{(n)})^2 &= \sum_{i=1}^n \left(\frac{b_i}{a_i} \right)^2 + 2 \sum_{i=1}^{n-1} \frac{(c_i)^2}{a_i a_{i+1}}, \\ \text{(III)} \quad \prod_{m=1}^n \lambda_m^{(n)} &= \frac{1}{\prod_{i=1}^n a_i} \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} \frac{(-1)^k}{k! (n-2k)!} \\ &\cdot \sum_{\pi \in S_n} \left\{ \prod_{v=1}^k d_{\pi(2v-1)}^{\pi(2v)} \prod_{\varrho=2k+1}^n b_{\pi(\varrho)} \right\} = \det(\tilde{B}_n). \end{aligned}$$

Note that (I) has been inserted into the expression for $l = n-2$ in order to obtain (II). Sum rules for powers higher than 2 can also be derived from Theorem 6, but it is quite tedious. An application of formula (I) to the Laguerre polynomials $L_n^{(\alpha)}(\lambda)$ results in

$$\sum_{m=1}^n \lambda_m^{(n)} = n(n+\alpha) \quad (51)$$

while formula (II), calculated for the Hermite polynomials $H_n(\lambda)$, yields

$$\sum_{m=1}^n (\lambda_m^{(n)})^2 = \frac{1}{2} n(n-1). \quad (52)$$

These two well-known equations (cf. [5]) are thus obtained from the recursion coefficients in a simple, but general way.

Let us close this Section with some remarks on the localization of the eigenfrequencies. From the intersection property of the roots of consecutive polynomials (cf. Sect. 3), the numerical determination of the roots is easy if one has – for each n – a sufficiently small interval that contains all roots of $P_n(\lambda)$. This can be obtained by means of Gerschgorin's theorem (cf. [18]). Weakening this theorem to the case of a real, symmetric matrix $A_n = (A_{ij}^{(n)})_{1 \leq i, j \leq n}$ we get the following inequality for its eigenvalues λ :

$$\min_{1 \leq i \leq n} (A_{ii}^{(n)} - \sum_{\substack{j=1 \\ j \neq i}}^n |A_{ij}^{(n)}|) \leq \lambda \leq \max_{1 \leq i \leq n} (A_{ii}^{(n)} + \sum_{\substack{j=1 \\ j \neq i}}^n |A_{ij}^{(n)}|). \quad (53)$$

Consider now the generalized eigenvalue problem $B_n x = \lambda A_n x$ described above in Sect. 3, where $A_n = \text{diag}(a_1, \dots, a_n)$ with positive constants a_k and

$$B_n = \begin{pmatrix} b_1 & -c_1 & & 0 \\ -c_1 & b_2 & \ddots & \\ & \ddots & \ddots & -c_{n-1} \\ 0 & & -c_{n-1} & b_n \end{pmatrix}.$$

In this case we obtain for the eigenvalues the inequality

$$\min_{1 \leq i \leq n} \left(\frac{b_i}{a_i} - \frac{|c_{i-1}|}{\sqrt{a_i a_{i-1}}} - \frac{|c_i|}{\sqrt{a_i a_{i+1}}} \right) \leq \lambda \leq \max_{1 \leq i \leq n} \left(\frac{b_i}{a_i} + \frac{|c_{i-1}|}{\sqrt{a_i a_{i-1}}} + \frac{|c_i|}{\sqrt{a_i a_{i+1}}} \right), \quad (54)$$

where $c_0 = c_n = 0$.

Note that the reduction to an ordinary eigenvalue problem has been used before application of (53). Going now to the limit $n \rightarrow \infty$ we have to replace ‘min’ and ‘max’ by ‘inf’ and ‘sup’, respectively. Then, the following statement can directly be derived from the last inequality.

Theorem 7: Suppose that the following boundaries exist, namely, $m = \inf_{i \in \mathbb{N}}(a_i) > 0$, $M = \sup_{i \in \mathbb{N}}(a_i) < \infty$, $v = \inf_{i \in \mathbb{N}}(b_i) > -\infty$, $V = \sup_{i \in \mathbb{N}}(b_i) < \infty$, and $R = \sup_{i \in \mathbb{N}}(|c_i|) < \infty$.

