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Eigenvalue asymptotic expansion for non-Hermitian tetradiagonal Toeplitz matrices with real spectrum

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ABSTRACT

In this paper we consider a family of tetradiagonal (= four non-zero diagonals) Toeplitz matrices with a limiting set consisting in one analytic arc only and obtain individual asymptotic expansions for all the eigenvalues, as the matrix size goes to infinity. Additionally, we provide specific expansions for the extreme eigenvalues which are the eigenvalues approaching the extreme points of the limiting set. In contrast to previous related works, we study non-Hermitian Toeplitz matrices having non-canonical distribution and a real limiting set. The considered family does not belong to the so-called simple-loop class, nevertheless we manage to extend the theory to this case. The achieved formulas reveal the fine details of the eigenvalue structure and allow us to directly calculate high accuracy eigenvalues, even for matrices of relatively small size.

1. Introduction

For an absolutely integrable function $a(z)$ over the complex unit circle $\mathbb{T}$, we denote by $T_n(a)$ the $n\times n$ Toeplitz matrix $(a_{j-k})_{j,k=0}^{n-1}$ where a_j stands for the jth Fourier coefficient of $a(z)$. Let $a(z)$ be a Laurent polynomial,

$$a(z)\equiv\sum_{j=-r}^{\ell}a_jz^j\quad\text{with}\quad r,\ell\geqslant 1,\ a_{-r},a_\ell\neq 0,\ z\in\mathbb{T}. \tag{1.1}$$

In this case $T_n(a)$ becomes a banded matrix, that is, a matrix having a finite number of non-zero diagonals, that is

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$$T_n(a) = \begin{pmatrix} a_0 & \cdots & a_{-r} & & & & & 0 \\ \vdots & \ddots & & \ddots & & & & \\ a_\ell & & \ddots & & \ddots & & & \\ & \ddots & & \ddots & & \ddots & & \\ & & \boxed{a_\ell \quad \cdots \quad a_0 \quad \cdots \quad a_{-r}} & & & & & \\ & & & \ddots & & \ddots & \ddots & \\ & & & & \ddots & & \ddots & a_{-r} \\ & & & & & \ddots & \ddots & \vdots \\ 0 & & & & & a_\ell & \cdots & a_0 \end{pmatrix},$$

where the non-zero "band" is highlighted in a rectangle.

The description and characterization of the different spectral features of finite Toeplitz matrices, such as determinant, eigenvalues, singular values, and pseudospectra, have been a fruitful research topic for more than a century. The huge amount of material is well collected in the books [6–8,18,19,22].

Toeplitz matrices have an important number of applications, including numerical analysis, engineering, stochastic processes, time series analysis, signal processing, quantum and statistical mechanics, and image processing; but the most popular nowadays is arguably the discretization of differential equations. A concrete application of a banded Toeplitz matrix is the numerical solution of a one-dimensional partial differential equation (PDE). In many cases, a PDE can be discretized on a uniform spatial grid, and the solution at each grid point can be represented by a vector, leading to a banded Toeplitz matrix. In this context, banded Toeplitz matrices are often used to represent discretizations of differential operators in one dimension, such as the second derivative or the Laplace operator.

If one has the task of calculating the spectrum of $T_n(a)$, the easiest option seems to be the usage of any commercial eigensolver (such as `Eigenvalues` in `Mathematica`, `eig` in `MATLAB`, or `eigvals` in `JULIA`) but they can dramatically fail producing fundamentally incorrect results. Consider for example the generating function $h(t) = (-2 + \mathrm{i})t^{-1} + 2 - t$, which produces a tridiagonal Toeplitz matrix $T_n(h)$. If we calculate the eigenvalues of $T_{200}(h)$ with double precision (approximately 64 precision digits), then we will obtain a result with only 1 correct digit. Generally speaking, those difficulties can be related with the condition number of the eigenvector matrix, the proximity between eigenvalues, and the sparse nature of the matrix. For instance, the eigenvector matrix arising from the discretization of a PDE, is known to be ill-conditioned polynomially in the matrix size, and the numerical calculation of its eigenvalues is, in general, a difficult task. In addition, all commercial eigensolvers are non-parallel and have time complexities approaching the order $O(n^3)$ where n is the matrix size. For structured matrices, such as the Toeplitz matrices, there exist specialized algorithms with a slight time complexity improvements. For example, the NAG library uses the Lanczos algorithm, which is an iterative method to find eigenvalues and eigenvectors of an $n \times n$ Hermitian matrix. The time complexity of the Lanczos algorithm is $O(dn^2)$ where d is the average number of non-zeros in a row. But beyond the time complexity, the available eigensolvers have a memory consumption which increases as n^2, therefore, it is important to have a more efficient alternative.

The classic results of Szegő [19] were the starting point of several studies that pursued the distribution for the spectrum of $T_n(a)$. This research line evolved for almost eight decades until the nice work of Tyrtyshnikov [23] described the $a \in L^1$ case. In some applications, i.e. when the extreme eigenvalues or the eigenvectors are required, the individual eigenvalue description is necessary because the distribution-like results are of little or no help (for a theoretical example see [2,9] and for a numerical one see [12,14]). In such a case, having access to an exact expression like $\lambda_j(T_n(a)) = \Phi_{j,n}(a)$ would constitute the best possible solution, because it can produce instantly individual eigenvalues for any matrix size n and any eigenvalue index $j \in \{1, \ldots, n\}$, without the necessity of even storing the matrix entries (a process known as *matrix-less*). Unfortunately, this kind of expressions is available only in very few situations (i.e. circulant

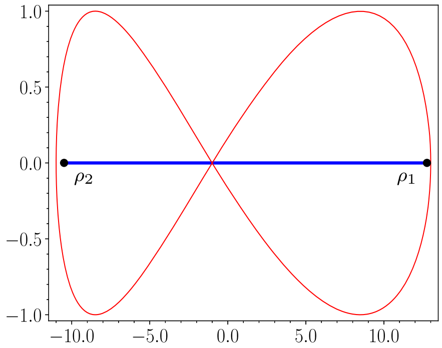

Fig. 1. The range of the generating function $a(z)$ (red curve) and the limiting set $\Lambda(a)$ (blue segment), for $a(z) = z^2 + cz + cz^{-1}$ with $c = 6$. (For interpretation of the colors in the figure(s), the reader is referred to the web version of this article.)

or some tridiagonal Toeplitz matrices, see [6]). If an exact expression is not known, then the second best option is (arguably) an asymptotic expansion, because it remains matrix-less, instantaneous, and can produce an approximation within machine precision. The article [10] is one of the first works producing individual asymptotic expansions for the eigenvalues of Toeplitz matrices, after this, a number of papers have followed the same research branch (see the reviews [3,5]).

For a Laurent polynomial $a(z)$, as n goes to infinity, Schmidt and Spitzer [20] proved that the spectrum of $T_n(a)$, $\operatorname{sp} T_n(a)$ converges in the Hausdorff metric, to a set called *limiting set* and denoted it by $\Lambda(a)$, that is the set of all $\lambda \in \mathbb{C}$ for which there exists $\lambda_n \in \operatorname{sp} T_n(a)$ such that $\lambda_n \to \lambda$. This set turns out to be the union of a finite number of analytic arcs together with the branch points.

For $\lambda \in \mathbb{C}$ and $a(z)$ given by (1.1), consider the equation $a(z) = \lambda$. We denote by $z_j(\lambda)$ ($j = 1, \ldots, r + \ell$) the respective solutions and label them in non-decreasing modulus order, that is,

$$|z_1(\lambda)| \leqslant |z_2(\lambda)| \leqslant \cdots \leqslant |z_{r+\ell}(\lambda)|.$$

One of the crucial results in [20] is that λ belongs to $\Lambda(a)$ if and only if $|z_r(\lambda)| = |z_{r+1}(\lambda)|$.

Recently, Böttcher, Gasca, Grudsky, and Kozak [11] considered the generating function (1.1) with $r = 1$, $\ell = 2$, and proved that the limiting set $\Lambda(a)$ coincides with a dilatation and a translation of the limiting set of either generating function $z^2 + z^{-1}$ or $z^2 + cz + cz^{-1}$ where $c \in \mathbb{C} \setminus \{0\}$. In any case, $\Lambda(a)$ is the union of finitely many analytic arcs together with their endpoints, and it does not contain isolated points (see Fig. 1). To be more precise, depending on the constant c, $\Lambda(a)$ can have 1, 2, or 3 analytic arcs. In the particular case $c \in (-\infty, -3\sqrt{3}] \cup [3\sqrt{3}, \infty)$ they proved that it is a closed real interval with endpoints $\rho_1 \equiv a(t_1)$ and $\rho_2 \equiv a(t_2)$, where t_1, t_2 are the two zeros of $a'(z)$ with the smallest modulus. For a generating function f, Shapiro and Štampach proved in [21] that $\Lambda(f) \subset \mathbb{R}$ if and only if $\operatorname{sp} T_n(f) \subset \mathbb{R}$, for each $n \in \mathbb{N}$, implying that, in the case at hand, each spectra $\operatorname{sp} T_n(a)$ must be a real set.

In the present article we bound ourselves to the case $\Lambda(a) \subset \mathbb{R}$ and use the Widom determinant formula [24] together with the simple-loop (SL) method (introduced in [1,10], see also [4] and the review [5]) to obtain an asymptotic expansion for each eigenvalue of $T_n(a)$.

The paper is organized as follows. In Section 2 we introduce the study objects and present our main results. In Section 3 we use the Widom formula for the determinants of finite Toeplitz matrices, to obtain a nonlinear equation for the localization of all the eigenvalues. In Section 4 we extend the SL theory to prove our main results, and finally, in Section 5 we present numerical examples.

2. Main results

Consider the generating function

$$a(z) \equiv a_2 z^2 + a_1 z + a_0 + a_{-1} z^{-1}, \qquad a_2, a_{-1} \neq 0.$$

In [20] Schmidt and Spitzer discovered the following trick for banded Toeplitz matrices: for $n \geqslant 0$ and a constant $\xi \in (0, \infty)$ consider the diagonal matrix $D_{\xi,n} \equiv \operatorname{diag}((\xi^{j-1})_{j=1}^{n})$ and the generating function $a_\xi(z) \equiv a(\xi z)$, then

$$D_{\xi,n} T_n(a) D_{\xi,n}^{-1} = \left(a_{j-k}\xi^{j-k}\right)_{j,k=1}^{n} = T_n(a_\xi),$$

and as a consequence $T_n(a_\xi)$ and $T_n(a)$ both share the same eigenvalues. If $a_1 = 0$ we can choose ξ such that $\xi^2 a_2 = \xi^{-1} a_{-1}$, to obtain

$$\operatorname{sp} T_n(a) = \operatorname{sp} T_n(a_\xi) = a_0 + \xi^2 a_2 \operatorname{sp} T_n(z^2 + z^{-1}).$$

Otherwise, taking ξ such that $\xi a_1 = \xi^{-1} a_{-1}$, it yields

$$\operatorname{sp} T_n(a) = \operatorname{sp} T_n(a_\xi) = a_0 + \xi^2 a_2 \operatorname{sp} T_n(z^2 + cz + cz^{-1}),$$

where $c = a_1(\xi a_2)^{-1}$. Therefore, the problem of calculating the eigenvalues of a tetradiagonal Toeplitz matrix can be reduced to the cases $a(z) = z^2 + z^{-1}$ or $a(z) = z^2 + cz + cz^{-1}$, $c \in \mathbb{C} \setminus \{0\}$.

In this article, we consider the second case,

$$a(z) \equiv z^2 + cz + cz^{-1} \quad \text{with} \quad c \in (-\infty, -3\sqrt{3}] \cup [3\sqrt{3}, \infty).$$

In general, we know that the eigenvalues of $T_n(a)$ approach $\Lambda(a)$, but from [11] and [21, Th.1], in our case we can go further and say that for each n, $\operatorname{sp} T_n(a)$ is contained in $\Lambda(a)$. Let $\Lambda^*(a) \equiv \Lambda(a) \setminus \{\rho_1, \rho_2\}$, where ρ_1 and ρ_2 are the two endpoints of $\Lambda(a)$; see Section 1 and item (ii) below. After [11], we know the following properties.

(i) Let $|t_1| \leqslant |t_2| \leqslant |t_3|$ be the zeros of $a'(z)$. All t_j turn out to be real numbers and there exist constants $b \in (-1/2, 0)$ and $\kappa \in \{-1, 1\}$ such that

$$t_1 = \kappa w, \quad t_2 = \frac{-\kappa w}{1+b}, \quad t_3 = \frac{\kappa w}{b}, \tag{2.1}$$

where $w = (1 + b + b^2)^{1/2}$.

(ii) Let $\rho_j \equiv a(t_j)$ for $j = 1, 2$. The points ρ_1, ρ_2 are branch points and $\Lambda(a)$ is the real segment joining them.

(iii) For $\lambda \in \Lambda(a)$ consider the function $a(z) - \lambda$ and let

$$|z_1(\lambda)| \leqslant |z_2(\lambda)| \leqslant |z_3(\lambda)|$$

be its zeros. Then $z_1(\lambda) = \overline{z_2(\lambda)}$ and $z_3(\lambda) \in \mathbb{R}$. Moreover, $|z_1(\lambda)| = |z_2(\lambda)| < |z_3(\lambda)|$ and for $\lambda \in \Lambda^*(a)$ we have $z_1(\lambda) \neq z_2(\lambda)$.

