J. Spectr. Theory 15 (2025), 441–477
DOI 10.4171/JST/538

Eigenvalues for a class of non-Hermitian tetradiagonal Toeplitz matrices

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Abstract. We study a family of non-Hermitian tetradiagonal Toeplitz matrices having a limiting set consisting of one analytic arc only. We derive individual asymptotic expansions for all eigenvalues as the matrix size grows to infinity. Additionally, we provide specific expansions for the extreme eigenvalues, which are those approaching the endpoints of the limiting set. Although this family does not belong to the simple-loop class, we managed to extend the existing theory to this case. Our results reveal the intricate details of the eigenvalue structure and allow a high accuracy direct calculation.

1. Introduction

For an absolutely integrable function a over the complex unit circle $\mathbb{T} = \partial\mathbb{D}$, we denote by $T_n(a)$ the $n \times n$ Toeplitz matrix $(a_{j-k})_{j,k=0}^{n-1}$, where a_k represents the kth Fourier coefficient of a, that is

$$a_k = \frac{1}{2\pi} \int_{-\pi}^{\pi} a(\mathrm{e}^{\mathrm{i}\sigma})\mathrm{e}^{-\mathrm{i}k\sigma}\,\mathrm{d}\sigma.$$

The matrix $T_n(a)$ is characterized by having constant entries along the main diagonals, and the function a is customarily called *symbol* or *generating function*.

The study of Toeplitz matrices started in the first decade of the 20th century with the classic works of O. Toeplitz and G. Szegő (see [15, 16] for the seminal papers or the book [11] for reviewing the classic works, see also [14]). Since then, these matrices have enjoyed popularity because of its many applications, including numerical analysis, engineering, stochastic processes, time series analysis, signal processing, quantum and statistical mechanics, and image processing. Nowadays, a very popular application is the numerical approximation for the solution to differential and integral

Mathematics Subject Classification 2020: 47B35 (primary); 15A18, 15B05, 65F15, 82B20 (secondary).
Keywords: Toeplitz matrix, asymptotic expansion, eigenvalues, simple loop method.

equations with local techniques of finite differences, finite elements, finite volumes, isogeometric analysis, and discontinuous Garlekin methods. The gathered research material is immense and we refer the interested readers to the books [5,7,8]. A recent approach named *generalized locally Toeplitz sequences* (GLT) can be found in [9,10].

The spectral characteristics of Toeplitz matrices, such as eigenvalues, eigenvectors, spectral distribution, clustering, and localization, have been a popular research topic for many decades now (see the beautiful paper [17] for a compendium and ultimate results about spectral distribution, localization, and clustering).

If tasked with computing the eigenvalues of $T_n(a)$, the most straightforward approach is the use of a commercial eigensolver (such as `Eigenvalues` in the software `Mathematica`, `eig` in `MATLAB`, or `eigvals` in `JULIA`). However, these methods can often yield fundamentally inaccurate results. To see that consider for example the generating function $a(z) = z^2 + (2 + 3\mathrm{i})z + (2 + 3\mathrm{i})z^{-1}$, which produces a tetradiagonal Toeplitz matrix, that is, a Toeplitz matrix with only four non-zero diagonals. Let $\lambda_{1,n}, \ldots, \lambda_{n,n}$ be the eigenvalues of $T_n(a)$ ordered by increasing real part, and let $\lambda_{j,n,d}$ be the numerical approximation of $\lambda_{j,n}$ computed with d precision digits, where $d = 16, 32, 64, 128, 500$. Additionally, consider the error

$$\mathbf{e}_{n,d} \equiv \max\{|\lambda_{j,n,d} - \lambda_{j,n,500}| : 1 \leqslant j \leqslant n\}, \quad d = 16, 32, 64, 128.$$

Given n and d, $\mathbf{e}_{n,d}$ indicates the maximum number of correct figures that the approximation $\lambda_{n,j,d}$ will have. From Table 1 we see that for a fixed d, as n increases, the number of correct figures decreases, meaning that an eigensolver may display d figures, but only some of them are correct. On the other hand, for a fixed n, as d increases, the number of correct figures increases. Therefore, increasing d ensures more correct figures. As time complexity and memory consumption highly increase with d, in practice, we want to know the minimum d producing certain quantity of correct figures. For instance, computing with 16 precision digits, the approximation of $\lambda_{j,n}$ will not have even one correct figure for matrices with n larger than 32. While working with 128 precision digits will make sense only for matrices with $n \leqslant 256$. In conclusion, as the matrix dimension grows, the required number of precision digits to maintain accuracy in computations becomes very hard to achieve. Figure 1 shows that working even with 128 precision digits produces a rough approximation of the spectrum.

Another factor to consider here is that all commercial eigensolvers lack parallelization capabilities and exhibit time complexities nearing the order $O(n^3)$ with n representing the size of the matrix. For structured matrices, such as the Toeplitz matrices, there exist specialized algorithms with 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

n	32	64	128	256	512	1024
$\mathbf{e}_{n,16}$	4.59×10^{-7}	3.94	6.89	10.44	15.60	22.73
$\mathbf{e}_{n,32}$	2.66×10^{-32}	1.48×10^{-9}	3.27	7.22	10.62	15.65
$\mathbf{e}_{n,64}$	3.46×10^{-64}	3.85×10^{-64}	6.80×10^{-15}	4.59	7.33	10.61
$\mathbf{e}_{n,128}$	2.90×10^{-128}	2.80×10^{-128}	2.64×10^{-128}	3.51×10^{-24}	4.71	7.40

Table 1. The errors $\mathbf{e}_{n,d}$ for different values of n and d.

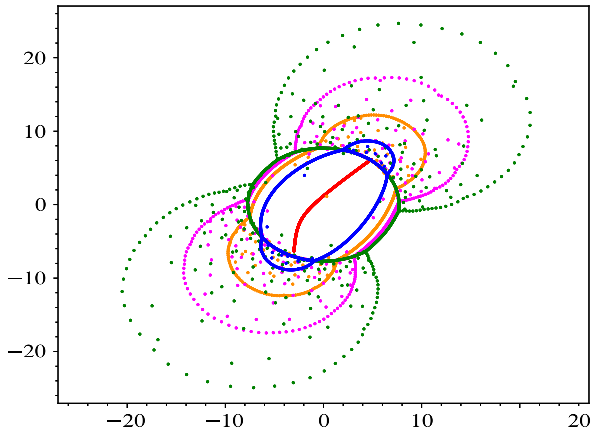


Figure 1. The set $\operatorname{sp} T_n(a)$ for $a(z) = z^2 + cz + cz^{-1}$ with $c = 2 + 3\mathrm{i}$ and $n = 1024$, computed with d precision digits for different values of d. The green, magenta, orange, blue, and red points correspond to $d = 16, 32, 64, 128$, and 500, respectively.

of the Lanczos algorithm is $O(rn^2)$ where r is the average number of non-zeros in a row. Beyond the time complexity, the available eigensolvers have a memory consumption which increases as n^2, and therefore, it is important to have a more efficient alternative.

Based on numerical experiments (see Figure 2), the asymptotic expansion developed for eigenvalues exhibits linear time complexity, representing a significant improvement over traditional eigenvalue solver methods. As previously said, standard eigensolvers are commonly accepted to have a time complexity of $O(n^3)$, where n denotes the size of the matrix, but Figure 2 shows that their practical time complexity can approach $O(n^4)$. This discrepancy highlights the inefficiency of standard methods for large matrices. Given the size of a matrix, the execution time of an eigensolver can vary significantly based on the desired precision and the condition number of the respective eigenvector matrix. For matrices of considerable size and "well" conditioning, computation with 16 precision digits can be relatively fast, as eigensolvers are typically optimized for such scenarios, delivering acceptable results within a reason-

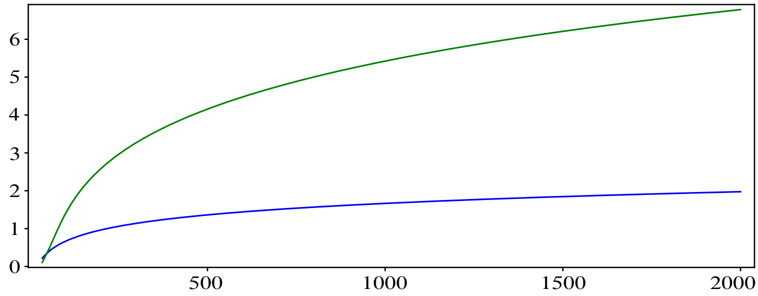


Figure 2. The 10-base logarithm of the execution time calculating the eigenvalues of $T_n(a)$ with $a(z) = z^2 + (2+3\mathrm{i})z + (2+3\mathrm{i})z^{-1}$, for the eigensolver `eigenvalues` in `SageMath`, working with 500 precision digits (green) and the asymptotic expansion in Theorem 2.4 with 16 precision digits (blue), considering matrix sizes ranging from 16 to 2000.

able timeframe. However, when higher precision is necessary or the matrix is poorly conditioned, the execution time can escalate notably. In contrast, for large matrices, asymptotic expansions can offer rapid eigenvalue estimates, reducing significantly the computational effort while maintaining accuracy. Thus, the proposed asymptotic expansion not only drastically reduces computation time but also provides an accurate solution for high-dimensional problems.