Then the generalized eigenvalues fulfil $\frac{v}{M} - \frac{2R}{m} \leq \lambda \leq \frac{2R + V}{m}$.

Note that the eigenvalues of an arbitrary subsystem also fulfil this inequality, where equality can then be excluded from the intersection properties of the zeros of Sturm sequences.

Let us go back to some earlier examples. In (5) we have $m = M = 1$, $v = V = 2$, and $R = 1$ which results in $0 < \lambda < 4$. This cannot be sharpened, which is also true of many other systems with bounded eigenfrequencies. If the assumption of Theorem 7 is violated, the inequality remains valid if one carefully arranges the limits, but in general the results is not sharp. In Sect. 2, we gave an example (see (18)) with $m = v = 1$ and $M = V = R = \infty$ that nevertheless possesses bounded eigenfrequencies. In the case of small oscillations, one additionally has $\lambda > 0$ from positive definiteness, which sometimes strengthens the lower boundary.

5. Concluding Remarks

Several structural properties of orthogonal polynomials have been presented from the viewpoint of the defining recurrence relations. The latter are connected to the generalized eigenvalue problem and the theory of Sturm sequences. The physical motivation was mainly taken from the theory of small oscillations of 1-D n -particle systems. Here, as in many other examples, orthogonal polynomials show up precisely

through the recurrence relations. Nevertheless, the actual treatment of the polynomials is often avoiding these relations – though it seems advantageous to extract as many properties as possible directly from these coefficients, which was the aim of this article.

At this point, we would like to mention two additional examples where one can profit from some knowledge of orthogonal polynomials and their properties. In view of the huge literature on this subject (presently, some 40 articles per year with “orthogonal polynomials” already in the title can be found in the Science Citation Index), this can, of course, only be illustrative. Firstly, the radial wave functions in elementary quantum mechanics (e.g., for the hydrogen atom) have the property that the roots of consecutive wave functions (w.r.t. the radial quantum number) possess the intersection property. But, as mentioned in Sect. 3, this is a key property of Sturm sequences, and the radial wave functions actually constitute such a Sturm sequence which can often be seen much easier than the intersection property itself. Secondly, the treatment of spin systems can profit from orthogonal polynomials. The classical example is the Ising quantum chain which can be solved by various techniques. The approach of [15] transforms it into an eigenvalue problem which allows immediate solution in some cases, compare Appendix C for an example. Moreover, various spin systems can be tackled by the corner transfer method, compare [23], and recent progress in this direction [24] was achieved by means of orthogonal polynomials.

Finally, the study of q -deformed Lie algebras (often mis-called quantum groups) has opened a new era also for the theory of special functions and their applications, compare [25] and references within: for almost every equation in this article there exists a q -analogue (and an exponentially growing amount of literature upon it), but a more detailed description of this is definitely a separate story.

Appendix A: A Generalization of Theorem 2

Consider the generalized eigenvalue problem $B_N \mathbf{w} = \lambda A_N \mathbf{w}$ with

$$A_N = \text{diag}(a_1, \dots, a_N), \quad B_N = \begin{pmatrix} b_1 & -c_1 & & \\ -\tilde{c}_1 & b_2 & & \\ & \ddots & \ddots & \\ & & -\tilde{c}_{N-1} & b_N \end{pmatrix}, \quad (55)$$

where $a_i, b_j, c_k, \tilde{c}_l$ are arbitrary complex numbers. For the characteristic polynomials $P_n(\lambda) = \det(B_n - \lambda A_n)$,

$1 \leq n \leq N$, we have the recurrence formula

$$P_{n+1}(\lambda) = (b_{n+1} - a_{n+1}\lambda)P_n(\lambda) - c_n \tilde{c}_n P_{n-1}(\lambda), \quad (56)$$

where $0 \leq n \leq N-1$ and $P_0 \equiv 1$, $P_{-1} \equiv 0$.