Since $T_n(a)$ and $T_n(a_\xi)$ have the same eigenvalues, taking $\xi = -1$ we seize

$$\operatorname{sp} T_n(z^2 + cz + cz^{-1}) = \operatorname{sp} T_n(z^2 - cz - cz^{-1}),$$

which means that the eigenvalues of the Toeplitz matrices with generating functions $z^2 + cz + cz^{-1}$ and $z^2 - cz - cz^{-1}$, coincide. As a consequence, it is enough to consider positive values of c only, therefore we bound ourselves to the generating function

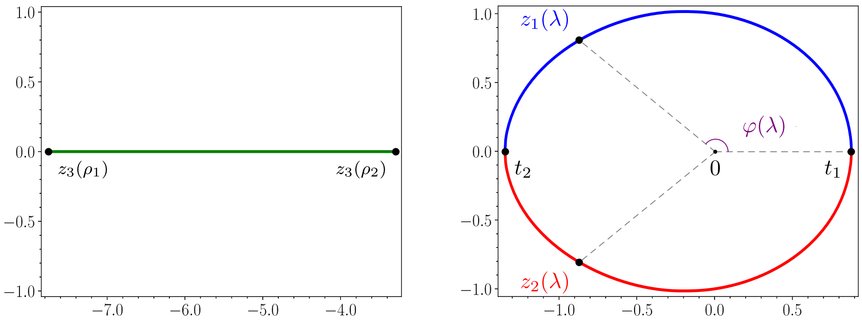

Fig. 2. The zeros of $a(z) - \lambda$ for $a(z) = z^2 + cz + cz^{-1}$, $c = 6$, and λ in the limiting set $\Lambda(a)$. Left: the real zero $z_3(\lambda)$ (green segment). Right: the complex-valued zeros $z_1(\lambda)$ (blue curve), $z_2(\lambda)$ (red curve), and the argument function $\varphi(\lambda)$ (purple).

$$a(z) \equiv z^2 + cz + cz^{-1} \quad \text{with} \quad c \in [3\sqrt{3}, \infty). \tag{2.2}$$

Consider the following continuous functions defined on the limiting set $\Lambda(a)$ by

$$\lambda \mapsto z_j(\lambda) \quad \text{for} \quad j = 1, 2, 3,$$

labeled such that, $\mathfrak{Im}\, z_1(\lambda) > 0$ and $\mathfrak{Im}\, z_2(\lambda) < 0$. From property (ii) we know that $\Lambda(a)$ is a compact real set. Combining this with the fact that all $z_j(\lambda)$ are continuous we infer that they are also bounded (see Fig. 2). In particular, $z_3(\lambda)$ is bounded away from zero, and there is a small real number $\Delta > 0$ satisfying

$$\sup_{\lambda \in \Lambda(a)} \frac{|z_1(\lambda)|}{|z_3(\lambda)|} < \mathrm{e}^{-\Delta}. \tag{2.3}$$

Furthermore, using property (i) it is clear that $t_1 t_2 < 0$. Since $c > 0$, it can be proven that $\kappa = 1$ in (2.1), yielding

$$t_1 \in \left(\frac{\sqrt{3}}{2}, 1\right), \quad t_2 \in (-\sqrt{3}, -1),$$

and $\rho_1 > 0$, $\rho_2 < 0$.

For every $\lambda \in \Lambda(a)$, we define the auxiliary real-valued functions $\varphi(\lambda)$ and $\sigma(\lambda)$ by,

$$\varphi(\lambda) \equiv \arg(z_1(\lambda)) \quad \text{and} \quad \sigma(\lambda) \equiv -\log(|z_1(\lambda)|), \tag{2.4}$$

see Fig. 3. Then, the function $\varphi(\lambda)$ satisfies

$$\varphi(\rho_1) = 0, \quad \varphi(\rho_2) = \pi, \quad \text{and} \quad \varphi(\Lambda(a)) = [0, \pi].$$

Using $\varphi(\lambda)$ and $\sigma(\lambda)$ we can write the zeros of $a(z) - \lambda$ as

$$z_1(\lambda) = \mathrm{e}^{\mathrm{i}\varphi(\lambda)} \mathrm{e}^{-\sigma(\lambda)}, \quad z_2(\lambda) = \mathrm{e}^{-\mathrm{i}\varphi(\lambda)} \mathrm{e}^{-\sigma(\lambda)}, \quad z_3(\lambda) = -c\mathrm{e}^{2\sigma(\lambda)}. \tag{2.5}$$

From property (ii) we know that $z_1(\rho_j) = t_j$ $(j = 1, 2)$ and in Lemma 3.3, we will see that the range of $\sigma(\lambda)$ is the real segment joining the points $-\log(|t_1|)$ and $-\log(|t_2|)$, see Fig. 3.

In Lemma 3.3 we will show that $\varphi(\lambda)$ is continuously differentiable, one-to-one, and that its inverse function $\psi\colon [0, \pi] \to \Lambda(a)$ is also continuously differentiable (see Figs. 3 and 4). As a consequence, $\psi(s)$ is a bijection between $s \in [0, \pi]$ and $\lambda \in \Lambda(a)$. In this article we prefer to work with the variable s instead of

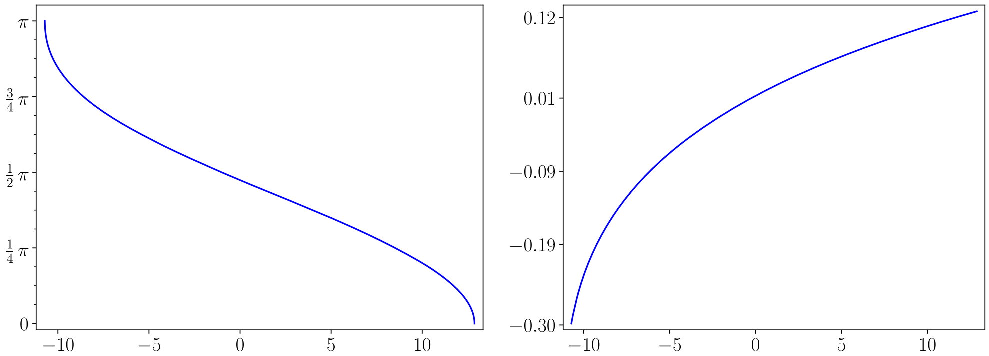

Fig. 3. The functions $\varphi(\lambda)$ (left) and $\sigma(\lambda)$ (right) for $\lambda \in \Lambda(a)$ with generating function $a(z) = z^2 + cz + cz^{-1}$ and $c = 6$.

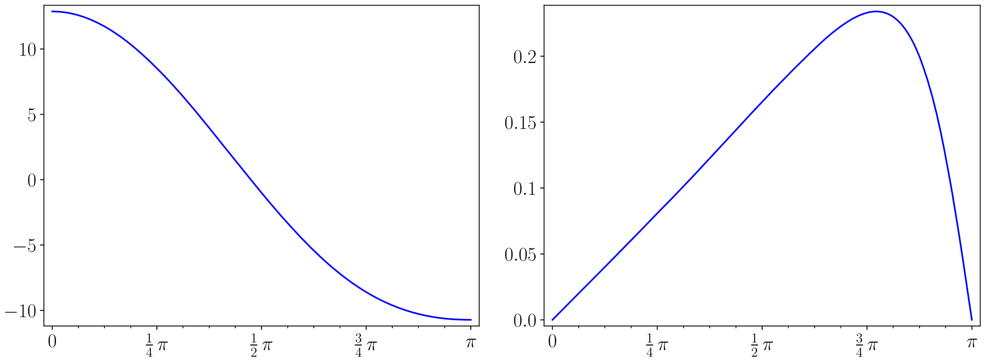

Fig. 4. The functions $\psi(s)$ (left) and $\theta(s)$ (right) for the generating function $a(z) = z^2 + cz + cz^{-1}$ with $c = 6$.

λ itself, because it will produce cleaner and simpler calculations. Accordingly, for $j = 1, 2, 3$, and $s \in [0, \pi]$, we introduce the functions

$$\hat{z}_j(s) \equiv z_j(\psi(s)) = z_j(\lambda), \qquad \hat{\sigma}(s) \equiv \sigma(\psi(s)) = \sigma(\lambda), \tag{2.6}$$

and from them, we define the auxiliary functions

$$f(s) \equiv \frac{\mathrm{e}^{-\hat{\sigma}(s)}}{\hat{z}_3(s)}, \qquad \eta(s) \equiv 1 - \mathrm{e}^{\mathrm{i}s} f(s), \qquad \theta(s) \equiv \arg(\eta(s)). \tag{2.7}$$

The fact that $\theta(s)$ is well-defined is a consequence of $f(s) = |\hat{z}_1(s)|/\hat{z}_3(s)$ from property (iii).

For $n \in \mathbb{N}$ and $j \in \{1, \ldots, n\}$, we consider the grid points

$$d_{j,n} \equiv \frac{\pi j}{n+1}, \quad e_{j,n} \equiv d_{j,n} - \frac{\theta(d_{j,n})}{n+1}, \tag{2.8}$$

and the neighborhoods

$$\Omega_{j,n} \equiv \big\{ s \in (0, \pi) \colon |s - e_{j,n}| \leqslant r_{j,n} \big\}, \tag{2.9}$$

where $r_{j,n} \equiv 3\|\theta'\|_\infty \theta(d_{j,n})/(n+1)^2$. For each n the sequence $(d_{j,n})_{j=1}^n$ is a regular mesh for the interval $[0, \pi]$, and the constants $r_{j,n}$ were selected in such a way that the sets $(\Omega_{j,n})_{j=1}^n$ become pairwise disjoint.

In asymptotic analysis, if $f_j(n)$ for $j \in \{1, \ldots, n\}$ and $g(n)$ are functions defined on $\mathbb{N}$, we say that $f_j(n) = O(g(n))$ as $n \to \infty$ uniformly with respect to j, if there exist positive numbers N and M not depending on j, such that for all $j \in \{1, \dots, n\}$ and $n > N$ we have $|f_j(n)| \leqslant M|g(n)|$. Now we write our main results.

Theorem 2.1. *Let $a(z)$ be the generating function in (2.2), $\psi(s)$ be the inverse function of $\varphi(\lambda)$ defined in (2.4), $\theta(s)$ be the function defined in (2.7), $\Omega_{j,n}$ be the set defined in (2.9) and let $\lambda_{1,n} \geqslant \lambda_{2,n} \geqslant \cdots \geqslant \lambda_{n,n}$ be the eigenvalues of $T_n(a)$. Then for each $j \in \{1, \dots, n\}$ and every sufficiently large $n \in \mathbb{N}$, the following statements hold.*

1. *The eigenvalues are pairwise distinct and $\lambda_{j,n} \in \psi(\Omega_{j,n})$.*
2. *The number $s_{j,n} \equiv \varphi(\lambda_{j,n})$ (equivalently $\lambda_{j,n} = \psi(s_{j,n})$) belongs to $\Omega_{j,n}$ and satisfies the equation*
$$(n+1)s_{j,n} + \theta(s_{j,n}) = \pi j + E_1(s_{j,n}),$$
where $E_1(s)$ is a differentiable function with $E_1(s_{j,n}) = O(\mathrm{e}^{-\Delta n})$, and whose derivative satisfies $E_1'(s_{j,n}) = O(n\mathrm{e}^{-\Delta n})$. Both order relations work as $n \to \infty$ uniformly in j.
3. *The equation*
$$(n+1)s + \theta(s) = \pi j,$$
has a unique solution $s^*_{j,n} \in \Omega_{j,n}$ and
$$\lambda_{j,n} = \psi(s^*_{j,n}) + E_2(s^*_{j,n}), \tag{2.10}$$
where $E_2(s^*_{j,n}) = O(n^{-1}\mathrm{e}^{-\Delta n})$, as $n \to \infty$ for certain $\Delta > 0$, uniformly in j.

Theorem 2.2. *Under the same hypothesis of Theorem 2.1, as $n \to \infty$ and for any $m \geqslant 1$, we have the following expansions,*

1. $s_{j,n} = \displaystyle\sum_{k=0}^{m-1} \frac{\mathfrak{s}_k(d_{j,n})}{(n+1)^k} + H_m(d_{j,n}),$
2. $\lambda_{j,n} = \displaystyle\sum_{k=0}^{m-1} \frac{\mathfrak{r}_k(d_{j,n})}{(n+1)^k} + \hat{H}_m(d_{j,n}),$

where $d_{j,n}$ is the number defined in (2.8) and the coefficients $\mathfrak{s}_k$ and $\mathfrak{r}_k$ can be exactly calculated, for instance

$$\mathfrak{s}_0 = \mathrm{id}, \qquad \mathfrak{s}_1 = -\theta, \qquad \mathfrak{s}_2 = \theta\theta',$$
$$\mathfrak{r}_0 = \psi, \qquad \mathfrak{r}_1 = -\psi'\theta, \qquad \mathfrak{r}_2 = \frac{1}{2}\psi''\theta^2 + \psi'\theta\theta';$$

$H_m(d_{j,n}) = O(d_{j,n}(\pi - d_{j,n})n^{-m})$ and $\hat{H}_m(d_{j,n}) = O(d_{j,n}(\pi - d_{j,n})n^{-m})$, as $n \to \infty$, are the remainder (error) terms with the order relations being uniform in j.

In our case the eigenvalues $\lambda_{j,n}$ can be classified into two types: the eigenvalues approaching either ρ_1 or ρ_2, that we called *extreme*, and the remaining ones that we called *inner*.

From properties (i) and (ii) we know that for $i = 1, 2$ and $j = 1, 2, 3$, the zeros of $a(z) - \rho_i$ are $z_j(\rho_i)$. The extreme eigenvalues have an important role in practice for estimating the norm of large matrices or its inverse. Here is our result for the extreme eigenvalues.