In 2010, a new research brand was initiated by A. Böttcher, E. Maximenko, and one of the authors with the paper [6], where they considered a class of real-valued symbols and developed a technique named now *simple-loop method* (SLM) to find individual asymptotic expressions for the eigenvalues of the respective Toeplitz matrices. Such an expansion can produce a very good approximation for each eigenvalue of $T_n(a)$ instantly and the whole spectrum in linear time.

More specifically, for a constant $\alpha \geqslant 0$, consider the well-known weighted Wiener algebra W^α, which is the collection of all functions $a\colon \mathbb{T} \to \mathbb{C}$ admitting the representation $a(z) = \sum_{k=-\infty}^{\infty} a_k z^k$ $(z \in \mathbb{T})$ and satisfying

$$\|a\|_\alpha \equiv \sum_{k=-\infty}^{\infty} |a_k|(|k|+1)^\alpha < \infty.$$

Let $g\colon \mathbb{R} \to \mathbb{R}$ be the 2π-periodic function given by $g(\sigma) \equiv a(\mathrm{e}^{\mathrm{i}\sigma})$. The simple-loop class SL^α is the set of all real-valued $a \in W^\alpha$ satisfying the following conditions.

(i) The range of g is a segment $[0, \mu]$ with $\mu > 0$.

(ii) $g(0) = g(2\pi) = 0$, $g'(0) = g'(2\pi) = 0$, and $g''(0) = g''(2\pi) > 0$.

(iii) There is a $\sigma_0 \in (0, 2\pi)$ such that $g(\sigma_0) = \mu$, $g'(\sigma) > 0$ for $0 < \sigma < \sigma_0$, $g'(\sigma) < 0$ for $\sigma_0 < \sigma < 2\pi$, $g'(\sigma_0) = 0$, and $g''(\sigma_0) < 0$.

The simple-loop method yields, among other results, that if $\lambda_{1,n} \leqslant \cdots \leqslant \lambda_{n,n}$ are the eigenvalues of $T_n(a)$, then there exists an integer $m \geqslant 2$ (depending on the symbol smoothness) such that

$$\lambda_{j,n} = \sum_{k=0}^{m-1} \frac{\mathbf{c}_k(\sigma_{j,n})}{(n+1)^k} + E_m(\sigma_{j,n}),$$

where

- $\sigma_{j,n} = \pi j/(n+1)$;
- the coefficients $\mathbf{c}_k : [0,\pi] \to \mathbb{R}$ are functions depending only on a that, in principle, can be found explicitly;
- the reminder, or *error term,* $E_m(\sigma_{j,n})$ equals $O(n^{-m})$ as $n \to \infty$ uniformly in $j = 1,\ldots,n$.

The SLM has inspired a number of theoretical and numerical works, starting with real-valued symbols including the cases of symmetric, non-symmetric with $\alpha \geqslant 4$ and then $\alpha \geqslant 2$, tetradiagonal, and more recently, non real-valued symbols with real limiting set. See the reviews [1, 3] and the references therein.

For a Laurent polynomial a,

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

the resulting matrix $T_n(a)$ is a sparse matrix having a finite number of non-zero diagonals, as we can see below:

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

Matrices of this kind are known as *banded* because of the non-zero band $a_\ell, \ldots, a_{-r}$.

In such a case, Schmidt and Spitzer [13] showed that, as n goes to infinity, the spectrum of $T_n(a)$, $\operatorname{sp} T_n(a)$, converges in the Hausdorff metric to a certain set called *limiting set* and denoted by $\Lambda(a)$, which turns out to be the union of finitely many analytic arcs together with their endpoints, not containing isolated points. Ullman [18] later proved that $\Lambda(a)$ is connected.

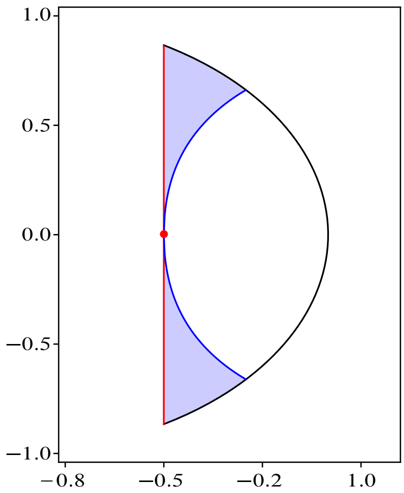


Figure 3. The curve γ (blue).

For $\lambda \in \mathbb{C}$ and a as in (1.1), consider the equation $a(z) = \lambda$. We denote by $z_k(\lambda)$ $(k = 1, \dots, r + \ell)$ the respective solutions and arrange 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 [13] is that the point λ belongs to $\Lambda(a)$ if and only if $|z_r(\lambda)| = |z_{r+1}(\lambda)|$. See [5, Section 11] for a complete treatment of this topic.

Let γ be the piece of the curve $\{b \in \mathbb{C} \colon |1 + b| = 2|b|^2\}$ that lies in the closed disk $\{b \in \mathbb{C} \colon |1 + b| \leqslant 1\}$ (see Figure 3) and let Γ be the curve

$$\Gamma \equiv \left\{\pm 2 \frac{(1 + b + b^2)^{3/2}}{b(1 + b)} \colon b \in \gamma\right\}.$$

The $\pm$ indicates that we take both values of $(1 + b + b^2)^{3/2}$. The curve Γ is the boundary of the blue domain Ω shown in Figure 4.

The authors of [4] considered the generating function (1.1) with $r = 1$, $\ell = 2$, and proved that $\Lambda(a)$ coincides with a dilatation and a translation of the limiting set of either the generating functions $z^2 + z^{-1}$ or $z^2 + cz + cz^{-1}$, where c is a non-zero complex constant. The authors were able to understand the relationship between the number of analytic arcs in $\Lambda(a)$ and the parameter c, obtaining the following. If $c \notin \Omega$ or $c = \pm 3\sqrt{3}$, then $\Lambda(a)$ consists of one analytic arc and two endpoints (Type 1); if $c \in \partial\Omega \setminus \{\pm 3\sqrt{3}\}$, then $\Lambda(a)$ consists of two analytic arcs and three endpoints, one of which joins the arcs (Type 2); and if $c \in \operatorname{int}\Omega$, then $\Lambda(a)$ consists of three analytic arcs and four endpoints one of them joining the arcs, and three endpoints (Type 3).

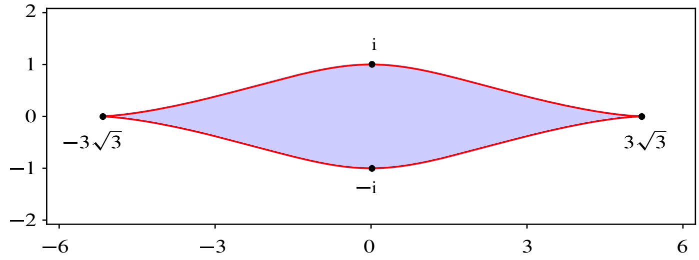


Figure 4. The set Ω.

When $c \in (-\infty, -3\sqrt{3}] \cup [3\sqrt{3}, \infty)$, the limiting set is a real line segment, which they called "degenerate case." See Figure 5.

In the paper [2], we made a more detailed study of the degenerate case. We computed the individual asymptotic expansions for all the eigenvalues, as the matrix size goes to infinity, and provided specific expansions for the extreme eigenvalues, which are those approaching the extreme points of the limiting set.

In the present article we bound ourselves to the case where $\Lambda(a)$ consists of one non-real analytic arc and use the Widom determinant formula [19] together with the SLM to obtain an asymptotic expansion for each eigenvalue of $T_n(a)$. We emphasize that it is the very first time that individual asymptotic expansions are obtained for complex-valued eigenvalues.