If none of the constants a_j , $1 \leq j \leq N$, and none of the products $c_k \cdot \tilde{c}_k$, $1 \leq k \leq N-1$, vanish, we can prove – in complete analogy to (27) – that $P_N(\lambda)$ has only simple roots $\lambda_j^{(N)}$, $1 \leq j \leq N$. But in this case, the procedure of (33) can be applied again (since $A_N^{-1} = \text{diag}(1/a_1, \dots, 1/a_N)$ exists), which results in

$$c_i u_{i+1,j}^{(N)} = (b_i - a_i \lambda_j^{(N)}) u_{i,j}^{(N)} - \tilde{c}_{i-1} u_{i-1,j}^{(N)} \quad (57)$$

with the solution

$$u_{i,j}^{(N)} = \frac{P_{i-1}(\lambda_j^{(N)})}{i-1} \cdot c_0 := 1. \quad (58)$$

$$\prod_{k=0}^{i-1} c_k$$

Notice that the case of hermitian matrices is contained for a_i, b_j real and $\tilde{c}_k = c_k^*$. The condition $c_k \cdot \tilde{c}_k \neq 0$ can be weakened to the condition that $c_k = 0$ if and only if $\tilde{c}_k = 0$, since then the problem reduces to block form and can be treated block by block.

Appendix B: A Proof of Theorem 5

First, for $n=1$ and $n=2$, the formula yields the coefficients $\alpha_0^{(1)} = b_1$, $\alpha_1^{(1)} = -a_1$, and $\alpha_0^{(2)} = b_1 b_2 - (c_1)^2$, $\alpha_1^{(2)} = -(a_1 b_2 + a_2 b_1)$, $\alpha_2^{(2)} = a_1 a_2$. This is in agreement with $P_1(x) = b_1 - a_1 x$ and $P_2(x) = (b_1 b_2 - (c_1)^2) - (a_1 b_2 + a_2 b_1)x + a_1 a_2 x^2$. Then, inserting $P_n(x) = \sum_{k=0}^n \alpha_k^{(n)} x^k$ into the recurrence relation for the polynomials, one obtains by comparison of coefficients

$$\alpha_l^{(n+1)} = b_{n+1} \alpha_l^{(n)} - a_{n+1} \alpha_{l-1}^{(n)} - d_n^{n+1} \alpha_l^{(n-1)}, \quad n \geq 1, \quad (59)$$

where $d_n^{n+1} = (c_n)^2$.

Now, assuming the formula to be true for $1 \leq m \leq n$, $n \geq 2$, we can evaluate $\alpha_l^{(n+1)}$ for an arbitrary l , $0 \leq l \leq n+1$:

$$\begin{aligned} \alpha_l^{(n+1)} &= \sum_{k=0}^{\lfloor \frac{n+1-l}{2} \rfloor} \frac{(-1)^{l+k}}{l! k! (n+1-l-2k)!} \\ &\cdot \sum_{\pi \in S_{n+1}} \left\{ \prod_{\mu=1}^l a_{\pi(\mu)} \prod_{v=1}^k d_{\pi(l+2v-1)}^{\pi(l+2v)} \prod_{q=l+2k+1}^{n+1} b_{\pi(q)} \right\} \\ &= \sum_{k=0}^{\lfloor \frac{n+1-l}{2} \rfloor} \frac{(-1)^{l+k}}{l! k! (n+1-l-2k)!} \{I + II + III\}, \quad (60) \end{aligned}$$

where

$$\begin{aligned} I &= \sum_{s=1}^l \sum_{\substack{\pi \in S_{n+1} \\ \pi(s) = n+1}} \\ &\cdot \left\{ \prod_{\mu=1}^l a_{\pi(\mu)} \prod_{v=1}^k d_{\pi(l+2v-1)}^{\pi(l+2v)} \prod_{q=l+2k+1}^{n+1} b_{\pi(q)} \right\} a_{n+1} \\ &= l \cdot a_{n+1} \sum_{\pi \in S_n} \left\{ \prod_{\mu=1}^{l-1} a_{\pi(\mu)} \prod_{v=1}^k d_{\pi(l+2v-2)}^{\pi(l+2v-1)} \prod_{q=l+2k}^n b_{\pi(q)} \right\}, \end{aligned} \quad (61)$$