Theorem 2.3. *Under the same hypothesis of Theorem 2.1, we have,*

1. *if* $j^2/n \to 0$*, then*

$$\lambda_{j,n} = \rho_1 + \frac{\mathfrak{u}_{1,1} j^2}{(n+1)^2} + \frac{\mathfrak{u}_{2,1} j^2}{(n+1)^3} + \frac{\mathfrak{u}_{3,1} j^2 + \mathfrak{u}_{4,1} j^4}{(n+1)^4} + o\Big(\frac{j^4}{n^5}\Big); \tag{2.11}$$

2. *if* $(n-j)^2/n \to 0$*, then*

$$\lambda_{j,n} = \rho_2 + \frac{\mathfrak{u}_{1,2}(n+1-j)^2}{(n+1)^2} + \frac{\mathfrak{u}_{2,2}(n+1-j)^2}{(n+1)^3} + \frac{\mathfrak{u}_{3,2}(n+1-j)^2}{(n+1)^4} + \frac{\mathfrak{u}_{4,2}(n+1-j)^4}{(n+1)^4} + o\Big(\frac{(n-j)^4}{n^5}\Big);$$

where the coefficients are given by

$$\mathfrak{u}_{1,i} \equiv -\frac{a^{(2)}(t_i)}{2}(t_i\pi)^2, \qquad \mathfrak{u}_{2,i} \equiv -\frac{2\mathfrak{u}_{1,i} t_i}{t_i - \tau_i}, \qquad \mathfrak{u}_{3,i} \equiv \frac{3\mathfrak{u}_{1,i} t_i^2}{(\tau_i - t_i)^2},$$

$$\mathfrak{u}_{4,i} \equiv \Big(\frac{a^{(4)}(t_i)t_i^4}{24} - \frac{a^{(3)}(t_i)t_i^3}{6} - \frac{5a^{(3)}(t_i)t_i^4}{72a^{(2)}(t_i)} - \frac{a^{(2)}(t_i)t_i^2}{3}\Big)\pi^4,$$

t_i *is the number defined in* (2.1)*,* $\rho_i = a(t_i)$*, and* τ_i *is the simple zero of* $a(z) - \rho_i$ $(i = 1, 2)$*. All the order relations are uniform in* j*.*

Remark 2.4. The results in Theorem 2.3 can be extended for as many terms as desired and specialized under different additional conditions, for instance,

- if $j/n \to 0$ or $(n-j)/n \to 0$, then

$$\lambda_{j,n} = \rho_1 + \frac{\mathfrak{u}_{1,1} j^2}{(n+1)^2} + o\Big(\frac{j^2}{n^3}\Big) + o\Big(\frac{j^4}{n^4}\Big),$$

$$\lambda_{j,n} = \rho_2 + \frac{\mathfrak{u}_{1,2}(n+1-j)^2}{(n+1)^2} + o\Big(\frac{(n-j)^2}{n^3}\Big) + o\Big(\frac{(n-j)^4}{n^4}\Big),$$

  respectively;
- or if $j^4/n^3 \to 0$ or $(n-j)^4/n^3 \to 0$, then

$$\lambda_{j,n} = \rho_1 + \frac{\mathfrak{u}_{1,1} j^2}{(n+1)^2} + \frac{\mathfrak{u}_{2,1} j^2}{(n+1)^3} + o\Big(\frac{j^4}{n^4}\Big),$$

$$\lambda_{j,n} = \rho_2 + \frac{\mathfrak{u}_{1,2}(n+1-j)^2}{(n+1)^2} + \frac{\mathfrak{u}_{2,2}(n+1-j)^2}{(n+1)^3} + o\Big(\frac{(n-j)^4}{n^4}\Big),$$

  respectively.

To compute the asymptotic expressions in Theorem 2.2 it is necessary to know the functions $\psi(s)$, $\theta(s)$, and some of their derivatives. These functions are defined in terms of $z_j(\lambda)$ $(j = 1, 2, 3)$ which don't have an easy analytic expression available, but can be found numerically with an appropriate interpolation process. However, in the case of the extreme eigenvalues, Theorem 2.3 gives us asymptotic expressions involving $a(z)$ and its derivatives only, which are available analytically.

3. Preliminaries

In the present section we derive a formula for the Toeplitz determinant $D_n(a-\lambda) \equiv \det T_n(a-\lambda)$, that will allow us to analyze the asymptotic behavior of the eigenvalues of $T_n(a)$ as n increases to ∞.

When the generating function $a(z)$ is a Laurent polynomial, the classic Widom determinant formula [24] gives us an expression for $D_n(a)$. For the reader convenience we report it here.

Proposition 3.1 *(Widom). Let $a(z)$ be the Laurent polynomial $a(z) = \sum_{j=-r}^{\ell} a_j z^j$. If its zeros $z_1, \ldots, z_{r+\ell}$, are pairwise distinct then, for every $n \geqslant 1$,*

$$D_n(a) = \sum_M c_M \omega_M^n,$$

where the sum runs over all sets $M \subset \{1, \ldots, r+\ell\}$ with cardinality $|M| = \ell$,

$$\omega_M \equiv (-1)^{\ell} a_{\ell} \prod_{j \in M} z_j, \quad c_M \equiv \prod_{j \in M} z_j^r \prod_{\substack{j \in M \\ k \in \overline{M}}} \frac{1}{z_j - z_k},$$

and $\overline{M} \equiv \{1, \ldots, r+\ell\} \setminus M$.

Consider the generating function $a(z)$ given in (2.2) and remember that $\rho_j = a(t_j)$ where t_j $(j = 1,2,3)$ are the three zeros of $a'(z)$. If we select a complex constant $\lambda \neq \rho_j$, then the solutions of $a(z) - \lambda = 0$, named $z_j(\lambda)$ $(j = 1,2,3)$ see (2.5), become pairwise distinct. Applying Proposition 3.1 we arrive at

$$D_n(a-\lambda) = c_1(\lambda)\omega_1^n(\lambda) + c_2(\lambda)\omega_2^n(\lambda) + c_3(\lambda)\omega_3^n(\lambda), \tag{3.1}$$

where

$$\begin{aligned} &\omega_1 \equiv z_1 z_3, && \omega_2 \equiv z_2 z_3, && \omega_3 \equiv z_1 z_2, \\ &c_1 \equiv \frac{\omega_1}{(z_1 - z_2)(z_3 - z_2)}, && c_2 \equiv \frac{\omega_2}{(z_2 - z_1)(z_3 - z_1)}, && c_3 \equiv \frac{\omega_3}{(z_1 - z_3)(z_2 - z_3)}. \end{aligned} \tag{3.2}$$

To exploit the relation (3.1) we now seek for an asymptotic expression for every term involved. Recall that $\Lambda^*(a) = \Lambda(a) \setminus \{\rho_1, \rho_2\}$.

Remark 3.2. From the open mapping theorem and the analyticity of $a(z)$, it follows that $z_j(\lambda)$ $(j = 1,2,3)$ are infinitely differentiable in $\Lambda^*(a)$. Moreover, each $z_j(\lambda)$ is one-to-one in $\Lambda^*(a)$. Property (iii) in Section 2, tells us that $z_3(\lambda)$ is a simple zero of $a(z) - \lambda$ for every $\lambda \in \Lambda(a)$, then there exists an open neighborhood Ω of $\Lambda(a)$ in $\mathbb{C}$ such that,

$$\lim_{\substack{\lambda \to \rho_j \\ \lambda \in \Omega}} z_3'(\lambda) = \frac{1}{a'(z_3(\rho_j))},$$

and $z_3(\lambda)$ is therefore, analytic in Ω.

Lemma 3.3. *The real-valued functions $\sigma(\lambda)$ and $\varphi(\lambda)$ defined in (2.4), are one-to-one and infinitely differentiable in $\Lambda^*(a)$.*

Proof. From (2.5) we know that $z_3(\lambda) = -c\mathrm{e}^{2\sigma(\lambda)}$. Thus by Remark 3.2 we conclude that $\sigma(\lambda)$ is infinitely differentiable in $\Lambda^*(a)$. Since $z_3(\lambda)$ is a root of $a(z) - \lambda$, we have $a(z_3(\lambda)) = \lambda$ for all $\lambda \in \Lambda(a)$, from which it follows that both $z_3(\lambda)$ and $\sigma(\lambda)$ are one-to-one, and using that they are real-valued, we deduce their monotonicity. To be more precise, $\sigma(\lambda)$ and $-z_3(\lambda)$ are both increasing.

Applying Vieta's theorem to the equation $a(z)-\lambda = 0$ and bearing in mind the first and second equations of (2.5), we seize

$$-c = z_1(\lambda) + z_2(\lambda) + z_3(\lambda) = 2\mathrm{e}^{-\sigma(\lambda)}\cos(\varphi(\lambda)) + z_3(\lambda).$$

Thus

$$\cos(\varphi(\lambda)) = -\frac{c + z_3(\lambda)}{2}\mathrm{e}^{\sigma(\lambda)},$$

and therefore, $\cos(\varphi(\lambda))$ is a monotonic function also. Since the range of $\varphi(\lambda)$ is $[0, \pi]$, $z_3(\lambda) = -c\mathrm{e}^{2\sigma(\lambda)}$, and $\arccos(-x) = \arcsin(x) + \pi/2$, we obtain

$$\varphi(\lambda) = \arcsin\left(\frac{c}{2}\mathrm{e}^{\sigma(\lambda)}(1 - \mathrm{e}^{2\sigma(\lambda)})\right) + \frac{\pi}{2}. \tag{3.3}$$

Recall that $\sigma(\lambda)$ is contained in the segment joining the points $-\log(|t_1|)$ and $-\log(|t_2|)$. From (2.1) we have $\sqrt{3}/2 \leqslant |t_1| \leqslant 1$ and $1 < |t_2| \leqslant \sqrt{3}$, then by Vieta's theorem, for all $\lambda \in \Lambda(a)$, we obtain

$$\sigma(\lambda) \in \left[\log\left(\frac{1}{\sqrt{3}}\right), \log\left(\frac{2}{\sqrt{3}}\right)\right].$$

Consider the function $p(x) \equiv cx(1 - x^2)/2$. Since $p(x)$ is one-to-one in $[1/\sqrt{3}, \infty)$ it follows that both $p(\mathrm{e}^{\sigma(\lambda)})$ and $\varphi(\lambda) = \arcsin(p(\mathrm{e}^{\sigma(\lambda)})) + \pi/2$ are one-to-one for the variable $\lambda \in \Lambda(a)$. Finally, from (3.3) $\varphi(\lambda)$ is infinitely differentiable in $\Lambda^*(a)$. $\square$

Let $\psi\colon [0, \pi] \to \Lambda(a)$ be the inverse function of $\varphi\colon \Lambda(a) \to [0, \pi]$. The fact that $\psi(s)$ is infinitely differentiable in $(0, \pi)$ is an immediate consequence of Lemma 3.3. Moreover, using the derivative chain rule to $\varphi(\psi(s)) = s$ together with $\varphi'(\lambda) \neq 0$ for $\lambda \in \Lambda^*(a)$, we seize

$$\psi'(s) = \frac{1}{\varphi'(\psi(s))}.$$

We know that, as $n \to \infty$, the biggest and smallest eigenvalues of $T_n(a)$ are arbitrarily close to ρ_1 and ρ_2, respectively, see Fig. 1. For the study of the extreme eigenvalues, we need to investigate the behavior of the functions $\varphi(\lambda)$ at ρ_i, and $\psi(s)$ at $\varphi(\rho_i)$. Since $z_1(\rho_i) = z_2(\rho_i)$ for $i = 1, 2$, we know that $a(z) - \rho_i$ has only two solutions, namely, $t_i = z_1(\rho_i)$ and $\tau_i \equiv z_3(\rho_i)$, moreover, τ_i is a simple zero, $a(t_i) = \rho_i$, $a'(t_i) = 0$, and $a''(t_i)\,\mathrm{sign}(t_i) > 0$.

Consider the coefficients

$$\mathfrak{a}_{k,i} \equiv \frac{a^{(k)}(t_i)}{k!}, \quad \mathfrak{b}_{k,i} \equiv \frac{a^{(k)}(\tau_i)}{k!}, \quad k \in \mathbb{N}. \tag{3.4}$$

Proposition 3.4. *For $i = 1, 2$, and every $m \in \mathbb{N}$ the real-valued functions $\varphi(\lambda)$ and $\psi(s)$ admit the following asymptotic expansions,*

$$\varphi(\lambda) = \varphi(\rho_i) + \sum_{k=1}^{m-1} \gamma_{k,i} |\lambda - \rho_i|^{\frac{k}{2}} + W_{1,i,m}(\lambda),$$
$$\psi(s) = \rho_i + \sum_{k=1}^{m-1} \nu_{k,i} (s - \varphi(\rho_i))^{2k} + W_{2,i,m}(s), \tag{3.5}$$

where

- *the coefficients $\gamma_{k,i}$ and $\nu_{k,i}$ can be calculated explicitly, for instance*

$$\gamma_{1,i} = \frac{1}{t_i |\mathfrak{a}_{2,i}|^{\frac{1}{2}}}, \quad \nu_{1,i} = -t_i^2 \mathfrak{a}_{2,i},$$
$$\gamma_{2,i} = \frac{\mathfrak{a}_{3,i}^2}{8\mathfrak{a}_{2,i}^4 t_i^2 \gamma_{1,i}} + (-1)^i \frac{3\mathfrak{a}_{3,i}^2 \gamma_{1,i}}{4\mathfrak{a}_{2,i}^3} + \frac{\mathfrak{a}_{4,i} t_i^2 \gamma_{1,i}^3}{2\mathfrak{a}_{2,i}} + (-1)^i \frac{\mathfrak{a}_{3,i} \gamma_{1,i}}{2\mathfrak{a}_{2,i}^2 t_i} - \frac{\gamma_{1,i}^3}{3},$$
$$\nu_{2,i} = \mathfrak{a}_{4,i} t_i^4 - \mathfrak{a}_{3,i} t_i^3 - \frac{5\mathfrak{a}_{3,i}^2 t_i^4}{4\mathfrak{a}_{2,i}} - \frac{2\mathfrak{a}_{2,i} t_i^2}{3};$$

- *$W_{1,i,m}(\lambda) = O(|\lambda - \rho_i|^{\frac{m}{2}})$ as $\lambda \to \rho_i$;*
- *in the particular case $m = 2m_0$, $m_0 \geqslant 1$, $W_{1,i,m}(\lambda)$ is differentiable in a neighborhood of ρ_i intersected with $\Lambda^*(a)$, and $W'_{1,i,m}(\lambda) = O(|\lambda - \rho_i|^{m_0 - 1})$;*
- *$W_{2,i,m}(s) = O((s - \varphi(\rho_i))^{2m})$ as $s \to \varphi(\rho_i)$;*
- *$W_{2,i,m}(s)$ is differentiable in a neighborhood of $\varphi(\rho_i)$ intersected with $(0, \pi)$, and $W'_{2,i,m}(s) = O(|s - \varphi(\rho_i)|^{2m-1})$.*

Proof. We start with the case $i = 1$. To simplify the notation and only in this proof, we will write $\mathfrak{a}_k$ instead of $\mathfrak{a}_{k,1}$.