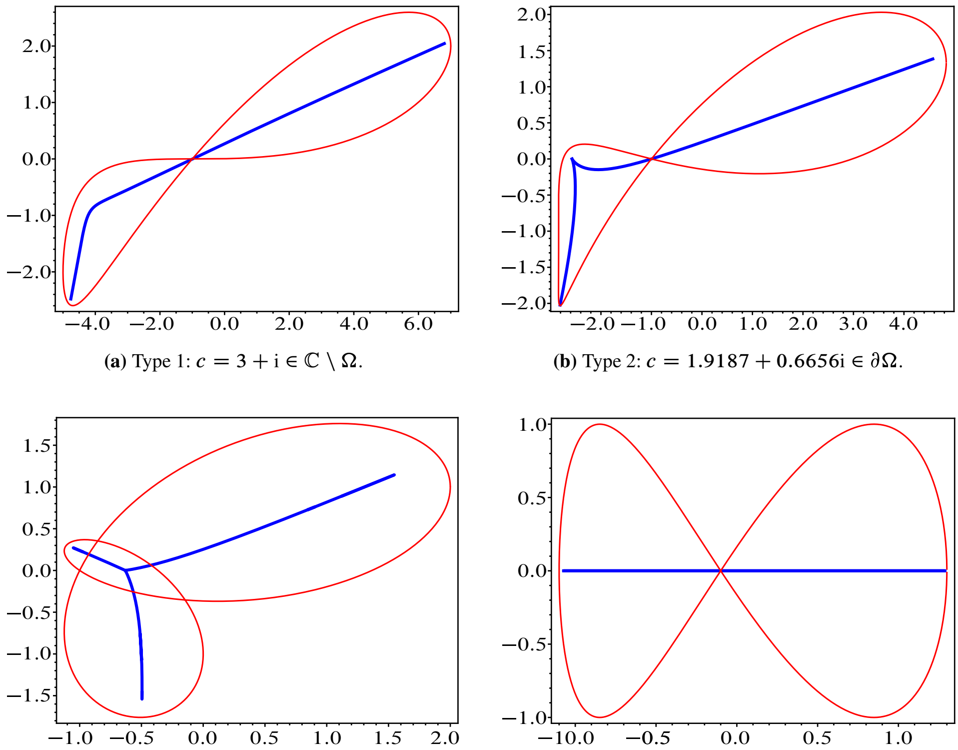
The paper is organized as follows. In Section 2 we introduce the study objects and present our main results. In Section 3 we present key findings for the limiting set as discussed in [4], with a specific focus on Type 1. Subsequently, we define a key function establishing a bijection between the limiting set and the real interval $[0, 2\pi]$, and 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 SLM to prove our main results, and finally, in Section 5 we present numerical examples illustrating the effectiveness of our results.

2. Main results

In [13] Schmidt and Spitzer discovered the following trick. 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 $a_\xi(z) \equiv a(\xi z)$, where a is a Laurent polynomial. Then we have the similarity relation

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

and as a consequence $T_n(a_\xi)$ and $T_n(a)$ both share the same eigenvalues.



(a) Type 1: $c = 3 + \mathrm{i} \in \mathbb{C} \setminus \Omega$.

(b) Type 2: $c = 1.9187 + 0.6656\mathrm{i} \in \partial\Omega$.

(c) Type 3: $c = 1/2 + \mathrm{i}/2 \in \operatorname{Int} \Omega$.

(d) Degenerate case: $c = 6 \in \mathbb{C} \setminus \Omega$.

Figure 5. The four types of limiting sets.

Consider the generating function

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

Thus, $T_n(a)$ is an arbitrary tetradiagonal Toeplitz matrix. According to [4], if $a_1 = 0$ we can choose ξ such that $\xi^2 a_2 = \xi^{-1} a_{-1}$, to obtain

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

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

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

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

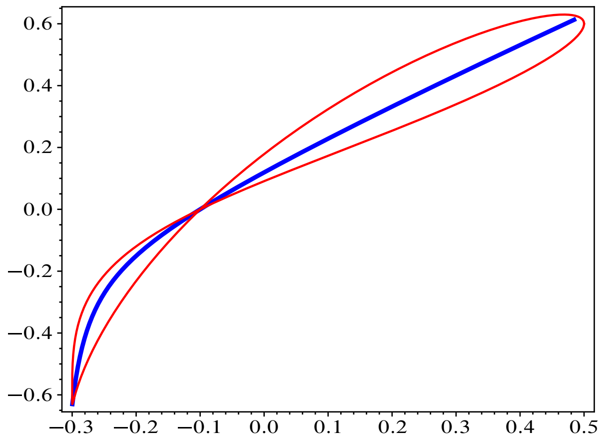


Figure 6. The range of the generating function a (red) and the limiting set $\Lambda(a)$ (blue), for $a(z) = z^2 + cz + cz^{-1}$ with $c = 2 + 3\mathrm{i} \in \mathbb{C} \setminus \Omega$.

From this point on, we bound ourselves to the generating function (see Figure 6),

$$a(z) \equiv z^2 + cz + cz^{-1}, \quad c \in \mathbb{C} \setminus \Omega. \tag{2.1}$$

By [13], we know that for every sufficiently large n, the spectrum of $T_n(a)$ is arbitrarily close to $\Lambda(a)$. In our case, [2] tells us that,, since $c \in \mathbb{C} \setminus \Omega$, the limiting set consists of one analytic arc and two endpoints. We denote the endpoints by ρ_1, ρ_2, and the analytic arc by $[\rho_1 \sim \rho_2]$.

Additionally, we will make use of the algorithm exposed in [4] for computing the limiting set. In order to present it here, we state first some key findings of [4] adapted to our case. If $\lambda \in \Lambda(a)$, then

- the equation $a(z) = \lambda$ has three solutions $z_1(\lambda)$, $z_2(\lambda)$, and $z_3(\lambda)$, satisfying

$$|z_1(\lambda)| = |z_2(\lambda)| < |z_3(\lambda)|,$$

  and hence, there exists a real number $s_0 \in [0, 2\pi]$ such that $z_2(\lambda) = \mathrm{e}^{\mathrm{i}s_0} z_1(\lambda)$;
- Vieta's theorem applied to the equation $a(z) = \lambda$ gives $z_3(\lambda) = -c\mathrm{e}^{-\mathrm{i}s_0} z_1(\lambda)^{-2}$, implying that $|z_2(\lambda)| < |z_3(\lambda)|$ is equivalent to $|z_1(\lambda)| < |c|^{1/3}$;
- $z_1(\lambda)$ solves the equation $a(z) - a(\mathrm{e}^{\mathrm{i}s_0} z) = 0$;
- if t_1, t_2, and t_3 are the zeros of $a'(z)$, labeled in such a way that $|t_1| \leqslant |t_2| \leqslant |t_3|$, then $\rho_k = a(t_k)$ $(k = 1, 2)$ are the endpoints of $\Lambda(a)$;
- for every $s \in [0, 2\pi]$, the equation $a(u) - a(\mathrm{e}^{\mathrm{i}s} u) = 0$ has three solutions $u_k(s)$ $(k = 1, 2, 3)$, and $\lambda_k(s) \equiv a(u_k(s))$ belongs to $\Lambda(a)$ if and only if $|u_k(s)| \leqslant |c|^{1/3}$.

Algorithm 2.1. The limiting set $\Lambda(a)$, with a given by (2.1), can be calculated as follows. For a fixed positive integer n and the step-size $h = 2\pi/(n+1)$, consider the regular grid $\sigma_{1,n}, \dots, \sigma_{n,n}$ with $\sigma_{j,n} \equiv jh$.

(1) For each $j = 1, \dots, n$, employ a numerical polynomial solver (such as `Root` in `Mathematica`, or `roots` in `SageMath`) to calculate the solutions of the equation $a(z) - a(\mathrm{e}^{\mathrm{i}\sigma_{j,n}} z) = 0$ for z, and name them as

$$u_{1,j,n}, \quad u_{2,j,n}, \quad u_{3,j,n}.$$

(2) Store only those $u_{k,j,n}$ satisfying $|u_{k,j,n}| < |c|^{1/3}$.

(3) Return the respective points $\lambda_{k,j,n} \equiv a(u_{k,j,n})$, which must belong to $\Lambda(a)$.

The endpoints of $\Lambda(a)$, ρ_1, and ρ_2, can be easily found numerically. Hence, together with Algorithm 2.1, we obtain $n+2$ points in $\Lambda(a)$. We highlight that the beauty of this algorithm, beyond its efficiency, is that it does not require to compute any eigenvalues at all.

Remark 2.2. Numerical experiments show that for a sufficiently large $n \in \mathbb{N}$, the points $z = u_{k,j,n}$ in the previous step (2) form a smooth path. Additionally, the solutions of $a(z) - a(u_{k,j,n}) = 0$ are

$$z = u_{k,j,n}, \quad z = \mathrm{e}^{\mathrm{i}\sigma_{j,n}} u_{k,j,n}, \quad z = -\frac{c\mathrm{e}^{-\mathrm{i}\sigma_{j,n}}}{u_{k,j,n}^2},$$

and they all satisfy $|z| < |c|^{1/3}$.