$$\begin{aligned} II &= \sum_{s=1}^k \sum_{\substack{\pi \in S_{n+1} \\ \pi(l+2s-1) = n \\ \pi(l+2s) = n+1}} \\ &\cdot \left\{ \prod_{\mu=1}^l a_{\pi(\mu)} \prod_{v=1}^k d_{\pi(l+2v-1)}^{\pi(l+2v)} \prod_{q=l+2k+1}^{n+1} b_{\pi(q)} \right\} d_n^{n+1} \\ &= k \cdot d_n^{n+1} \sum_{\pi \in S_{n-1}} \\ &\cdot \left\{ \prod_{\mu=1}^l a_{\pi(\mu)} \prod_{v=1}^{k-1} d_{\pi(l+2v-1)}^{\pi(l+2v)} \prod_{q=l+2k-1}^{n-1} b_{\pi(q)} \right\}, \quad (62) \end{aligned}$$

and

$$\begin{aligned} III &= \sum_{s=l+2k+1}^{n+1} \sum_{\substack{\pi \in S_{n+1} \\ \pi(s) = n+1}} \\ &\cdot \left\{ \prod_{\mu=1}^l a_{\pi(\mu)} \prod_{v=1}^k d_{\pi(l+2v-1)}^{\pi(l+2v)} \prod_{q=l+2k+1}^{n+1} b_{\pi(q)} \right\} b_{n+1} \\ &= (n+1-l-2k) \cdot b_{n+1} \sum_{\pi \in S_n} \\ &\cdot \left\{ \prod_{\mu=1}^l a_{\pi(\mu)} \prod_{v=1}^k d_{\pi(l+2v-1)}^{\pi(l+2v)} \prod_{q=l+2k+1}^n b_{\pi(q)} \right\}. \quad (63) \end{aligned}$$

In the first term we have contributions from $0 \leq k \leq \lfloor \frac{n+1-l}{2} \rfloor$, in the second one from $1 \leq k \leq \lfloor \frac{n+1-l}{2} \rfloor$,

and in the third one from $0 \leq k \leq \lfloor \frac{n-l}{2} \rfloor$.

Inserting these expressions into (60) and replacing the summation index k for the second term by $k' = k-1$, we obtain, from the above assumption, the formula

$$\alpha_l^{(n+1)} = b_{n+1} \alpha_l^{(n)} - a_{n+1} \alpha_{l-1}^{(n)} - d_n^{n+1} \alpha_l^{(n-1)}. \quad (64)$$

Consequently, $\alpha_l^{(n+1)}$ fits into the recurrence relation (59) of the coefficients which are equivalent to the corresponding relation for the polynomials themselves. This completes the proof.

Appendix C:**An Application to the Ising Quantum Chain**

Let us consider the Ising Hamiltonian

$$H(\kappa) = -\frac{1}{2} \left(\lambda \sum_{j=1}^N \sigma_j^z + \sum_{j=1}^{N-1} \sigma_j^x \cdot \sigma_{j+1}^x + \kappa \sigma_N^x \cdot \sigma_1^x \right) \quad (65)$$

with Pauli matrices σ^x and σ^z . Here, κ is the strength of a real defect in the closed chain with N sites. We are interested in the point $\lambda=1$ where the system is known to be critical in the thermodynamic limit and has been solved completely by algebraic techniques [15].

Nevertheless, it might be instructive to rewrite the Hamiltonian by means of the Jordan-Wigner transformation and to take a look at it from the viewpoint of orthogonal polynomials. To do so, let us first remark that H commutes with the charge operator

$$\hat{Q} = \frac{1}{2} \left(1 - \sum_{j=1}^N \sigma_j^z \right), \quad (66)$$

wherefore we have two sectors, and the projectors onto the eigenspaces with charge 0 (1) are denoted by P_0 (P_1), respectively. As is well known [15, 26], one has to consider the mixed sector Hamiltonian

$$\tilde{H}(\kappa) = H(\kappa) P_0 + H(-\kappa) P_1 \quad (67)$$

in order to avoid contributions from a nonlocal number operator and to obtain the limit of a free Majorana fermion. Obviously, one also has $H(\kappa) = \tilde{H}(\kappa) P_0 + \tilde{H}(-\kappa) P_1$, wherefore $\tilde{H}(\kappa)$ contains the same information as $H(\kappa)$.