Recall that $\varphi(\lambda)$ is the argument of $z_1(\lambda)$ which is the complex-valued zero of $a(z) - \lambda$ having non-negative imaginary part. The asymptotic expansion of $a(z)$ centered at t_1 for $\operatorname{im} z \geqslant 0$, yields

$$a(z) = \rho_1 + \sum_{k=2}^{m-1} \mathfrak{a}_k (z - t_1)^k + P_{1,m}(z),$$

where $m \geqslant 3$ and $P_{1,m}(z) = O(|z - t_1|^m)$ as $z \to t_1$, is a differentiable function. Here the term corresponding to $k = 1$ is missing because of $\mathfrak{a}_1 = a'(t_i) = 0$. Hence, taking $z = z_1(\lambda)$ for $\lambda \in \Lambda^*(a)$ and any $m \geqslant 3$, we arrive at

$$\lambda - \rho_1 = \sum_{k=2}^{m-1} \mathfrak{a}_k (z_1(\lambda) - t_1)^k + \hat{P}_{1,m}(\lambda), \tag{3.6}$$

where $\hat{P}_{1,m}(z) = O(|z_1(\lambda) - t_1|^m)$ as $\lambda \to \rho_1$, is a differentiable function in $\Lambda^*(a)$. Since by continuity, $\lambda \to \rho_1$ implies $z_1(\lambda) \to t_1$, we can solve (3.6) for $z_1(\lambda)$ (see [17, Sc.1.5]), resulting in

$$z_1(\lambda) = t_1 + \sum_{k=1}^{m-1} \alpha_k (\rho_1 - \lambda)^{\frac{k}{2}} + K_{1,m}(\lambda), \tag{3.7}$$

where $m \geqslant 2$ and the coefficients α_k, can be computed by formal substitution, for example

$$\alpha_1 = \mathrm{i}\frac{1}{|\mathfrak{a}_2|^{\frac{1}{2}}}, \quad \alpha_2 = \frac{\mathfrak{a}_3}{2\mathfrak{a}_2^2}, \quad \alpha_3 = \mathrm{i}\left(\frac{\mathfrak{a}_3^2|\mathfrak{a}_2|^{\frac{1}{2}}}{8\mathfrak{a}_2^4} - \frac{3\mathfrak{a}_3^2}{4\mathfrak{a}_2^3|\mathfrak{a}_2|^{\frac{1}{2}}} + \frac{\mathfrak{a}_4}{2\mathfrak{a}_2|\mathfrak{a}_2|^{\frac{3}{2}}}\right).$$

Moreover, $K_{1,m}(\lambda) = O((\rho_1 - \lambda)^{\frac{m}{2}})$ as $\lambda \to \rho_1$. Solving (3.7) for $K_{1,m}(\lambda)$ we can see that it is infinitely differentiable in the real interval $(\rho_1 - \varepsilon, \rho_1)$ for some $\varepsilon > 0$.

To obtain an asymptotic expansion for $\varphi(\lambda)$, we use the representation

$$\varphi(\lambda) = \arg(z_1(\lambda)) = \arctan\left(\frac{\mathfrak{Im}\, z_1(\lambda)}{\mathfrak{Re}\, z_1(\lambda)}\right),$$

which combined with (3.7), the geometric series, and the Maclaurin series of arctan, yields

$$\varphi(\lambda) = \sum_{k=1}^{m-1} \gamma_k(\rho_1 - \lambda)^{\frac{k}{2}} + K_{2,m}(\lambda), \tag{3.8}$$

where the coefficients γ_k can be found explicitly, for example

$$\gamma_1 = \frac{\mathfrak{Im}\,\alpha_1}{t_1}, \quad \gamma_2 = \frac{\mathfrak{Im}\,\alpha_3}{t_1} - \frac{\alpha_2\,\mathfrak{Im}\,\alpha_1}{t_1^2} - \frac{(\mathfrak{Im}\,\alpha_1)^3}{3t_1^3},$$

and $K_{2,m}(\lambda) = O((\rho_1 - \lambda)^{\frac{m}{2}})$ as $\lambda \to \rho_1$. Using that $\varphi(\lambda)$ is infinitely differentiable in $\Lambda^*(a)$, we deduce the same for $K_{2,m}(\lambda)$ in the real interval $(\rho_1 - \varepsilon, \rho_1)$ for some $\varepsilon > 0$. Finally, differentiating term-by-term the expansion (3.8) we obtain the first assertion.

We now prove our second assertion. For $s \in (0, \pi)$ we know that $\lambda = \psi(s) \in \Lambda^*(a)$ and $s = \varphi(\psi(s))$. Furthermore, by Lemma 3.3 it follows that $\psi(s)$ is infinitely differentiable in $(0, \pi)$. Expanding $\psi(s)$ around $s = 0$ we reach

$$\psi(s) = \rho_1 + \sum_{k=1}^{\infty} \nu_k s^k, \tag{3.9}$$

where $\nu_k = \psi^{(k)}(0)/k!$. Additionally, by composing the expansions (3.8) and (3.9), we can seize the values of ν_k in terms of γ_k, for instance

$$\nu_1 = 0, \quad \nu_2 = -\frac{1}{\gamma_1^2}, \quad \nu_3 = 0, \quad \nu_4 = 2\frac{\gamma_3}{\gamma_1^5}, \quad \nu_5 = 0,$$

finishing the proof for the case $i = 1$. The case $i = 2$ can be readily proven. □

Mimicking the proof of Proposition 3.4, for any $m \geqslant 2$ as $\lambda \to \rho_i$, we obtain the following asymptotic expansions,

$$z_1(\lambda) = t_i + \sum_{k=1}^{m-1} \alpha_{k,i}|\lambda - \rho_i|^{\frac{k}{2}} + G_{1,i,m}(\lambda), \tag{3.10}$$

$$z_3(\lambda) = \tau_i + \sum_{k=1}^{m-1} \beta_{k,i}|\lambda - \rho_i|^{k} + G_{2,i,m}(\lambda), \tag{3.11}$$

where

- the coefficients $\alpha_{k,i}$ and $\beta_{k,i}$ can be found explicitly, for instance

$$\alpha_{1,i} = \frac{\mathrm{i}}{|\mathfrak{a}_{2,i}|^{\frac{1}{2}}}, \quad \alpha_{3,i} = \frac{\mathrm{i}}{2\mathfrak{a}_{2,i}}\left(\frac{\mathfrak{a}_{3,i}^2|\mathfrak{a}_{2,i}|^{\frac{1}{2}}}{4\mathfrak{a}_{2,i}^3} + \frac{3\mathfrak{a}_{3,i}^2(-1)^i}{2\mathfrak{a}_{2,i}^2|\mathfrak{a}_{2,i}|^{\frac{1}{2}}} + \frac{\mathfrak{a}_{4,i}}{|\mathfrak{a}_{2,i}|^{\frac{3}{2}}}\right),$$
$$\alpha_{2,i} = (-1)^{i+1}\frac{\mathfrak{a}_{3,i}}{2\mathfrak{a}_{2,i}^2}, \qquad \beta_{1,i} = \frac{1}{\mathfrak{b}_{1,i}}, \qquad \beta_{2,i} = -\frac{\mathfrak{b}_{2,i}}{\mathfrak{b}_{1,i}^3};$$

  where $t_i = z_1(\rho_i)$ and $\tau_i = z_3(\rho_i)$ are the zeros of $a(z) - \rho_i$, and the numbers $\mathfrak{a}_{k,i}$ and $\mathfrak{b}_{k,i}$ are defined in (3.4).
- $G_{1,i,m}(\lambda) = O(|\lambda - \rho_i|^{\frac{m}{2}})$ and $G_{2,i,m}(\lambda) = O(|\lambda - \rho_i|^m)$ are infinitely differentiable functions in a neighborhood of ρ_i intersected with $\Lambda^*(a)$.

The respective expansion for $z_2(\lambda)$ can be obtained using $z_2(\lambda) = \overline{z_1(\lambda)}$.

Since the zeros of $a(z) - \psi(s)$ are given by $\hat{z}_j(s) = z_j(\psi(s))$ for $j = 1, 2, 3$, see (2.6), the relation $\hat{\sigma}(s) = -\log(|\hat{z}_1(s)|)$ combined with (2.5), produces the simpler equalities,

$$\hat{z}_1(s) = \mathrm{e}^{\mathrm{i}s}\mathrm{e}^{-\hat{\sigma}(s)}, \quad \hat{z}_2(s) = \mathrm{e}^{-\mathrm{i}s}\mathrm{e}^{-\hat{\sigma}(s)}, \quad \hat{z}_3(s) = -c\mathrm{e}^{2\hat{\sigma}(s)}, \tag{3.12}$$

which are the protagonists of our next result.

Proposition 3.5. *For $j = 1, 2, 3$, the functions $\hat{z}_j(s)$ defined in (2.6) are infinitely differentiable on $[0, \pi]$ and for any $m \geqslant 1$, they admit the expansions*

$$\hat{z}_1(s) = t_i + \sum_{k=1}^{m-1} \mathfrak{h}_k(s - \varphi(\rho_i))^k + F_{1,i,m}(s), \tag{3.13}$$
$$\hat{z}_3(s) = \tau_i + \sum_{k=1}^{m-1} \mathfrak{g}_k(s - \varphi(\rho_i))^{2k} + F_{2,i,m}(s), \tag{3.14}$$

where

- *$t_i = z_1(\rho_i)$, $\tau_i = z_3(\rho_i)$ are the zeros of $a(z) - \rho_i$ where ρ_i is the branch point of $\Lambda(a)$ and the function $\varphi(\lambda)$ defined in (2.4);*
- *the coefficients $\mathfrak{h}_k$ and $\mathfrak{g}_k$ can be found explicitly, for instance*

$$\mathfrak{h}_1 = \mathrm{i}t_i, \quad \mathfrak{h}_2 = \frac{\mathfrak{a}_{3,i}t_i^2}{2}, \quad \mathfrak{h}_3 = \mathrm{i}\left(\frac{\mathfrak{a}_{3,i}t_i^2}{2\mathfrak{a}_{2,i}} + \frac{t_i}{3}\right),$$
$$\mathfrak{g}_1 = -\frac{\mathfrak{a}_{2,i}t_i^2}{\mathfrak{b}_{1,i}}, \quad \mathfrak{g}_2 = \frac{1}{\mathfrak{b}_{1,i}}\left(\mathfrak{a}_{4,i}t_i^4 - \mathfrak{a}_{3,i}t_i^3 - \frac{5\mathfrak{a}_{3,i}^2t_i^4}{4\mathfrak{a}_{2,i}} - \frac{2\mathfrak{a}_{2,i}t_i^2}{3}\right) - \frac{\mathfrak{b}_{2,i}\mathfrak{a}_{2,i}^2t_i^4}{\mathfrak{b}_{1,i}^3},$$

  where the numbers $\mathfrak{a}_{k,i}$ and $\mathfrak{b}_{k,i}$ are defined in (3.4);
- *$F_{1,i,m}(s) = O(|s - \varphi(\rho_i)|^m)$ and $F_{2,i,m}(s) = O(|s - \varphi(\rho_i)|^{2m})$ as $s \to \varphi(\rho_i)$ with $i = 1, 2$;*
- *the functions $F_{1,i,m}(s)$ and $F_{2,i,m}(s)$ are differentiable in the intersection of $(0, \pi)$ with a neighborhood of $\varphi(\rho_i)$ and satisfy $F'_{1,i,m}(s) = O(|s - \varphi(\rho_i)|^{m-1})$ and $F'_{2,i,m}(s) = O(|s - \varphi(\rho_i)|^{2m-1})$ as $s \to \varphi(\rho_i)$ with $i = 1, 2$.*

The respective expansion for $\hat{z}_2(s)$ can be obtained using $\hat{z}_2(s) = \overline{\hat{z}_1(s)}$.