Remark 2.2 suggests the existence of a continuous function $u\colon [0, 2\pi] \to \mathbb{C}$ satisfying $a(u([0, 2\pi])) = \Lambda(a)$. In the next section, we will prove this and derive some properties of u. Sadly, we were not able to find an analytic expression for u, but in our numerical experiments, we could approximate it using interpolation of the data $(\sigma_{j,n}, u_{k,j,n})$ $(j = 1, \dots, n)$ $(k = 1, 2, 3)$. The importance of u rests mainly in the fact that

$$\psi(s) \equiv a(u(s)) \tag{2.2}$$

maps the interval $[0, 2\pi]$ to the limiting set $\Lambda(a)$. Such a function is called *spectral symbol* and is the leading coefficient of our asymptotic expansion.

Our main goal is to provide individual asymptotic expansions for the eigenvalues of $T_n(a)$. To achieve this, we need to introduce the following auxiliary functions:

$$h_1(s) \equiv 1 + \frac{1}{c}\mathrm{e}^{2\mathrm{i}s} u(s)^3, \quad h_2(s) \equiv 1 + \frac{1}{c}\mathrm{e}^{\mathrm{i}s} u(s)^3, \quad \theta(s) \equiv -\mathrm{i}\log\Big(\frac{h_1(s)}{h_2(s)}\Big).$$

From Remark 2.2, we know that $|u(s)| < |c|^{1/3}$, whence $|h_k(s)| > 0$ $(k = 1, 2)$, and, as a consequence, θ is well defined.

As in Algorithm 2.1, for $n \in \mathbb{N}$ and $j \in \{1, \dots, n\}$, we consider the grid points

$$\sigma_{j,n} \equiv \frac{2\pi j}{n+1}, \quad d_{j,n} \equiv \sigma_{j,n} - \frac{\theta(\sigma_{j,n})}{n+1},$$

and the neighborhoods

$$\Omega_\delta \equiv \{z \in \mathbb{C}\colon \mathfrak{Re}(z) \in (0, 2\pi),\ |\mathfrak{Im}(z)| < \delta\}, \tag{2.3}$$

for some sufficiently small number $\delta > 0$, and

$$\Theta_{j,n} \equiv \{s \in \Omega_\delta\colon |s - d_{j,n}| \leqslant r_{j,n}\}, \tag{2.4}$$

where $r_{j,n} \equiv 3\sup\{|\theta'(s)||\theta(\sigma_{j,n})|(n+1)^{-2}\colon s \in \Omega_\delta\}$. The sequence $(\sigma_{j,n})_{j=1}^n$ is a regular mesh for the interval $[0, 2\pi]$, and the constants $r_{j,n}$ were selected in such a way that the sets $(\Theta_{j,n})_{j=1}^n$ become pairwise disjoint.

Recall that $\Lambda(a)$, with a given by (2.1), consists of one analytic arc without self-intersections. We will prove that ψ can be continued to an analytic and one-to-one function on Ω_δ, concluding that ψ restricted to $(0, 2\pi)$ is an smooth parametrization of $\Lambda(a)$.

The following are our main results.

Theorem 2.3. *Let a be the generating function in (2.1) and take an small $\delta > 0$. Then, for every sufficiently large $n \in \mathbb{N}$ and each $j \in \{1, \dots, n\}$, the following statements hold.*

(1) *The eigenvalues of $T_n(a)$, $\lambda_{1,n}, \dots, \lambda_{n,n}$, are pairwise distinct and there is a number $s_{j,n} \in \Theta_{j,n}$ such that $\lambda_{j,n} = \psi(s_{j,n})$, where ψ is given by (2.2).*

(2) *The number $s = s_{j,n}$ satisfies the equation*

$$(n+1)s + \theta(s) = 2\pi j + E_1(s),$$

where $E_1(s)$ is an analytic function in a complex neighborhood of $(0, 2\pi)$, with $E_1(s) = O(\mathrm{e}^{-n\Delta})$, and whose derivative satisfies $E_1'(s) = O(n\mathrm{e}^{-n\Delta})$. Both order relations work as $n \to \infty$ for certain $\Delta > 0$, uniformly in $s \in \Omega_\delta$.

(3) *The equation*

$$(n+1)s + \theta(s) = 2\pi j,$$

has a unique solution $s_{j,n}^* \in \Theta_{j,n}$, and we can write

$$\lambda_{j,n} = \psi(s_{j,n}^*) + E_2(s_{j,n}^*),$$

where $E_2(s_{j,n}^*) = O(\mathrm{e}^{-n\Delta}/n)$, as $n \to \infty$ for certain $\Delta > 0$, uniformly in j.

Theorem 2.4. *Under the same hypothesis of Theorem 2.3, as $n \to \infty$, we have the following expansions:*

$$s_{j,n} = \mathbf{q}_0(\sigma_{j,n}) + \frac{\mathbf{q}_1(\sigma_{j,n})}{n+1} + \frac{\mathbf{q}_2(\sigma_{j,n})}{(n+1)^2} + H(\sigma_{j,n}),$$
$$\lambda_{j,n} = \mathbf{r}_0(\sigma_{j,n}) + \frac{\mathbf{r}_1(\sigma_{j,n})}{n+1} + \frac{\mathbf{r}_2(\sigma_{j,n})}{(n+1)^2} + \widehat{H}(\sigma_{j,n}),$$

where

$$\mathbf{q}_0(s) = s, \qquad \mathbf{q}_1(s) = -\theta(s), \qquad \mathbf{q}_2(s) = \theta(s)\theta'(s),$$
$$\mathbf{r}_0(s) = \psi(s), \quad \mathbf{r}_1(s) = -\psi'(s)\theta(s), \quad \mathbf{r}_2(s) = \frac{1}{2}\psi''(s)\theta(s)^2 + \psi'(s)\theta(s)\theta'(s),$$

$H(\sigma_{j,n}) = O(\sigma_{j,n}(\sigma_{j,n} - 2\pi)/n^3)$, and $\widehat{H}(\sigma_{j,n}) = O(\sigma_{j,n}^2(\sigma_{j,n} - 2\pi)^2/n^3)$ are the remainder (error) terms. The order relations work as $n \to \infty$ uniformly in j.

A consequence of Theorem 2.4 is that

$$\begin{aligned} &\text{if} \quad j/n \to 0 \quad \text{then} \quad \lambda_{j,n} \to \psi(0) = \rho_1, \\ &\text{if} \quad j/n \to 1 \quad \text{then} \quad \lambda_{j,n} \to \psi(2\pi) = \rho_2. \end{aligned}$$

Therefore, in our case, the eigenvalues $\lambda_{j,n}$ can be classified as follows: the eigenvalues satisfying $j/n \to 0$ or $(n-j)/n \to 0$, which we call *extreme*, and the remaining ones, which we call *inner*. The extreme eigenvalues have an important role in practice for estimating the norm of large matrices or its inverse, and the accuracy of certain algorithms.

If a is given by (2.1), then ρ_1 and ρ_2 belong to the limiting set $\Lambda(a)$, and we know that, as $n \to \infty$, there are eigenvalues of $T_n(a)$ arbitrarily close to them, see Figure 6. For $k = 1, 2$, Vieta's theorem tells us that $a(z) - \rho_k$ has exactly two solutions, t_k and $-c\mathrm{e}^{-\mathrm{i}s} t_k^{-2}$. Hence, we can write

$$a(z) = \rho_k + \sum_{\ell=1}^{\infty} \mathbf{a}_{\ell,k}(z - t_k)^\ell, \tag{2.5}$$

where $\mathbf{a}_{\ell,k} = a^{(\ell)}(t_k)/\ell!$ and the variable z belongs to some neighborhood of t_k. Moreover, we know that $a'(t_k) = 0$ and $a^{(\ell)}(t_k) \neq 0$, for $k = 1, 2$ and $\ell \geqslant 2$. As a consequence, $\mathbf{a}_{1,k} = 0$ and $\mathbf{a}_{\ell,k} \neq 0$ for $k = 1, 2$ and $\ell \geqslant 2$. Here is our result for the extreme eigenvalues.

Theorem 2.5. *Under the same hypothesis of Theorem 2.3, the following statements hold:*

(1) *if* (j_n) *is a sequence satisfying* $j_n^2/n \to 0$ *and* $j \in \{1, \dots, j_n\}$*, then*

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

(2) *if* (j_n) *is a sequence satisfying* $(n-j_n)^2/n \to 0$ *and* $j \in \{j_n, \dots, n\}$*, then*

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

the coefficients are given by

$$\mathbf{u}_{1,k} \equiv -\mathbf{a}_{2,k}(t_k\pi)^2, \quad \mathbf{u}_{2,k} \equiv 2\mathbf{a}_{2,k}\frac{t_k^5\pi^2}{c+t_k^3}, \quad \mathbf{u}_{3,k} \equiv -3\mathbf{a}_{2,k}\frac{t_k^8\pi^2}{(c+t_k^3)^2},$$

$$\mathbf{u}_{4,k} \equiv \Big(\mathbf{a}_{4,k}t_k^4 - \mathbf{a}_{3,k}t_k^3 - \frac{5\mathbf{a}_{3,k}^2}{4\mathbf{a}_{2,k}}t_k^4 - \frac{2\mathbf{a}_{2,k}}{3}\Big)t_k^2\pi^4,$$

and the order relations are uniform in j.