The Jordan-Wigner transformation, compare [15], reads

$$d_n^- = \prod_{j=1}^{n-1} \sigma_j^z \sigma_n^+, \quad d_n^+ = \prod_{j=1}^{n-1} \sigma_j^z \sigma_n^-, \quad (68)$$

and we obtain

$$\sum_{j=1}^N \sigma_j^z = e^{i\pi \hat{N}}, \quad \hat{N} = \sum_{j=1}^N d_j^+ d_j, \quad (69)$$

together with

$$\begin{aligned} \tilde{H}(\kappa) = & -\lambda \cdot \frac{N}{2} \\ & + \sum_{j,k} \left(d_j^+ A_{jk} d_k + \frac{1}{2} (d_j^+ B_{jk} d_k^+ + h.c.) \right). \end{aligned} \quad (70)$$

Here, $A^t = A$, $B^t = -B$, and (71)

$$A = \frac{1}{2} \begin{pmatrix} 2\lambda & -1 & & \kappa \\ -1 & 2\lambda & \ddots & \\ & \ddots & \ddots & -1 \\ \kappa & & -1 & 2\lambda \end{pmatrix}, \quad B = \frac{1}{2} \begin{pmatrix} 0 & -1 & & -\kappa \\ 1 & 0 & \ddots & \\ & \ddots & \ddots & -1 \\ \kappa & & 1 & 0 \end{pmatrix},$$

where all matrix elements (off the tridiagonal block) not shown vanish.

We can now perform a suitable Bogoljubov-Valatin transformation to bring \tilde{H} to the form

$$\tilde{H} = \sum_{k=1}^N \eta_k a_k^+ a_k + \text{const} \quad (72)$$

with fermionic creation and annihilation operators a_k^+ , a_k and frequencies η_k . The general case (arbitrary κ) is solved in [26], in this Appendix we will only consider free boundary conditions, i.e., $\kappa=0$. From (72) one also has

$$[a_k, \tilde{H}] = \eta_k \cdot a_k. \quad (73)$$

The ansatz $a_k = \frac{1}{2} \sum \left(\frac{\Phi + \Psi}{2} d_j + \frac{\Phi - \Psi}{2} d_j^+ \right) (a_k^+)$ taken accordingly) with *real* matrices Φ and Ψ then leads to

$$\Psi_k (A+B) = \eta_k \cdot \Phi_k, \quad \Phi_k (A+B) = \eta_k \cdot \Psi_k, \quad (74)$$

where Φ_k and Ψ_k denote the k 's row vectors of the matrices Φ and Ψ , respectively. Slightly rewriting (74) one arrives at $\Phi_k (A-B) (A+B) = \eta_k^2 \cdot \Phi_k$ and $\Psi_k = \eta_k \Phi_k (A+B)^{-1}$. This left eigenvector problem is equivalent to a right eigenvector problem, because $(A-B) (A+B)$ is symmetric:

$$(A-B) (A+B) \Phi_k^t = \eta_k^2 \cdot \Phi_k^t, \quad \Psi_k^t = \eta_k (A-B)^{-1} \Phi_k^t. \quad (75)$$

The explicit form of $(A-B) (A+B)$ for free boundary conditions reads

$$(A-B) (A+B) = \begin{pmatrix} \lambda^2 & -\lambda & & \mathbf{0} \\ -\lambda & 1+\lambda^2 & \ddots & \\ & \ddots & \ddots & -\lambda \\ \mathbf{0} & & -\lambda & 1+\lambda^2 \end{pmatrix} \quad (76)$$

and is of the tridiagonal form treated in Sect. 3. For $\lambda=1$, one is back to (12), wherefore we obtain from (14):

$$\eta_k^{(N)} = 2 \sin \left(\frac{2k-1}{2N+1} \cdot \frac{\pi}{2} \right), \quad 1 \leq k \leq N, \quad (77)$$

together with the closed expression for the eigenvectors

$$\Phi_{kl}^{(N)} = E_{l-1}(\eta_k^{(N)}). \quad (78)$$

Though, admittedly, this example is rather simple, we would like to stress that similar techniques have recently led to new results through the method of corner transfer matrices, compare [24].

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