Proof. By Lemma 3.3 and Proposition 3.4, we know that the real-valued function $\psi(s)$ is infinitely differentiable in $[0,\pi]$. The composition of the asymptotic expansion (3.5) with (3.10) and (3.11), yields (3.13) and (3.14), respectively. Moreover, the existence of the limits of $\hat{z}_j^{(\ell)}(s)$ $(\ell \in \mathbb{N})$ at $s = 0, \pi$ is a consequence of Proposition 3.4, therefore, $\hat{z}_j(s)$ is infinitely differentiable in the interval $[0,\pi]$, and the proof is over. □

Because of (3.12) an immediate consequence of Proposition 3.5 is that $\hat{\sigma}(s)$ is infinitely differentiable in the whole set $[0,\pi]$, where the derivatives on the extreme points $\{0,\pi\}$ are defined in the lateral sense. Lemma 3.3 tells us, in particular, that the function $\psi(s)$ is an infinitely differentiable bijection between $\Lambda(a)$ and $[0,\pi]$. Hence to easy the reading of the paper and to simplify some proofs, we decide to work with the variable $s \in [0,\pi]$ rather that $\lambda \in \Lambda(a)$. With this change, the Toeplitz determinant defined in (3.1), becomes

$$D_n(a-\lambda) = D_n(a-\psi(s)) = \hat{c}_1(s)\hat{\omega}_1^n(s) + \hat{c}_2(s)\hat{\omega}_2^n(s) + \hat{c}_3(s)\hat{\omega}_3^n(s), \tag{3.15}$$

where

$$\hat{\omega}_j(s) \equiv \omega_j(\psi(s)) = \omega_j(\lambda), \quad \hat{c}_j(s) \equiv c_j(\psi(s)) = c_j(\lambda), \quad j = 1,2,3;$$

and ω_j, c_j are defined in (3.2).

Lemma 3.6. *Let $s \in (0,\pi)$, then the terms in the Widom determinant formula (3.15), can be written as*

$$\hat{\omega}_1(s) = g(s)\mathrm{e}^{\mathrm{i}s}, \qquad \hat{\omega}_2(s) = g(s)\mathrm{e}^{-\mathrm{i}s}, \qquad \hat{\omega}_3(s) = g(s)f(s),$$

$$\hat{c}_1(s) = \frac{\mathrm{e}^{\mathrm{i}s}}{2\mathrm{i}\sin(s)\overline{\eta(s)}}, \qquad \hat{c}_2(s) = -\frac{\mathrm{e}^{-\mathrm{i}s}}{2\mathrm{i}\sin(s)\eta(s)}, \qquad \hat{c}_3(s) = \frac{g(s)f(s)}{(\hat{z}_3(s)|\eta(s)|)^2};$$

where

$$g(s) \equiv \hat{z}_3(s)\mathrm{e}^{-\hat{\sigma}(s)}, \quad f(s) \equiv \frac{\mathrm{e}^{-\hat{\sigma}(s)}}{\hat{z}_3(s)}, \quad \eta(s) \equiv 1 - \mathrm{e}^{\mathrm{i}s}f(s).$$

Proof. The expressions for each $\hat{\omega}_j(s)$ follow from the Widom formulas (3.2) together with (3.12). Since $\hat{z}_1(s) = \overline{\hat{z}_2(s)}$ then $\hat{c}_1(s) = \overline{\hat{c}_2(s)}$, hence it is enough to prove the equalities for $\hat{c}_1(s)$ and $\hat{c}_3(s)$. We have

$$\hat{c}_1(s) = \Big(1 - \frac{\hat{z}_2(s)}{\hat{z}_1(s)}\Big)^{-1}\Big(1 - \frac{\hat{z}_2(s)}{\hat{z}_3(s)}\Big)^{-1} = \frac{1}{(1-\mathrm{e}^{-2\mathrm{i}s})\eta(-s)} = \frac{\mathrm{e}^{\mathrm{i}s}}{2\mathrm{i}\sin(s)\overline{\eta(s)}},$$

$$\hat{c}_3(s) = \frac{\hat{z}_1(s)\hat{z}_2(s)}{\hat{z}_3^2(s)\eta(s)\eta(-s)} = \frac{g(s)f(s)}{\hat{z}_3^2(s)\eta(s)\overline{\eta(s)}} = \frac{g(s)f(s)}{\hat{z}_3^2(s)|\eta(s)|^2},$$

and the lemma is proved. □

From the previous lemma, we deduce that $\eta(s) = 1 - \hat{z}_1(s)/\hat{z}_3(s)$ which combined with (2.3) show us that $\eta(s)$ is bounded and bounded away from zero on $[0,\pi]$, making

$$\theta(s) \equiv \arg(\eta(s)), \tag{3.16}$$

a well-defined function. Additionally, from properties (ii) and (iii) in Section 2, it follows that $\hat{z}_j(\varphi(\rho_i)) \in \mathbb{R}$ for $j = 1,2,3$ and $i = 1,2$. Therefore, $\eta(\varphi(\rho_i)) \in \mathbb{R}$ and $\theta(\varphi(\rho_i)) = 0$. Recall that $\varphi(\rho_1) = 0$ and $\varphi(\rho_2) = \pi$.

Lemma 3.7. *The function $f(s)$ given in Lemma 3.6, is infinitely differentiable in $[0, \pi]$. Moreover, for $i = 1, 2$, we have $f'(\varphi(\rho_i)) = 0$.*

Proof. Since $\hat{z}_3(s)$ and $\hat{\sigma}(s)$ are infinitely differentiable in $[0, \pi]$ so is $f(s)$. Now, differentiating the relation (3.14) we can see that $\hat{z}_3'(\varphi(\rho_i)) = 0$, which combined with the representation $\hat{z}_3(s) = -c\mathrm{e}^{2\hat{\sigma}(s)}$ produces $\hat{\sigma}'(\varphi(\rho_i)) = 0$. Finally, the fact that $f'(\varphi(\rho_i)) = 0$ is the result of $f'(s) = -3\hat{\sigma}'(s)f(s)$. $\square$

Proposition 3.8. *The real-valued function $\theta(s)$ defined in (3.16), is infinitely differentiable in $[0, \pi]$. Moreover, for $i = 1, 2$, we have $\theta'(\varphi(\rho_i)) \neq 0$.*

Proof. For a complex number z and under the usual writing $z = x + \mathrm{i}y$, we know that $\arg(z) = \arctan(y/x)$ when $x \neq 0$. Since $f(s)$ is real-valued and

$$|f(s)| = \frac{|\hat{z}_1(s)|}{|\hat{z}_3(s)|} < 1,$$

a simple calculation shows that $0 < 1 - \cos(s)f(s) < 2$ for all $s \in (0, \pi)$. We now want to express $\theta(s)$ as an algebraic function of $f(s)$. It can be done by using the relation $\eta(s) = 1 - \mathrm{e}^{\mathrm{i}s}f(s)$, which yields

$$\theta(s) = \arg(\eta(s)) = \arctan\left(\frac{-\sin(s)f(s)}{1 - \cos(s)f(s)}\right).$$

Hence, Lemma 3.7 tells us that $\theta(s)$ is infinitely differentiable in $[0, \pi]$. Differentiating the previous expression we obtain

$$\theta'(s) = \frac{f^2(s) - f(s)\cos(s) - f'(s)\sin(s)}{1 + f^2(s) - 2\cos(s)f(s)},$$

whose denominator coincides with $|\eta(s)|^2$ which is bounded away from zero. Finally, the fact that $\theta'(\varphi(\rho_i)) \neq 0$ is a consequence of $\varphi(\rho_i) \in \{0, \pi\}$ combined with $f(\varphi(\rho_i)) = |t_i|/\tau_i \neq \pm 1$ for $i = 1, 2$. $\square$

Proposition 3.9. *For any $m \geqslant 1$, the real-valued function $\theta(s)$ defined in (3.16), admits the following asymptotic expansion at the points $\varphi(\rho_i)$ for $i = 1, 2$,*

$$\theta(s) = \sum_{k=1}^{m-1} \varkappa_{k,i}(s - \varphi(\rho_i))^{2k-1} + K_{m,i}(s), \quad s \to \varphi(\rho_i), \tag{3.17}$$

where

- *the coefficients $\varkappa_{k,i}$ can be found explicitly, for instance*

$$\varkappa_{1,i} = \frac{t_i}{t_i - \tau_i},$$

$$\varkappa_{2,i} = (-1)^i \frac{3\mathfrak{a}_{3,i} - 2\mathfrak{a}_{2,j}}{6\mathfrak{a}_{2,j}^2 t_i(\tau_i - t_i)} + \frac{t_i^2}{\tau_i(\tau_i - t_i)}\left(\frac{|\mathfrak{a}_{2,i}|^{\frac{1}{2}}}{\mathfrak{b}_{1,i}} + (-1)^i \frac{\mathfrak{a}_{2,i} t_i^2}{\mathfrak{b}_{1,i}\tau_i} + \frac{\mathfrak{a}_{3,i} t_i}{2\mathfrak{a}_{2,i}} + \frac{t_i}{\tau_i}\right);$$

  where $t_i = z_1(\rho_i)$ and $\tau_i = z_3(\rho_i)$ are the zeros of $a(z) - \rho_i$, and the numbers $\mathfrak{a}_{k,i}$ and $\mathfrak{b}_{k,i}$ are defined in (3.4).
- *$K_{m,i}(s) = O(|s - \varphi(\rho_i)|^{2m-1})$ as $s \to \varphi(\rho_i)$, is differentiable in $(0, \pi)$.*

Proof. In order to find an asymptotic expansion for $\eta(s)$ we use the equality

$$\eta(s) = 1 - \frac{\hat{z}_1(s)}{\hat{z}_3(s)},$$

the relations (3.13), (3.14), and the geometric series, to obtain

$$\eta(s) \equiv 1 - \frac{t_i}{\tau_i} + \sum_{k=1}^{\infty} \mathfrak{e}_{k,i}(s - \varphi(\rho_i))^k,$$

where the coefficients $\mathfrak{e}_{k,i}$ can be calculated explicitly, for instance

$$\mathfrak{e}_{1,i} = -\mathrm{i}\frac{t_i}{\tau_i}, \quad \mathfrak{e}_{2,i} = (-1)^{i+1}\frac{\mathfrak{a}_{2,i}t_i^3}{\mathfrak{b}_{1,i}\tau_i^2} - \frac{\mathfrak{a}_{3,i}t_i^2}{2\mathfrak{a}_{2,i}\tau_i},$$
$$\mathfrak{e}_{3,i} = \mathrm{i}\left(\frac{t_i^2|\mathfrak{a}_{2,i}|^{\frac{1}{2}}}{\mathfrak{b}_{1,i}\tau_i^2} + (-1)^i\frac{3\mathfrak{a}_{3,i} - 2\mathfrak{a}_{2,i}}{6\mathfrak{a}_{2,i}^2\tau_i t_i}\right).$$

To finish the proof, it is enough to use that $\theta(s)$ is the argument of $\eta(s)$ together with an application of the Maclaurin series for arctan. □

We are ready to combine the (rather) technical results of the present section to produce an expansion for the Toeplitz determinant at hand.

Proposition 3.10. *Let the generating function $a(z)$ have the form (2.2), then for $s \in (0, \pi)$ we have*

$$D_n(a - \psi(s)) = \frac{g^n(s)}{\sin(s)|\eta(s)|}\left\{\sin\big((n+1)s + \theta(s)\big) + R_n(s)\right\}, \tag{3.18}$$

where the functions $f(s), g(s), \eta(s)$ are given in Lemma 3.6 and

$$R_n(s) = \frac{\sin(s)}{|\eta(s)|}f^{n+2}(s).$$

Moreover, $R_n(s) = O(\mathrm{e}^{-\Delta n})$ and $R_n'(s) = O(n\mathrm{e}^{-\Delta n})$ for some $\Delta > 0$.

Proof. From Widom determinant formula (3.15) and Lemma 3.6, we have

$$D_n(a - \psi(s)) = \frac{\mathrm{e}^{\mathrm{i}(n+1)s}g^n(s)}{2\mathrm{i}\sin(s)\overline{\eta(s)}} - \frac{\mathrm{e}^{-\mathrm{i}(n+1)s}g^n(s)}{2\mathrm{i}\sin(s)\eta(s)} + \frac{(g(s)f(s))^{n+1}}{(\hat{z}_3(s)|\eta(s)|)^2}.$$

Hence $D_n(a - \psi(s))$ equals

$$\begin{aligned}
&\frac{g^n(s)}{\sin(s)}\left(\frac{1}{2\mathrm{i}|\eta(s)|^2}\left\{\mathrm{e}^{\mathrm{i}(n+1)s}\eta(s) - \mathrm{e}^{-\mathrm{i}(n+1)s}\overline{\eta(s)}\right\} + \frac{g(s)f^{n+1}(s)\sin(s)}{\hat{z}_3^2(s)|\eta(s)|^2}\right)\\
=&\frac{g^n(s)}{\sin(s)|\eta(s)|}\left(\frac{1}{2\mathrm{i}}\left\{\mathrm{e}^{\mathrm{i}(n+1)s}\mathrm{e}^{\mathrm{i}\theta(s)} - \mathrm{e}^{-\mathrm{i}(n+1)s}\mathrm{e}^{-\mathrm{i}\theta(s)}\right\} + \frac{\sin(s)}{|\eta(s)|}f^{n+2}(s)\right)\\
=&\frac{g^n(s)}{\sin(s)|\eta(s)|}\left(\sin\big((n+1)s + \theta(s)\big) + R_n(s)\right),
\end{aligned}$$

where $R_n(s) = \sin(s)f^{n+2}(s)/|\eta(s)|$. From Lemma 3.7 we know that $\eta(s)$ is bounded away from zero and from (2.3) it follows that $|f(s)| \leqslant \mathrm{e}^{-\Delta}$ for some $\Delta > 0$, hence $|R_n(s)| = O(\mathrm{e}^{-\Delta n})$.