Remark 2.6. The results in Theorem 2.5 can be specified as follows:

- if (j_n) is a sequence satisfying $j_n/n \to 0$ and $j \in \{1, \dots, j_n\}$, then

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

- if (j_n) is a sequence satisfying $(n-j_n)/n \to 0$ and $j \in \{j_n, \dots, n\}$, then

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

- if (j_n) is a sequence satisfying $j_n^4/n^3 \to 0$ and $j \in \{1, \dots, j_n\}$, then

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

- if (j_n) is a sequence satisfying $(n-j_n)^4/n^3 \to 0$ and $j \in \{j_n, \dots, n\}$, then

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

3. Preliminaries

3.1. Limiting set

Assume that the generating function a has the form

$$a(z) = z^2 + cz + cz^{-1}, \tag{3.1}$$

for a non-zero complex constant c. Then we know that the respective limiting set admits the representation

$$\Lambda(a) = \{\lambda \in \mathbb{C}\colon |z_1(\lambda)| = |z_2(\lambda)| \leqslant |z_3(\lambda)|\},$$

where $z_k(\lambda)$ $(k = 1, 2, 3)$ are zeros of $a(z) - \lambda$. The points $\lambda \in \Lambda(a)$ have the following analytical classification.

- We call λ a *simple point* if $|z_2(\lambda)| < |z_3(\lambda)|$ and $z_1(\lambda) \neq z_2(\lambda)$.
- A *branch point* is a $\lambda \in \Lambda(a)$ such that two or all three of $z_1(\lambda), z_2(\lambda), z_3(\lambda)$, coincide. In such a case, they may be labeled so that $|z_2(\lambda)| \leqslant |z_3(\lambda)|$ and $z_1(\lambda) = z_2(\lambda)$.
- The remaining points in $\Lambda(a)$ are called *multiple points* and produce pairwise distinct $z_1(\lambda), z_2(\lambda), z_3(\lambda)$, with $|z_2(\lambda)| = |z_3(\lambda)|$.

Clearly, the union of simple, branch, and multiple points is the whole set $\Lambda(a)$. In our case, the respective topological classification is as follows. The simple points have a neighborhood where the limiting set is an analytic arc starting and ending at the boundary, a branch point is where an analytic arc starts without intersecting any other arc, and a multiple point is where two or more arcs coincide.

The following Theorems 3.1, 3.2, 3.3, and 3.4 can be found in [4], and, since they are important for the present work, we present them here without a proof.

Theorem 3.1. *Let a be the generating function in* (3.1). *Then $\Lambda(a)$ has a multiple point if only if $c \in \operatorname{int}\Omega$.*

Theorem 3.2. *Let a be the generating function* (3.1). *If $\lambda \in \Lambda(a)$ is simple then there is a unique number $s \in (0, 2\pi)$ such that $z_1(\lambda)/z_2(\lambda) = \mathrm{e}^{\mathrm{i}s}$ and*

$$a'(z_1(\lambda)) - \mathrm{e}^{\mathrm{i}s} a'(\mathrm{e}^{\mathrm{i}s} z_1(\lambda)) \neq 0.$$

Moreover, there is a neighborhood of λ which intersected with $\Lambda(a)$ is an analytic arc (without self-intersection) starting and finishing on its boundary.

Theorem 3.3. *Let a be the generating function in* (3.1) *with $c \notin \overline{\operatorname{int}\Omega}$. Then ρ_1 and ρ_2 are branch points of $\Lambda(a)$.*

Theorem 3.4. *Under the same hypothesis of Theorem 3.3, there are two analytic arcs ℓ_1 and ℓ_2 belonging to $\Lambda(a)$, coming from the points ρ_1 and ρ_2, respectively, and near them we have the representation*

$$\ell_j = s\Big\{\lambda \in \mathbb{C}\colon \lambda = \rho_j - \frac{a''(t_j)}{8} t_j^2 s^2 + O(s^3),\ s \in (0, \varepsilon)\Big\},$$

for some $\varepsilon > 0$ and $j = 1, 2$.

Theorem 3.5. *Under the same hypothesis of Theorem 3.3, the set $\Lambda(a)$ consists of one analytic arc $[\rho_1 \sim \rho_2]$, without self-intersection.*

Proof. By Theorems 3.3 and 3.4, $\Lambda(a)$ has ρ_1 and ρ_2 as branch points with one outgoing arc coming from each of them. Due to Theorem 3.1, there is no multiple point. Therefore, $\Lambda(a)$ consists exactly of simple points and two branch points. Since $\Lambda(a)$ is the union of a finite number of pairwise disjoint (open) connected analytic arcs and there are no multiple points, we must have $\Lambda(a) = [\rho_1 \sim \rho_2]$. ∎

3.2. Spectral symbol

We now justify the existence and properties of the function ψ given by (2.2), which is our spectral symbol for the eigenvalues of $T_n(a)$. Let us start with the function u introduced in (2.2).

For $\lambda \in \Lambda(a)$, let

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

be the zeros of $a(z) - \lambda$. Then we must have $|z_1(\lambda)| = |z_2(\lambda)|$. From the open mapping theorem and the analyticity of a, each $z_j(\lambda)$ ($j = 1, 2, 3$) turns out to be a continuous function.

Consider the auxiliary function $\varphi\colon \Lambda(a) \to \mathbb{R}$ given by

$$\varphi(\lambda) \equiv -\mathrm{i} \log\Big(\frac{z_2(\lambda)}{z_1(\lambda)}\Big).$$

The fact that $\varphi(\lambda) \in \mathbb{R}$ is a consequence of $|z_1(\lambda)| = |z_2(\lambda)|$. Since $\varphi(\lambda)$ is continuous and $\Lambda(a)$ is compact and connected, so is $\varphi(\Lambda(a))$. Additionally, $z_1(\lambda)$ and $z_2(\lambda)$ can be labeled so that $\varphi(\rho_1) = 0$ and $\varphi(\rho_2) = 2\pi$, and hence we have $\varphi(\Lambda(a)) = [0, 2\pi]$, which implies that for every $s \in [0, 2\pi]$ there exists $\lambda \in \Lambda(a)$ (an inverse image of s under $\varphi(\lambda)$) such that $z_2(\lambda)/z_1(\lambda) = \mathrm{e}^{\mathrm{i}s}$ and $\lambda = a(z_1(\lambda)) = a(z_2(\lambda))$.

Thus, $z_1(\lambda)$ solves $a(z) - a(\mathrm{e}^{\mathrm{i}s} z) = 0$, $a(z) - \lambda = 0$, and $|z_1(\lambda)| < |c|^{1/3}$ simultaneously, and, according to Algorithm 2.1, a point $\lambda \in \mathbb{C}$ belongs to $\Lambda(a)$ if and only if $z_1(\lambda)$ satisfies these three relations. For example, for $\lambda = -1$, the solutions of $a(z) - \lambda = 0$ are

$$z_1(\lambda) = \mathrm{i}, \quad z_2(\lambda) = -\mathrm{i}, \quad z_3(\lambda) = -c,$$

with $s = \pi$. Thus, $z = z_1(-1) = \mathrm{i}$ solves $a(z) - a(-z) = 0$, $a(z) = -1$, and $|z_1(\lambda)| = 1 < |c|^{1/3}$, and therefore $\lambda = -1$ belongs to $\Lambda(a)$.

Let $D \equiv z_1(\Lambda(a)) \subset \mathbb{C}$. Since $z_1(\lambda)$ is a continuous function and $\Lambda(a)$ is a compact and connected set, so is D, and obviously we have $a(D) = \Lambda(a)$.

Proposition 3.6. *There exists a function u, analytic in a complex neighborhood of $[0, 2\pi]$, such that $a(u([0, 2\pi])) = \Lambda(a)$.*

Proof. As previously discussed, we know that for each $s \in [0, 2\pi]$ there is a solution $z = u(s)$ of

$$a(z) - a(\mathrm{e}^{\mathrm{i}s} z) = 0, \tag{3.2}$$

satisfying $a(u(s)) \in \Lambda(a)$. The following diagram shows the interplay between the sets $\Lambda(a)$, D, and $[0, 2\pi]$, and the functions connecting them:

$$\begin{tikzcd}
\Lambda(a) \arrow[rr, shift left, "z_1"] \arrow[dr, shift right, "\varphi"'] & & D \arrow[ll, shift left, "a"] \\
& {[0, 2\pi]} \arrow[ul, shift right, "\psi"'] \arrow[ur, "u"'] &
\end{tikzcd}$$

We want to extend u to a function analytic on a certain complex neighborhood of s. By noticing that

$$u(0) = t_1, \quad u(2\pi) = t_2, \quad a(u(0)) = \rho_1, \quad a(u(2\pi)) = \rho_2,$$

we can see that $a(u(s))$ is branch point of $\Lambda(a)$ if and only if $s \in \{0, 2\pi\}$; otherwise, it is a simple point if and only if $s \in (0, 2\pi)$. Then, we divide the proof in two cases: $s \in (0, 2\pi)$ and $s \in \{0, 2\pi\}$.