Finally, to verify the smoothness of $R_n(s)$, we recall that $f(s)$ is infinitely differentiable in $[0, \pi]$, then so is $|\eta(s)| = (1 + 2f(s)\cos(s) + f(s)^2)^{\frac{1}{2}}$ in $(0, \pi)$. Moreover, from Lemma 3.7 $f'(s)$ is continuous in $[0, \pi]$ and therefore $R_n'(s) = O(n\mathrm{e}^{-\Delta n})$, which finishes the proof. □

Using Proposition 3.10 we can see that the extreme points of the limiting set $\Lambda(a)$, that is ρ_1 and ρ_2, are not eigenvalues of $T_n(a)$ for any sufficiently large n, as follows. From Remark 3.2, Lemma 3.7, and Proposition 3.8 we know that

$$f(\varphi(\rho_i)) \neq 0, \qquad f'(\varphi(\rho_i)) = 0, \qquad \theta(\varphi(\rho_i)) = 0, \qquad \theta'(\varphi(\rho_i)) \neq 0.$$

Then, using $\psi'(\varphi(\rho_i)) = 0$ and the above conditions, we arrive at

$$\begin{aligned} g(\varphi(\rho_i)) &\neq 0, & \eta(\varphi(\rho_i)) &\neq 0, & R_n(\varphi(\rho_i)) &= 0, \\ g'(\varphi(\rho_i)) &= 0, & \eta'(\varphi(\rho_i)) &\neq 0, & R_n'(\varphi(\rho_i)) &\neq 0. \end{aligned}$$

Since the numerator and the denominator of $D_n(a - \psi(s))$ in (3.18) go to 0 as $s \to \varphi(\rho_i)$, an application of the L'Hôpital rule produces

$$\lim_{s \to \varphi(\rho_i)} D_n(a - \psi(s)) = -g^n(\varphi(\rho_i)) \frac{(-1)^{n+1}\{n + 1 + \theta'(\varphi(\rho_i))\} + R_n'(\varphi(\rho_i))}{|\eta(\varphi(\rho_i))|},$$

which shows that, for every sufficiently large n this limit exists and is nonzero.

4. Proof of the main theorems

Since the function $g(s) = \hat{z}_3(s)\mathrm{e}^{-\hat{\sigma}(s)} = \hat{z}_3(s)|\hat{z}_1(s)|$ in Lemma 3.6, does not take the value zero, Proposition 3.10 tells us that $\lambda = \psi(s)$ is an eigenvalue of $T_n(a)$ if and only if

$$\sin\big((n + 1)s + \theta(s)\big) + R_n(s) = 0,$$

or equivalently

$$(n + 1)s + \theta(s) + (-1)^j E_n(s) = \pi j, \tag{4.1}$$

where $j \in \mathbb{Z}$, $s \in (0, \pi)$, and $E_n(s) \equiv \arcsin(R_n(s))$. We are going to show that the term $E_n(s)$ being relatively small, plays the role of a remainder which suggests the usage of the reduced equation

$$(n + 1)s^* + \theta(s^*) = \pi j. \tag{4.2}$$

We now introduce the necessary auxiliary elements to prove our main results. Consider the functions

$$\begin{aligned} H_{j,n}(s) &\equiv d_{j,n} - \frac{\theta(s)}{n + 1}, \\ \tilde{H}_{j,n}(s) &\equiv d_{j,n} - \frac{\theta(s) + (-1)^j E_n(s)}{n + 1}, \end{aligned}$$

where $d_{j,n} = \pi j/(n + 1)$, the function $\theta(s)$ is defined in (3.16), and note that if $s_{j,n}$ and $s^*_{j,n}$ are solutions of the equations (4.1) and (4.2), respectively, we obtain

$$H_{j,n}(s^*_{j,n}) = s^*_{j,n} \quad \text{and} \quad \tilde{H}_{j,n}(s_{j,n}) = s_{j,n}. \tag{4.3}$$

From Proposition 3.8 we know that $\|\theta\|_\infty \equiv \sup_{s\in[0,\pi]} |\theta(s)|$ and $\|\theta'\|_\infty \equiv \sup_{s\in[0,\pi]} |\theta'(s)|$ are both finite. Lastly, for each $n \in \mathbb{N}$ and $j \in \{1,\ldots,n\}$, we consider the set

$$\Omega_{j,n} \equiv \bigl\{s \in (0,\pi)\colon |s - e_{j,n}| \leqslant r_{j,n}\bigr\},$$

where $e_{j,n} \equiv d_{j,n} - \theta(d_{j,n})/(n+1)$ and $r_{j,n} \equiv 3\theta(d_{j,n})\|\theta'\|_\infty/(n+1)^2$.

Lemma 4.1. *Let $a(z)$ be the function given by (2.2). For $n \in \mathbb{N}$ and $j \in \{1,\ldots,n\}$, the functions $H_{j,n}(s)$ and $\tilde{H}_{j,n}(s)$ are contractive maps on $\Omega_{j,n}$ to itself.*

Proof. Take $s \in \Omega_{j,n}$. We start with $\tilde{H}_{j,n}(s)$. From the mean value theorem it follows,

$$\begin{aligned}|\tilde{H}_{j,n}(s) - e_{j,n}| &= \left|\frac{\theta(s) - \theta(d_{j,n})}{n+1} + \frac{(-1)^j E_n(s)}{n+1}\right| \\ &\leqslant \|\theta'\|_\infty \frac{|s - d_{j,n}|}{n+1} + \frac{|E_n(s)|}{n+1}.\end{aligned}$$

Proposition 3.10 together with the Maclaurin series of arcsin tells us that $|E_n(s)| = O(\mathrm{e}^{-\Delta n})$. We now manipulate the last expression in order to include the term $|s - e_{j,n}|$,

$$\begin{aligned}|\tilde{H}_{j,n}(s) - e_{j,n}| &\leqslant \|\theta'\|_\infty \frac{|(n+1)(s - e_{j,n}) + \theta(d_{j,n})|}{(n+1)^2} + O\Bigl(\frac{\mathrm{e}^{-\Delta n}}{n}\Bigr) \\ &\leqslant \|\theta'\|_\infty \Bigl(\frac{|s - e_{j,n}|}{n+1} + \frac{\theta(d_{j,n})}{(n+1)^2}\Bigr) + O\Bigl(\frac{\mathrm{e}^{-\Delta n}}{n}\Bigr) \\ &\leqslant r_{j,n}\Bigl(\frac{1}{3} + \frac{\|\theta'\|_\infty}{n+1} + O(n\mathrm{e}^{-\Delta n})\Bigr),\end{aligned}$$

the last bound being strictly smaller than $r_{j,n}$ tells us that $\tilde{H}_{j,n}(s)$ is an element of $\Omega_{j,n}$, for every sufficiently large n.

Suppose now that $s_1, s_2 \in \Omega_{j,n}$. We have

$$\begin{aligned}|\tilde{H}_{j,n}(s_1) - \tilde{H}_{j,n}(s_2)| &\leqslant \frac{|\theta(s_1) - \theta(s_2)|}{n+1} + \frac{|E_n(s_1) - E_n(s_2)|}{n+1} \\ &\leqslant \|\theta'\|_\infty \frac{|s_1 - s_2|}{n+1} + |E_n'(\varsigma)|\frac{|s_1 - s_2|}{n+1},\end{aligned}$$

for some ς between s_1 and s_2. The bound $E_n'(s) = O(n\mathrm{e}^{-\Delta n})$ uniformly in $s \in (0,\pi)$, is a consequence of Proposition 3.10, therefore

$$|\tilde{H}_{j,n}(s_1) - \tilde{H}_{j,n}(s_2)| \leqslant \Bigl(\frac{\|\theta'\|_\infty}{n+1} + O(\mathrm{e}^{-\Delta n})\Bigr)|s_1 - s_2| = O\Bigl(\frac{1}{n}\Bigr)|s_1 - s_2|,$$

and hence, $\tilde{H}_{j,n}$ is contractive on $\Omega_{j,n}$ for every sufficiently large n.

Finally, a similar calculation for $H_{j,n}(s)$ yields

$$|H_{j,n}(s) - \mathrm{e}_{j,n}| \leqslant r_{j,n}\Bigl(\frac{1}{3} + \frac{\|\theta'\|_\infty}{n+1}\Bigr),$$

which tells us that $H_{j,n}(s) \in \Omega_{j,n}$ for every sufficiently large n. Moreover

$$|H_{j,n}(s_1) - H_{j,n}(s_2)| \leqslant \frac{\|\theta'\|_\infty}{n+1}\,|s_1 - s_2|,$$

showing that $H_{j,n}(s)$ is contractive on $\Omega_{j,n}$ and finishing the proof. □

With the previous theorem and the Banach fixed point theorem, we deduce that for each $j \in \{1, \ldots, n\}$ and every sufficiently large n, there are points $s_{j,n}$ and $s^*_{j,n}$ in $\Omega_{j,n}$, satisfying (4.3), and being the solutions of (4.1) and (4.2), respectively.

Proof of Theorem 2.1. A simple calculation shows that

$$|e_{j+1,n} - e_{j,n}| \geqslant \frac{\pi - |\theta(d_{j,n}) - \theta(d_{j+1,n})|}{n+1} \geqslant \frac{\pi}{n+1}\left(1 - \frac{\|\theta'\|_\infty}{n+1}\right),$$

which means that $|e_{j+1,n} - e_{j,n}| \geqslant O(n^{-1})$ while $r_{j,n} = O(n^{-2})$, and therefore for every sufficiently large n the domains $\Omega_{j,n}$ pairwise disjoint. Thus for every $j \in \{1, \ldots, n\}$, $H_{j,n}(s) = s$ has a unique solution $s_{j,n} \in \Omega_{j,n}$ satisfying (4.1) which proves the second statement.

By Proposition 3.10 we know that $\lambda_{j,n} = \psi(s_{j,n})$ is an eigenvalue of $T_n(a)$ lying on $\psi(\Omega_{j,n})$. Moreover, the points $\lambda_{j,n}$ with $j \in \{1, \ldots, n\}$ are pairwise distinct, which proves the first statement.

We are left with the proof of the third statement. From Lemma 4.1, for each $j \in \{1, \ldots, n\}$, we know that the point $s^*_{j,n}$ is the unique solution of (4.2) belonging to $\Omega_{j,n}$. Consider the function

$$F_n(s) \equiv s(n+1) - \theta(s),$$

and note that

$$F_n(s_{j,n}) - F_n(s^*_{j,n}) = (n+1)(\tilde{H}_{j,n}(s_{j,n}) - H_{j,n}(s^*_{j,n})) = (-1)^j E_n(s_{j,n}),$$

where $E_n(s)$ is given by (4.1), then by the mean value theorem it follows that there is an $\tilde{s}$ between $s^*_{j,n}$ and $s_{j,n}$, such that

$$F_n(s_{j,n}) - F_n(s^*_{j,n}) = F'_n(\tilde{s})(s_{j,n} - s^*_{j,n}),$$

and therefore

$$|s^*_{j,n} - s_{j,n}| = \frac{|E_n(s_{j,n})|}{|F'_n(\tilde{s})|}.$$

The bound $|E_n(s)| = O(\mathrm{e}^{-\Delta n})$ uniformly in $s \in (0, \pi)$, together with

$$|F'_n(s)| = |n + 1 - \theta'(s)| \geqslant n + 1 - \|\theta'\|_\infty > \frac{n+1}{2},$$

produces the estimation

$$|s^*_{j,n} - s_{j,n}| = O\left(\frac{\mathrm{e}^{-\Delta n}}{n}\right).$$

To finish the proof we merge $\|\psi'\|_\infty < \infty$ (see Lemma 3.7) with

$$|\lambda_{j,n} - \psi(s^*_{j,n})| = |\psi(s_{j,n}) - \psi(s^*_{j,n})| \leqslant \|\psi'\|_\infty |s^*_{j,n} - s_{j,n}|,$$

and write

$$\lambda_{j,n} = \psi(s^*_{j,n}) + E(s^*_{j,n}),$$

where $E(s^*_{j,n}) = O(n^{-1}\mathrm{e}^{-\Delta n})$ uniformly in j. $\square$

Remark 4.2. Since $H_{j,n}(s)$ is contractive on $\Omega_{j,n}$, it admits a unique fixed-point, namely $s^*_{j,n}$. Furthermore, the recursive sequence

$$s^{(1)}_{j,n} \equiv e_{j,n}, \quad s^{(k)}_{j,n} \equiv H_{j,n}\big(s^{(k-1)}_{j,n}\big) \quad (k \geqslant 2),$$

satisfies $s^{(k)}_{j,n} \to s^*_{j,n}$ as $k \to 0$, together with the bound

$$|s^{(k)}_{j,n} - s^*_{j,n}| \leqslant \frac{6\|\theta'\|^k_\infty \theta(d_{j,n})}{(n+1)^{k+1}}.$$

By (3.17) it follows that $\theta(d_{j,n}) = O(d_{j,n}(\pi - d_{j,n}))$ as $n \to \infty$ uniformly in j. Thus, we can write

$$s^*_{j,n} = s^{(k)}_{j,n} + O\left(\frac{d_{j,n}(\pi - d_{j,n})}{n^{k+1}}\right),$$

as $n \to \infty$ uniformly in j.