Case 1. Assume that $s_0 \in (0, 2\pi)$ and let $\Theta(z, s) \equiv a(z) - a(\mathrm{e}^{\mathrm{i}s} z)$. We know that $a(u(s_0))$ is a simple point of $\Lambda(a)$, and in such a case, Theorem 3.2 tells us that

$$\frac{\partial \Theta}{\partial z}(u, s_0) = a'(u) - \mathrm{e}^{\mathrm{i}s_0} a'(\mathrm{e}^{\mathrm{i}s_0} u(s_0)) \neq 0.$$

Thus, by (3.2), and the implicit function theorem for complex variables (see [12]) applied to Θ, we conclude the existence of a complex neighborhood N_{s_0} of s_0, such that (3.2) has a unique solution $z = u(s)$ for any in $s \in N_{s_0}$. Moreover, u is single-valued and analytic in N_{s_0}.

The previous construction was made locally for each $s_0 \in (0, 2\pi)$. Then let u be the respective analytic continuation to the set $\bigcup_{s_0 \in (0, 2\pi)} N_{s_0}$.

Case 2. Assume that $s = 0$. A simple calculation shows that

$$a(z) - a(\mathrm{e}^{\mathrm{i}s}z) = (1 - \mathrm{e}^{\mathrm{i}s})\Phi(z, s),$$

where

$$\Phi(z, s) \equiv (1 + \mathrm{e}^{\mathrm{i}s})z^2 + cz - c\mathrm{e}^{-\mathrm{i}s}z^{-1}.$$

Therefore, $\Phi(z, s) = 0$ and $a(z) - a(\mathrm{e}^{\mathrm{i}s}z) = 0$ have the same solutions with respect to the variable z. In particular, $\Phi(t_1, 0) = 0$.

According to the implicit function theorem for complex variables, by showing that $\partial\Phi/\partial z(t_1, 0) \neq 0$, we obtain the existence of a function u analytic in a complex neighborhood of 0 satisfying $\Phi(u(s), s) = 0$ there, with $u(0) = t_1$.

Fortunately, the case $\partial\Phi/\partial z(t_1, 0) = 0$ is not possible because, in such a case, we have $\partial\Phi/\partial z(t_1, 0) = 4t_1 + c + ct_1^{-2}$, which combined with $0 = a'(t_1) = 2t_1 + c - ct_1^{-2}$ produces

$$0 = \Phi_z(t_1, 0) - a'(t_1) = 6t_1 + 2c,$$

and thus, $t_1 = -c/3$. Therefore, $0 = a'(t_1) = a'(-c/3)$ is a quadratic equation with solution $c = \pm 3\sqrt{3} \in \partial\Omega$, contrary to our general assumption (2.1). Hence, we arrive at $\partial\Phi/\partial z(t_1, 0) \neq 0$ and the existence of the required function u. The case $s = 2\pi$ can be proven in a similar manner. ∎

Proposition 3.7. *For $k = 1, 2$, the function u in Proposition 3.6 admits the following expansion at the points $\varsigma_1 = 0$ and $\varsigma_2 = 2\pi$:*

$$u(s) = t_k + \sum_{\ell=1}^{\infty} \mathbf{d}_{\ell,k}(s - \varsigma_k)^{\ell},$$

where the coefficients $\mathbf{d}_{\ell,k}$ can be calculated in terms of $\mathbf{a}_{\ell,k}$ and t_k, for instance

$$\begin{aligned}
\mathbf{d}_{1,k} &= -\mathrm{i}\frac{t_k}{2},\\
\mathbf{d}_{2,k} &= \frac{1}{8}\frac{\mathbf{a}_{3,k}}{\mathbf{a}_{2,k}}t_k^2,\\
\mathbf{d}_{3,k} &= \frac{-\mathrm{i}}{2}\Big(\frac{1}{8}\frac{\mathbf{a}_{3,k}}{\mathbf{a}_{2,k}}t_k^2 + \frac{t_k}{12}\Big).
\end{aligned}$$

Proof. We start with the case $k = 1$. Since u is analytic in a complex neighborhood of 0 and $u(0) = t_1$, we can write

$$u(s) = t_1 + \sum_{\ell=1}^{\infty} \mathbf{d}_{\ell,1}s^{\ell}. \tag{3.3}$$

Expanding $\mathrm{e}^{\mathrm{i}s}$ around $s=0$ and multiplying we obtain

$$\mathrm{e}^{\mathrm{i}s}u(s) = t_1 + \sum_{\ell=1}^{\infty} \alpha_\ell s^\ell, \tag{3.4}$$

where the coefficients α_ℓ can be computed in terms of $\mathbf{d}_{\ell,1}$, for example

$$\alpha_1 = \mathbf{d}_{1,1} + \mathrm{i}t_1, \quad \alpha_2 = \mathbf{d}_{2,1} + \mathrm{i}\mathbf{d}_{1,1} - \frac{t_1}{2}, \quad \alpha_3 = \mathbf{d}_{3,1} + \mathrm{i}\mathbf{d}_{2,1} - \frac{\mathbf{d}_{1,1}}{2} - \mathrm{i}\frac{t_1}{6}.$$

We now compose (3.3) with (2.5) and (3.4) with (2.5), and subtract them to reach

$$a(u(s)) - a(\mathrm{e}^{\mathrm{i}s}u(s)) = \sum_{\ell=1}^{\infty} \beta_\ell s^\ell,$$

where the coefficients β_ℓ can be found in terms of $\mathbf{a}_{\ell,k}$ and $\mathbf{d}_{\ell,k}$, for example

$$\begin{aligned}
\beta_1 &= t_1^2 - 2\mathrm{i}\mathbf{d}_{1,1}t_1,\\
\beta_2 &= 2\mathrm{i}\Big(\mathbf{a}_{2,1}t_1\mathbf{d}_{2,1} - \frac{\mathbf{a}_{3,1}t_1^3}{8}\Big),\\
\beta_3 &= 2\mathrm{i}t_1\mathbf{a}_{2,1}\mathbf{d}_{3,1} - \mathbf{a}_{2,1}t_1\mathbf{d}_{2,1} - \frac{\mathbf{a}_{2,1}t_1^2}{12}.
\end{aligned}$$

Finally, since $a(u(s)) - a(\mathrm{e}^{\mathrm{i}s}u(s)) = 0$, we obtain $\beta_\ell = 0$ for $\ell \geqslant 1$, and, using that $\mathbf{a}_{2,1} \neq 0$, the equations $\beta_\ell = 0$ with $\ell = 1,2,3$, yield

$$\mathbf{d}_{1,1} = -\mathrm{i}\frac{t_1}{2}, \quad \mathbf{d}_{2,1} = \frac{1}{8}\frac{\mathbf{a}_{3,1}}{\mathbf{a}_{2,1}}t_1^2, \quad \mathbf{d}_{3,1} = \frac{-\mathrm{i}}{2}\Big(\frac{1}{8}\frac{\mathbf{a}_{3,1}}{\mathbf{a}_{2,1}}t_1^2 + \frac{t_1}{12}\Big).$$

The case $k=2$ can be proven in a similar manner. ∎

Remark 3.8. The function u can be defined on the whole real line as follows. Define first $u(s) \equiv \mathrm{e}^{-\mathrm{i}s}u(-s)$ for $s \in [-2\pi, 0)$. Note that the resulting function is defined in $[-2\pi, 2\pi]$ and satisfies $u(-2\pi) = u(2\pi)$. Finally, extend the function u periodically over all $\mathbb{R}$. The obtained extended version is 4π-periodic, and satisfies $u(-s) = \mathrm{e}^{\mathrm{i}s}u(s)$ and $u(2\pi+s) = u(2\pi-s)$ for every $s \in \mathbb{R}$.

By Proposition 3.6, the function ψ given by (2.2) is analytic in a complex neighborhood of $[0,2\pi]$ with $\psi([0,2\pi]) = \Lambda(a)$, $\psi(0) = \rho_1$, $\psi(\pi) = -1$, and $\psi(2\pi) = \rho_2$. The following result shows that it is also injective.

Proposition 3.9. *The function ψ in (2.2) is one-to-one on $[0,2\pi]$.*

Proof. We will show that ψ is one-to-one on the intervals $[0,\pi]$ and $[\pi,2\pi]$ independently, and afterwards, we will show that

$$\psi([0,\pi]) \cap \psi([\pi,2\pi]) = \{\psi(\pi)\},$$

making ψ one-to-one on the whole interval $[0,2\pi]$.

Suppose by contradiction that ψ is not one-to-one on $[0,\pi]$. Then there exist distinct points $s_1, s_2 \in [0,\pi]$ such that $\psi(s_1) = \psi(s_2)$. For $k = 1, 2$, the rational function $a(z) - \psi(s_k)$ has three roots, namely $u(s_k)$, $\mathrm{e}^{\mathrm{i}s_k} u(s_k)$, and a third one that we call w_k. Therefore,

$$\{u(s_1), \mathrm{e}^{\mathrm{i}s_1} u(s_1), w_1\} = \{u(s_2), \mathrm{e}^{\mathrm{i}s_2} u(s_2), w_2\}.$$

According to the properties of $\Lambda(a)$ described immediately before Algorithm 2.1, from $\psi([0, 2\pi]) = \Lambda(a)$ we know that $|u(s_k)| < |w_k|$. Hence, a little thought tells us that the possible cases are $u(s_1) = u(s_2)$ or $u(s_1) = \mathrm{e}^{\mathrm{i}s_2} u(s_2)$ with $u(s_2) = \mathrm{e}^{\mathrm{i}s_1} u(s_1)$. In the former case, we obtain $\mathrm{e}^{\mathrm{i}(s_1 - s_2)} = 1$, implying that $s_1 = s_2$, which is not possible. In the latter case, we obtain $\mathrm{e}^{\mathrm{i}(s_1 + s_2)} = 1$, meaning that $s_1 + s_2 \in \{0, 2\pi\}$, which is also not possible. Therefore, ψ is one-to-one on $[0,\pi]$. By mimicking the previous approach, we can prove that ψ is also one-to-one on $[\pi, 2\pi]$.

Finally, from Theorem 3.5 we know that $\Lambda(a)$ consists of one analytic arc without self-intersections, and it follows that both $\psi([0,\pi])$ and $\psi([\pi, 2\pi])$ have the same property. Moreover, since $\psi(0) = \rho_1$, $\psi(\pi) = -1$, and $\psi(2\pi) = \rho_2$, we obtain $\psi([0,\pi]) = [\rho_1 \sim -1]$ and $\psi([\pi, 2\pi]) = [-1 \sim \rho_2]$, which in particular implies that $\psi([0,\pi]) \cap \psi([\pi, 2\pi]) = \{\psi(\pi)\}$. ■

Proposition 3.10. *The function ψ in (2.2) can be extended to the whole real line in such a way that it becomes even, that is, $\psi(-s) = \psi(s)$ for every $s \in \mathbb{R}$.*

Proof. Take the function u extended as instructed in Remark 3.8. Then we obtain an extension of ψ to the entire real line $\mathbb{R}$, satisfying

$$\psi(-s) = a(u(-s)) = a(\mathrm{e}^{\mathrm{i}s} u(s)) = a(u(s)) = \psi(s),$$

and the proposition is proved. ■

Proposition 3.11. *Let $\varsigma_1 = 0$ and $\varsigma_2 = 2\pi$. For $k = 1, 2$, the function ψ admits the following expansion at ς_k:*

$$\psi(s) = \rho_k + \sum_{\ell=1}^{\infty} \nu_{\ell,k} (s - \varsigma_k)^{2\ell},$$

where the coefficients $\nu_{\ell,k}$ can be calculated in terms of $\mathbf{a}_{\ell,k}$ and t_k, for instance

$$\nu_{1,k} = -t_k^2 \frac{\mathbf{a}_{2,k}}{4},$$

$$\nu_{2,k} = \frac{\mathbf{a}_{4,k}}{16} t_k^4 - \frac{\mathbf{a}_{3,k}}{16} t_k^3 - \frac{5\mathbf{a}_{3,k}^2}{64\mathbf{a}_{2,k}} t_k^4 - \frac{\mathbf{a}_{2,k}}{24} t_k^2.$$

Proof. We start with the case $k = 1$. Using the expansion in (2.5) and noticing that $\mathbf{a}_{1,1} = a'(t_1) = 0$, we can write

$$a(z) = \rho_1 + \sum_{\ell=2}^{\infty} \mathbf{a}_{\ell,1}(z - t_1)^{\ell}.$$

Now, taking $z = u(s)$, Proposition 3.7 gives us an expansion for $u(s) - t_1$ which combined with the previous expression produces

$$\psi(s) = \rho_1 + \sum_{\ell=1}^{\infty} \nu_{\ell,1} s^{2\ell},$$

where the coefficients $\nu_{\ell,1}$ can be obtained in two different ways: first, by direct composition of the mentioned expansions and second, by noticing that ψ is analytic, being the composition of two analytic functions, producing the well-known expression $\nu_{\ell,1} = \psi^{(2\ell)}(0)/(2\ell)!$. By comparison of these two alternatives, we can find the values of $\nu_{\ell,1}$ in terms of $\mathbf{a}_{\ell,1}$ and $\mathbf{d}_{\ell,1}$, for instance

$$\begin{aligned}
\nu_{1,1} &= \mathbf{a}_{2,1}\mathbf{d}_{1,1}^2, \\
\nu_{2,1} &= \mathbf{a}_{2,1}\mathbf{d}_{2,1}^2 + 2\mathbf{a}_{2,1}\mathbf{d}_{1,1}\mathbf{d}_{3,1} + 3\mathbf{a}_{3,1}\mathbf{d}_{1,1}^2\mathbf{d}_{2,1} + \mathbf{a}_{4,1}\mathbf{d}_{1,1}^4.
\end{aligned}$$

Finally, using the expression for $\mathbf{d}_{\ell,1}$ in terms of $\mathbf{a}_{\ell,1}$ and t_k, given by Proposition 3.7, we obtain the required statement. The case $k = 2$ can be proven analogously. ∎

3.3. Determinant

We now obtain an expression for the determinant of $T_n(a) - \lambda I_n = T_n(a - \lambda)$. Recall the set Ω_δ defined in (2.3) and fix a sufficiently small $\delta > 0$. The following key statements are direct consequences of the previous section.

(1) By Proposition 3.9, ψ is analytic and one-to-one on Ω_δ.

(2) From Proposition 3.6, $\Lambda(a) = \psi([0, 2\pi])$ with $\psi(0) = \rho_1$ and $\psi(2\pi) = \rho_2$.

(3) The properties of $\Lambda(a)$ listed immediately before Algorithm 2.1 tell us that if $\lambda = a(u(s)) \in \Lambda(a)$, then the roots of $a(z) - \lambda(s)$ are $u(s)$, $\mathrm{e}^{\mathrm{i}s}u(s)$, and $w(s)$ where $|u(s)| \leqslant |c|^{1/3}$ and $w(s) \equiv -c\mathrm{e}^{-\mathrm{i}s}/u(s)^2$.

(4) From Proposition 3.6, u and, hence, w are analytic on Ω_δ.

(5) The properties of $\Lambda(a)$ listed immediately before Algorithm 2.1 also tell us that $|u(s)| < |w(s)|$ for any $s \in [0, 2\pi]$. Then, we can extend that property by the continuity of u and w to the set Ω_δ. Therefore, there exists a constant $\Delta > 0$ such that $\sup\{|u(s)|/|w(s)| \colon s \in \Omega_\delta\} < \mathrm{e}^{-\Delta}$. See Figure 7.

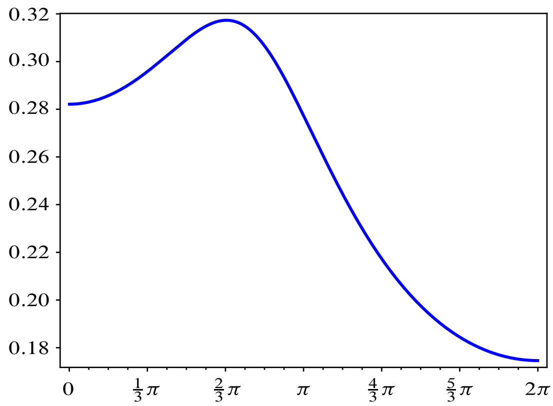


Figure 7. The absolute value of the quotient $u(s)/w(s)$ for the generating function $a(z) = z^2 + cz + cz^{-1}$ with $c = 2 + 3\mathrm{i}$.

Denote by $D_n(a)$ the determinant of the matrix $T_n(a)$. When the generating function a is a Laurent polynomial, the classic Widom determinant formula [19] gives us an expression for $D_n(a)$. For the reader's convenience we report it here, without a proof.