Proof of Theorem 2.2. Suppose that $m = 2$, consider the second term in the recursive sequence $(s^{(k)}_{j,n})_k$, and write

$$\begin{aligned} s^{(2)}_{j,n} = H_{j,n}(s^{(1)}_{j,n}) = d_{j,n} - \frac{\theta(s^{(1)}_{j,n})}{n+1} \\ &= d_{j,n} - \frac{\theta\left(d_{j,n} - \frac{\theta(d_{j,n})}{n+1}\right)}{n+1} \\ &= d_{j,n} - \frac{\theta(d_{j,n})}{n+1} + \frac{\theta'(d_{j,n})\theta(d_{j,n})}{(n+1)^2} + O\left(\frac{\theta''(d_{j,n})\theta^2(d_{j,n})}{n^3}\right). \end{aligned}$$

To improve the previous bound, from Proposition 3.8 we know that $\|\theta''\| < \infty$ and from (3.17) it follows that $\theta(d_{j,n}) = O(d_{j,n}(\pi - d_{j,n}))$ uniformly in j. Thus

$$s^{(2)}_{j,n} = d_{j,n} - \frac{\theta(d_{j,n})}{n+1} + \frac{\theta'(d_{j,n})\theta(d_{j,n})}{(n+1)^2} + O\left(\frac{d^2_{j,n}(\pi - d_{j,n})^2}{n^3}\right),$$

which combined with $s^*_{j,n} = s^{(2)}_{j,n} + O(d_{j,n}(\pi - d_{j,n})n^{-3})$ (see Remark 4.2), produces

$$s^*_{j,n} = d_{j,n} - \frac{\theta(d_{j,n})}{n+1} + \frac{\theta'(d_{j,n})\theta(d_{j,n})}{(n+1)^2} + O\left(\frac{d_{j,n}(\pi - d_{j,n})}{n^3}\right), \tag{4.4}$$

finishing the proof of the first statement.

Let us now work with the second statement. By (2.10) we know that

$$\lambda_{j,n} = \psi(s^*_{j,n}) + O(n^{-1}\mathrm{e}^{-\Delta n}),$$

and (4.4) tells us that the main term in the expansion of $s^*_{j,n}$ is $d_{j,n}$, hence in order to obtain an expression for $\lambda_{j,n}$, we need to expand $\psi(s)$ around $d_{j,n}$. For that purpose, we merge

$$\psi(s^*_{j,n}) = \psi(d_{j,n}) + \psi'(d_{j,n})(s^*_{j,n} - d_{j,n}) + \frac{\psi''(d_{j,n})}{2}(s^*_{j,n} - d_{j,n})^2 + O(|s^*_{j,n} - d_{j,n}|^3),$$

with (4.4) to reach

$$\psi(s^*_{j,n}) = \psi(d_{j,n}) + \frac{\mathfrak{r}_1(d_{j,n})}{n+1} + \frac{\mathfrak{r}_2(d_{j,n})}{(n+1)^2} + E_{j,n},$$

where $E_{j,n}$ plays the role of a remainder term and satisfies

$$E_{j,n} = O\left(\frac{\psi'(d_{j,n})d_{j,n}(\pi - d_{j,n})}{n^3}\right) + O\left(\frac{\psi''(d_{j,n})\theta'(d_{j,n})\theta(d_{j,n})}{n^3}\right) + O\left(\frac{\psi'''(d_{j,n})\theta(d_{j,n})}{n^3}\right),$$

while the coefficients $\mathfrak{r}_k$ are given by,

$$\mathfrak{r}_1(d_{j,n}) \equiv -\psi'(d_{j,n})\theta(d_{j,n}), \quad \mathfrak{r}_2(d_{j,n}) \equiv \frac{1}{2}\psi''(d_{j,n})\theta(d_{j,n})^2 + \psi'(d_{j,n})\theta(d_{j,n})\theta'(d_{j,n}).$$

Finally, the bound

$$E_{j,n} = O\left(\frac{d^2_{j,n}(\pi - d_{j,n})^2}{n^3}\right),$$

is a consequence of (3.5), (3.17), and the fact that $\psi(s)$ is infinitely differentiable in the interval $[0, \pi]$. The cases $m > 2$ can be readily shown. □

Theorem 2.2 shows in particular that, as n increases, there are eigenvalues arbitrarily close to the points ρ_1 and ρ_2. This situation happens, for instance, when either $j/n \to 0$ or $j/n \to 1$. The respective eigenvalues are called *extreme*. With the aid of Propositions 3.4 and 3.9, together with Theorem 2.2, we now give specialized asymptotic expansions for the extreme eigenvalues.

Proof of Theorem 2.3. We prove (2.11) first. For simplicity, we write ν_k instead of $\nu_{k,1}$. From Propositions 3.4 and 3.9, we know that as $s \to 0$, we have

$$\psi'(s) = 2\nu_1 s + 4\nu_2 s^3 + O(s^5), \quad \psi''(s) = 2\nu_1 + 12\nu_2 s^2 + O(s^4), \quad \theta'(s) = \varkappa_1 + O(s^2).$$

Then, as $s \to 0$,

$$\mathfrak{r}_1(s) = -2\varkappa_1\nu_1 s^2 + O(s^4) \quad \text{and} \quad \mathfrak{r}_2(s) = 3\nu_1\varkappa_1^2 s^2 + O(s^4).$$

Take $s = d_{j,n}$ and use the second statement in Theorem 2.2, to obtain

$$\begin{aligned}\lambda_{j,n} = \rho_1 + \nu_1 d^2_{j,n} + \nu_2 d^4_{j,n} - 2\varkappa_1\nu_1\frac{d^2_{j,n}}{n+1} + 3\nu_1\varkappa_1^2\frac{d^2_{j,n}}{(n+1)^2} \\ + O(d^6_{j,n}) + O\left(\frac{d^4_{j,n}}{n^2}\right) + O\left(\frac{d^4_{j,n}}{n}\right) + O\left(\frac{d^2_{j,n}(\pi - d_{j,n})^2}{n^3}\right),\end{aligned}$$

which combined with the fact $O(d^2_{j,n}(\pi - d_{j,n})^2 n^{-3}) = O(j^2 n^{-5})$ together with the assumption $j^2/n \to 0$ gives us the first statement of the theorem. The second statement can be readily proved. □

Table 1
The condition number κ_n for the eigenvector matrix of $T_n(a)$, the generating function $a(t) = t^2 + 6t + 6t^{-1}$, and different values of n.

n	128	256	512	1024	2048	4096
κ_n	3.40×10^{15}	6.39×10^{19}	3.17×10^{20}	3.43×10^{21}	5.16×10^{22}	7.08×10^{22}

5. Numerical experiments

In this section we test the asymptotic expansions in Theorems 2.2 and 2.3 for the Toeplitz matrices $T_n(a)$ with generating function

$$a(t) = t^2 + 6t + 6t^{-1}.$$

We split our experiments into inner and extreme eigenvalues.

To make an appropriate estimation of the errors, we need “exact” eigenvalues $\lambda_{j,n}$ for the largest attainable n. But, as mentioned in Section 1, the numerical computation of eigenvalues can be extremely difficult, which was our case. The condition number of the respective eigenvector matrix can explain those difficulties. Table 1 shows that the eigenvector matrix of $T_n(a)$ is severely ill-conditioned. Then, to guarantee accurate exact eigenvalues, we employed the software `Wolfram Mathematica v.13` and perform eigenvalue computations using no less than 300 and some times, 1000 precision digits.

We highlight here that our asymptotic expansions can be used to implement a matrix-less algorithm in the same fashion of [13,15,16].

5.1. General eigenvalues

We introduce the term-by-term approximation of $\lambda_{j,n}$, given by our expansion in Theorem 2.2, by

$$\begin{aligned}
\lambda_{j,n}^{\mathrm{SL}(1)} &\equiv \psi(d_{j,n}), \\
\lambda_{j,n}^{\mathrm{SL}(2)} &\equiv \psi(d_{j,n}) + \frac{\mathfrak{r}_1(d_{j,n})}{n+1}, \\
\lambda_{j,n}^{\mathrm{SL}(3)} &\equiv \psi(d_{j,n}) + \frac{\mathfrak{r}_1(d_{j,n})}{n+1} + \frac{\mathfrak{r}_2(d_{j,n})}{(n+1)^2},
\end{aligned} \tag{5.1}$$

where

$$\mathfrak{r}_1(s) \equiv -\psi'(s)\theta(s) \quad \text{and} \quad \mathfrak{r}_2(s) \equiv \frac{1}{2}\psi''(s)\theta^2(s) + \psi'(s)\theta(s)\theta'(s).$$

To implement the approximations in (5.1), we need the values of $\psi(s)$, $\theta(s)$, and its first derivatives. Those values can be obtained numerically but the computation is slow, hence we opted to record a sample over a regular mesh of 6000 nodes, and to perform a local interpolation.

Trying to understand how good the approximation given by $\lambda_{j,n}^{\mathrm{SL}(1)}$ is, we can proceed as follows. From the second statement in Theorem 2.1, we know that $\lambda_{j,n} = \psi(s_{j,n})$ satisfies

$$|\lambda_{j,n} - \lambda_{j+1,n}| \leqslant \|\psi'\|_\infty |s_{j,n} - s_{j+1,n}| \leqslant \frac{\|\psi'\|_\infty M}{n+1}, \quad j \in \{1, \ldots, n-1\},$$

where $M = 6\|\theta\|_\infty \|\theta'\|_\infty + \pi(1 + \|\theta'\|_\infty)$, hence the distance between two consecutive eigenvalues has order $O(n^{-1})$. On the other hand, by Theorem 2.2 we easily deduce $|\lambda_{j,n} - \lambda_{j,n}^{\mathrm{SL}(1)}| = O(n^{-1})$, which means that the one term eigenvalue approximation $\lambda_{j,n}^{\mathrm{SL}(1)}$, produces an error comparable with the distance between

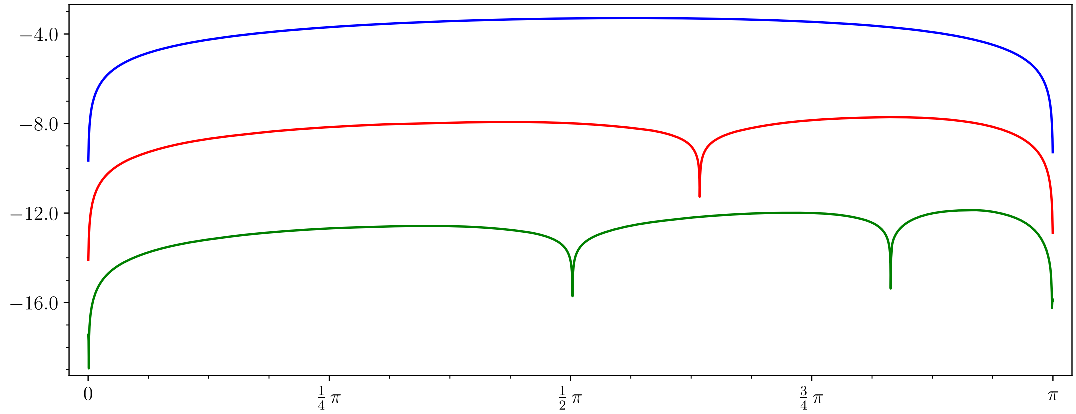

Fig. 5. The 10-base logarithm of the individual absolute error $\mathrm{AE}_{j,n}^{\mathrm{SL}(k)}$ for $n = 4096$ and different values of k: $k = 1$ (blue), $k = 2$ (red), and $k = 3$ (green). For the eigenvalue $\lambda_{j,n} = \psi(s_{j,n})$ we took as independent variable $s_{j,n}$ and plotted the errors over the grid $j\pi/(n+1)$ for $j \in \{1, \ldots, n\}$.

Table 2
The maximum and normalized errors $\mathrm{AE}_n^{\mathrm{SL}(k)}$ and $\mathrm{NE}_n^{\mathrm{SL}(k)}$, respectively, given by (5.2) with $k = 1, 2, 3$, for different values of n.

n	$\mathrm{AE}_n^{\mathrm{SL}(1)}$	$\mathrm{NE}_n^{\mathrm{SL}(1)}$	$\mathrm{AE}_n^{\mathrm{SL}(2)}$	$\mathrm{NE}_n^{\mathrm{SL}(2)}$	$\mathrm{AE}_n^{\mathrm{SL}(3)}$	$\mathrm{NE}_n^{\mathrm{SL}(3)}$
16	1.232×10^{-1}	2.094	1.115×10^{-3}	0.322	1.549×10^{-5}	0.076
32	6.379×10^{-2}	2.105	2.944×10^{-4}	0.320	2.633×10^{-6}	0.094
64	3.244×10^{-2}	2.108	7.672×10^{-5}	0.324	3.430×10^{-7}	0.094
128	1.635×10^{-2}	2.110	1.947×10^{-5}	0.324	4.407×10^{-8}	0.094
256	8.213×10^{-3}	2.110	4.908×10^{-6}	0.324	5.571×10^{-9}	0.094
512	4.114×10^{-3}	2.110	1.231×10^{-6}	0.324	7.010×10^{-10}	0.094
1024	2.059×10^{-3}	2.111	3.085×10^{-7}	0.324	8.787×10^{-11}	0.094
2048	1.030×10^{-3}	2.111	7.721×10^{-8}	0.324	1.100×10^{-11}	0.094
4096	5.152×10^{-4}	2.111	1.931×10^{-8}	0.324	2.891×10^{-12}	0.094

consecutive eigenvalues, and as a consequence, it is good enough only for distribution purposes. In that case, we use to say that *the approximation* $\lambda_{j,n}^{\mathrm{SL}(1)}$ *does not separate the eigenvalues.*

For the individual and maximum absolute eigenvalue errors, we introduce the notation,

$$\mathrm{AE}_{j,n}^{\mathrm{SL}(k)} \equiv |\lambda_{j,n} - \lambda_{j,n}^{\mathrm{SL}(k)}|, \qquad \mathrm{AE}_n^{\mathrm{SL}(k)} \equiv \max_{1 \leqslant j \leqslant n} \mathrm{AE}_{j,n}^{\mathrm{SL}(k)}. \tag{5.2}$$

Fig. 5 and Table 2 show the data. According to the second statement in Theorem 2.2, we must have $\mathrm{AE}_n^{\mathrm{SL}(k)} = O(n^{-k})$, then the respective normalized error,

$$\mathrm{NE}_n^{\mathrm{SL}(k)} \equiv (n+1)^k \, \mathrm{AE}_n^{\mathrm{SL}(k)},$$

should have a bounded behavior, as a matter of fact, in Table 2 we can see that in our case, it has an almost constant behavior.

5.2. Extreme eigenvalues

The extreme eigenvalues have attracted the attention of the mathematicians since the middle part of the last century, they constitute an important parameter in the design of numerical algorithms and can be used to estimate the operator norm of a matrix.

In our case, we know that $\rho_1 > \lambda_{1,n} > \cdots > \lambda_{n,n} > \rho_2$ with $\rho_1\rho_2 < 0$. Thus

$$\max_{1 \leqslant j \leqslant n} |\lambda_{j,n}| = \max\{|\lambda_{1,n}|, |\lambda_{n,n}|\}.$$

Table 3
The relative and normalized extreme errors $\mathrm{RE}_{1,n}^{\mathrm{EXT}(k)}$ and $\mathrm{NE}_{1,n}^{\mathrm{EXT}(k)}$, respectively, for the eigenvalue $\lambda_{1,n}$ of $T_n(a)$, $k = 1, 2, 3$, and different values of n.

n	$\mathrm{RE}_{1,n}^{\mathrm{EXT}(1)}$	$\mathrm{NE}_{1,n}^{\mathrm{EXT}(1)}$	$\mathrm{RE}_{1,n}^{\mathrm{EXT}(2)}$	$\mathrm{NE}_{1,n}^{\mathrm{EXT}(2)}$	$\mathrm{RE}_{1,n}^{\mathrm{EXT}(3)}$	$\mathrm{NE}_{1,n}^{\mathrm{EXT}(3)}$
16	1.617×10^{-2}	0.274	4.000×10^{-3}	1.156	9.925×10^{-5}	0.487
32	7.280×10^{-3}	0.240	1.065×10^{-3}	1.160	1.301×10^{-5}	0.457
64	3.418×10^{-3}	0.222	2.752×10^{-4}	1.162	1.665×10^{-6}	0.457
128	1.650×10^{-3}	0.212	6.996×10^{-5}	1.164	2.107×10^{-7}	0.452
256	8.105×10^{-4}	0.208	1.763×10^{-5}	1.165	2.649×10^{-8}	0.447
512	4.014×10^{-4}	0.205	4.428×10^{-6}	1.154	3.321×10^{-9}	0.448
1024	1.997×10^{-4}	0.204	1.109×10^{-6}	1.165	4.158×10^{-10}	0.447
2048	9.965×10^{-5}	0.204	2.776×10^{-7}	1.165	5.201×10^{-11}	0.447
4096	4.976×10^{-5}	0.205	6.945×10^{-8}	1.165	6.504×10^{-12}	0.447

According to the first and second statements in Theorem 2.3, there are two types of extreme eigenvalues: the ones approaching either ρ_1 or ρ_2. We start by analyzing the eigenvalues $\lambda_{j,n}$ that are arbitrarily close to ρ_1. Take $1 \leqslant j_0 < \lceil \sqrt{n}\,\rceil$, then for $j \in \{1, \ldots, j_0\}$ we define

$$\begin{aligned}
\lambda_{j,n}^{\mathrm{EXT}(1)} &\equiv \rho_1 + \frac{\mathfrak{u}_{1,1} j^2}{(n+1)^2}, \\
\lambda_{j,n}^{\mathrm{EXT}(2)} &\equiv \rho_1 + \frac{\mathfrak{u}_{1,1} j^2}{(n+1)^2} + \frac{\mathfrak{u}_{2,1} j^2}{(n+1)^3}, \\
\lambda_{j,n}^{\mathrm{EXT}(3)} &\equiv \rho_1 + \frac{\mathfrak{u}_{1,1} j^2}{(n+1)^2} + \frac{\mathfrak{u}_{2,1} j^2}{(n+1)^3} + \frac{\mathfrak{u}_{3,1} j^4 + \mathfrak{u}_{4,1} j^2}{(n+1)^4};
\end{aligned} \tag{5.3}$$

where

$$\mathfrak{u}_{1,1} \equiv -\frac{a^{(2)}(t_1)}{2}(t_1\pi)^2, \qquad \mathfrak{u}_{2,1} \equiv -\frac{2\mathfrak{u}_{1,1} t_1}{t_1 - \tau_1}, \qquad \mathfrak{u}_{3,1} \equiv \frac{3\mathfrak{u}_{1,1} t_1^2}{(\tau_1 - t_1)^2},$$

$$\mathfrak{u}_{4,1} \equiv \left(\frac{a^{(4)}(t_1) t_1^4}{24} - \frac{a^{(3)}(t_1) t_1^3}{6} - \frac{5a^{(3)}(t_1) t_1^4}{72 a^{(2)}(t_1)} - \frac{a^{(2)}(t_1) t_1^2}{3}\right)\pi^4,$$

and τ_1, t_1 are the zeros of $a(z) - \rho_1$.

Now, we define the individual relative and normalized relative errors by,

$$\mathrm{RE}_{j,n}^{\mathrm{EXT}(k)} \equiv \frac{|\lambda_{j,n} - \lambda_{j,n}^{\mathrm{EXT}(k)}|}{|\lambda_{j,n} - \rho_1|}, \quad \mathrm{NE}_{j,n}^{\mathrm{SL}(k)} \equiv (n+1)^k \, \mathrm{RE}_{j,n}^{\mathrm{EXT}(k)}.$$

The reason behind these definitions is that when the eigenvalues $\lambda_{j,n}$ are arbitrarily close to ρ_1, that is, when $|\lambda_{j,n} - \rho_1|$ is arbitrarily small, the relative error $\mathrm{RE}_{j,n}^{\mathrm{EXT}(k)}$ shows how precise the approximation really is, on the other hand, when $|\lambda_{j,n} - \rho_1|$ is *big*, the relative error $\mathrm{RE}_{j,n}^{\mathrm{EXT}(k)}$ is close to the value $|\lambda_{j,n} - \lambda_{j,n}^{\mathrm{EXT}(k)}|$, that is, the absolute error. Moreover, a value of $\mathrm{RE}_{j,n}^{\mathrm{EXT}(k)}$ close to 1, says that the measured object and its approximation are comparable. Table 3 and Fig. 6 show the data for the very first eigenvalue $\lambda_{1,n}$.

Now, we study the eigenvalues $\lambda_{j,n}$ which are arbitrarily close to ρ_2. Let j_0 be such that $1 \leqslant n - j_0 < \lceil \sqrt{n}\,\rceil$, then for $j \in \{j_0, \ldots, n\}$ we introduce the approximations

$$\begin{aligned}
\lambda_{j,n}^{\mathrm{EXT}(1)} &\equiv \rho_2 + \frac{\mathfrak{u}_{1,2}(n+1-j)^2}{(n+1)^2}, \\
\lambda_{j,n}^{\mathrm{EXT}(2)} &\equiv \rho_2 + \frac{\mathfrak{u}_{1,2}(n+1-j)^2}{(n+1)^2} + \frac{\mathfrak{u}_{2,2}(n+1-j)^2}{(n+1)^3},
\end{aligned}$$

Table 4
The relative and normalized extreme errors $\mathrm{RE}_{n,n}^{\mathrm{EXT}(k)}$ and $\mathrm{NE}_{n,n}^{\mathrm{EXT}(k)}$, respectively, for the eigenvalue $\lambda_{n,n}$ of $T_n(a)$, $k = 1, 2, 3$, and different values of n.

n	$\mathrm{RE}_{n,n}^{\mathrm{EXT}(1)}$	$\mathrm{NE}_{n,n}^{\mathrm{EXT}(1)}$	$\mathrm{RE}_{n,n}^{\mathrm{EXT}(2)}$	$\mathrm{NE}_{n,n}^{\mathrm{EXT}(2)}$	$\mathrm{RE}_{n,n}^{\mathrm{EXT}(3)}$	$\mathrm{NE}_{n,n}^{\mathrm{EXT}(3)}$
16	1.000×10^{-1}	1.700	2.720×10^{-2}	7.862	3.416×10^{-3}	16.784
32	4.793×10^{-2}	1.581	8.232×10^{-3}	8.964	3.652×10^{-4}	13.127
64	2.292×10^{-2}	1.489	2.234×10^{-3}	9.442	3.938×10^{-5}	10.817
128	1.112×10^{-2}	1.435	5.799×10^{-4}	9.650	4.458×10^{-6}	9.571
256	5.472×10^{-3}	1.406	1.475×10^{-4}	9.745	5.261×10^{-7}	8.931
512	2.712×10^{-3}	1.391	3.720×10^{-5}	9.790	6.376×10^{-8}	8.608
1024	1.350×10^{-3}	1.383	9.339×10^{-6}	9.812	7.842×10^{-9}	8.445
2048	6.734×10^{-4}	1.379	2.339×10^{-6}	9.823	9.723×10^{-10}	8.364
4096	3.363×10^{-4}	1.378	5.855×10^{-7}	9.828	1.210×10^{-10}	8.323

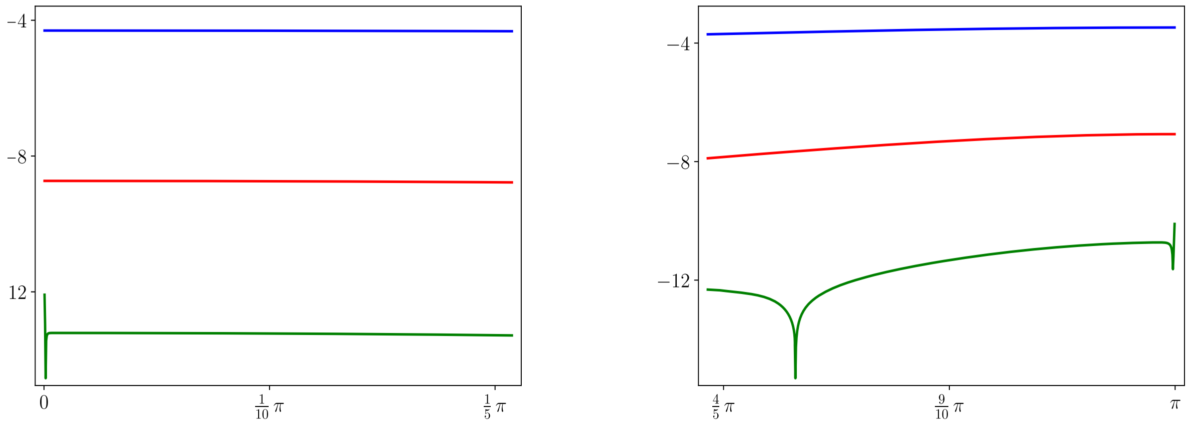

Fig. 6. The 10-base logarithm of the individual relative error $\mathrm{RE}_{j,n}^{\mathrm{EXT}(k)}$ for $n = 4096$, using the approximations (5.3) and (5.4) for different values of k: $k = 1$ (blue), $k = 2$ (red), and $k = 3$ (green). The left and right panels show the errors corresponding to the extreme eigenvalues $\lambda_{j,n} = \psi(s_{j,n})$ such that $s_{j,n}$ approaches 0 and π, respectively.

$$\lambda_{j,n}^{\mathrm{EXT}(3)} \equiv \rho_2 + \frac{\mathfrak{u}_{1,2}(n+1-j)^2}{(n+1)^2} + \frac{\mathfrak{u}_{2,2}(n+1-j)^2}{(n+1)^3} + \frac{\mathfrak{u}_{3,2}(n+1-j)^2 + \mathfrak{u}_4(n+1-j)^4}{(n+1)^4}; \tag{5.4}$$

where

$$\mathfrak{u}_{1,2} \equiv -\frac{a^{(2)}(t_2)}{2}(t_2\pi)^2, \qquad \mathfrak{u}_{2,2} \equiv -\frac{2\mathfrak{u}_{1,2}t_2}{t_2 - \tau_2}, \qquad \mathfrak{u}_{3,2} \equiv \frac{3\mathfrak{u}_{1,2}t_i^2}{(\tau_2 - t_2)^2},$$

$$\mathfrak{u}_4 \equiv \left(\frac{a^{(4)}(t_2)t_2^4}{24} - \frac{a^{(3)}(t_2)t_2^3}{6} - \frac{5a^{(3)}(t_2)t_2^4}{72a^{(2)}(t_2)} - \frac{a^{(2)}(t_2)t_2^2}{3}\right)\pi^4,$$

and τ_2, t_2 are the zeros of $a(z) - \rho_2$. In this case, the individual relative error is given by

$$\mathrm{RE}_{j,n}^{\mathrm{EXT}(k)} \equiv \frac{|\lambda_{j,n} - \lambda_{j,n}^{\mathrm{EXT}(k)}|}{|\lambda_{j,n} - \rho_2|}.$$

Table 4 and Fig. 6 show the data for the very last eigenvalue $\lambda_{n,n}$.

Remark 5.1. Theorem 2.3 contains asymptotic expansions for the extreme eigenvalues, derived from Theorem 2.2. Therefore, the respective relative errors are asymptotically equivalent. For instance when the eigenvalues are arbitrarily close to ρ_1, we obtain

$$\frac{|\lambda_{j,n}-\lambda_{j,n}^{\mathrm{SL}(k)}|}{|\lambda_{j,n}-\rho_1|}-\frac{|\lambda_{j,n}-\lambda_{j,n}^{\mathrm{EXT}(k)}|}{|\lambda_{j,n}-\rho_1|}=O\Big(\frac{1}{n^{k+1}}\Big),\quad j=1,\ldots,j_0,\quad n\to\infty,$$

while a similar relation holds for the eigenvalues arbitrarily close to ρ_2. This situation can be appreciated by making a comparison between Figs. 5 and 6, along with Tables 3 and 4.

Declaration of competing interest

The authors declare no potential conflict of interests.

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