Proposition 3.12 (Widom). *Let a be the Laurent polynomial $a(z) = \sum_{j=-r}^{\ell} a_j z^j$, $r, \ell \geqslant 1$, $a_{-r}a_\ell \neq 0$. 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 $|M| = \ell$,

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

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

Let a be given by (2.1). Applying Proposition 3.12 to the Laurent polynomial $a(z) - \psi(s)$ we obtain

$$D_n(a - \psi(s)) = p_1(s) + p_2(s) + p_3(s), \tag{3.5}$$

where

$$p_1(s) = \frac{\big(u(s)w(s)\big)^{n+1}}{(u(s) - \mathrm{e}^{\mathrm{i}s}u(s))(w(s) - \mathrm{e}^{\mathrm{i}s}u(s))},$$

$$p_2(s) = \frac{e^{is(n+1)}\big(u(s)w(s)\big)^{n+1}}{(e^{is}u(s) - u(s))(w(s) - u(s))},$$

$$p_3(s) = \frac{u(s)^{2(n+1)}e^{is(n+1)}}{(u(s) - w(s))(e^{is}u(s) - w(s))}.$$

For $s \in \Omega_\delta$, we define the following auxiliary complex-valued functions:

$$g(s) \equiv u(s)w(s), \quad f(s) \equiv \frac{u(s)}{w(s)}, \quad h_1(s) \equiv 1 - e^{is} f(s), \quad h_2(s) \equiv 1 - f(s). \tag{3.6}$$

Proposition 3.13. *Let $s \in \Omega_\delta$. The terms in (3.5) can be written as*

$$p_1(s) = -\frac{e^{-i\frac{s}{2}} g(s)^n}{2i \sin\left(\frac{s}{2}\right) h_1(s)},$$

$$p_2(s) = \frac{e^{is(n+\frac{1}{2})} g(s)^n}{2i \sin\left(\frac{s}{2}\right) h_2(s)},$$

$$p_3(s) = \frac{e^{is(n+1)} f(s)^{n+2} g(s)^n}{h_1(s)h_2(s)}.$$

Proof. The proposition follows after inserting (3.6) into (3.5). ∎

Proposition 3.14. *The function f in (3.6) is analytic, bounded, and non-zero in Ω_δ. Moreover, for $k = 1, 2$, we have $f'(\varsigma_k) = it_k^3/(2c)$, where $\varsigma_1 = 0$ and $\varsigma_2 = 2\pi$.*

Proof. By statement (4), f is the quotient of two analytic functions in Ω_δ, hence it is analytic there too. Additionally, statement (5) tells us that

$$|f(s)| \leqslant \sup_{s \in \Omega_\delta} \frac{|u(s)|}{|w(s)|} < e^{-\Delta}.$$

Moreover, since $u(s) \neq 0$ (otherwise $a(0) = 0$, which is not possible), by statement (3), we have

$$f(s) = -\frac{e^{is} u(s)^3}{c} \neq 0. \tag{3.7}$$

From Proposition 3.7, we know that $u(\varsigma_k) = t_k$ and $u'(\varsigma_k) = -t_k/2$, and so the required value of $f'(\varsigma_k)$ follows easily. ∎

Proposition 3.15. *The complex-valued function*

$$\theta(s) \equiv -i \log\left(\frac{h_1(s)}{h_2(s)}\right)$$

is analytic in Ω_δ and can be extended to $\mathbb{R}$ in such a way that it becomes odd, that is, $\theta(-s) = -\theta(s)$ for every $s \in \mathbb{R}$.

Proof. The proof of Proposition 3.14 tells us that $|f(s)| < \mathrm{e}^{-\Delta}$ for some $\Delta > 0$ and all $s \in \Omega_\delta$. Hence, we have

$$|1 - h_1(s)| \leqslant \mathrm{e}^{-\Delta} \quad \text{and} \quad |1 - h_2(s)| \leqslant \mathrm{e}^{-\Delta},$$

which in particular means that h_1 and h_2 are bounded and bounded away from zero, making θ well defined. Now, it is clear that θ inherits its analyticity from the one of f.

We now turn to the extension of θ. Consider the extended version of u constructed in Remark 3.8. This function is defined in $\mathbb{R}$ and satisfies $u(-s) = \mathrm{e}^{\mathrm{i}s}u(s)$ for every $s \in \mathbb{R}$.

Using (3.7), we can write

$$\theta(s) = -\mathrm{i}\log\Bigl(\frac{c + \mathrm{e}^{2\mathrm{i}s}u(s)^3}{c + \mathrm{e}^{\mathrm{i}s}u(s)^3}\Bigr).$$

Therefore, θ is now defined in $\mathbb{R}$ and satisfies

$$\begin{aligned}\theta(-s) &= -\mathrm{i}\log\Bigl(\frac{c + \mathrm{e}^{-2\mathrm{i}s}u(-s)^3}{c + \mathrm{e}^{-\mathrm{i}s}u(-s)^3}\Bigr),\\ &= -\mathrm{i}\log\Bigl(\frac{c + \mathrm{e}^{\mathrm{i}s}u(s)^3}{c + \mathrm{e}^{2\mathrm{i}s}u(s)^3}\Bigr),\\ &= \mathrm{i}\log\Bigl(\frac{c + \mathrm{e}^{2\mathrm{i}s}u(s)^3}{c + \mathrm{e}^{\mathrm{i}s}u(s)^3}\Bigr) = -\theta(s),\end{aligned}$$

as needed. ■

Proposition 3.16. *The function θ admits the following expansion at the points $\varsigma_1 = 0$ and $\varsigma_2 = 2\pi$:*

$$\theta(s) = \sum_{\ell=1}^{\infty} \varkappa_{\ell,k}(s - \varsigma_k)^{2\ell-1} \quad (k = 1, 2)$$

where the coefficients $\varkappa_{\ell,k}$ can be expressed in terms of $\mathbf{a}_{\ell,k}$ and t_k, for instance

$$\begin{aligned}\varkappa_{1,k} &= \frac{t_k^3}{c + t_k^3},\\ \varkappa_{2,k} &= \Bigl(\frac{3\mathbf{a}_{3,k}^2}{8\mathbf{a}_{2,k}}t_k^4 - \frac{1}{3}t_k^3\Bigr)\frac{1}{c + t_k^3} - \Bigl(\frac{3\mathbf{a}_{3,k}^2}{8\mathbf{a}_{2,k}}t_k^7 - \frac{1}{4}t_k^4\Bigr)\frac{1}{(c + t_k^3)^2} - \frac{t_k^9}{12(c + t_k^3)^3}.\end{aligned}$$

Proof. In order to find an expansion for θ, we use (3.7) and write

$$\frac{h_1(s)}{h_2(s)} = \frac{c + \mathrm{e}^{\mathrm{i}2s} u(s)^3}{c + \mathrm{e}^{\mathrm{i}s} u(s)^3}.$$

Then, Proposition 3.7, combined with the geometric series, produces

$$\frac{h_1(s)}{h_2(s)} \equiv 1 + \sum_{\ell=1}^{\infty} \mathbf{h}_{\ell,k}(s - \varsigma_k)^{\ell},$$

where the coefficients $\mathbf{h}_{\ell,k}$ can be calculated in terms of $\mathbf{a}_{\ell,k}$ and t_k, for instance

$$\begin{aligned}
\mathbf{h}_{1,k} &= \frac{\mathrm{i}t_k^3}{c + t_k^3}, \\
\mathbf{h}_{2,k} &= -\frac{t_k^6}{2(c + t_k^3)^2}, \\
\mathbf{h}_{3,k} &= \Big(\frac{\mathrm{i}3\mathbf{a}_{3,k}}{8\mathbf{a}_{2,k}} t_k^4 + \frac{\mathrm{i}}{3} t_k^3\Big) \frac{1}{c + t_k^3} - \Big(\frac{\mathrm{i}3\mathbf{a}_{3,k}}{8\mathbf{a}_{2,k}} t_k^7 + \frac{\mathrm{i}}{4} t_k^6\Big) \frac{1}{(c + t_k^3)^2} - \frac{\mathrm{i}t_k^9}{(c + t_k^3)^3}.
\end{aligned}$$

To finish the proof, we take the logarithm of $h_1(s)/h_2(s)$ and expand with the Maclaurin series for $\log(1 + z)$. ∎

Most of the technical work done so far culminates in the following key expression for $D_n(a - \psi(s))$.

Theorem 3.17. *Let a have the form (2.1). Then, for every $s \in \Omega_\delta$, the determinant $D_n(a - \psi(s))$ can be written as*

$$D_n(a - \psi(s)) = \frac{g(s)^n \mathrm{e}^{\mathrm{i}\frac{n}{2}s}}{\sin(\frac{s}{2})\sqrt{h_1(s)h_2(s)}} \Big[\sin\Big(\frac{(n + 1)s + \theta(s)}{2}\Big) + R_n(s)\Big],$$

where R_n is given by

$$R_n(s) = \frac{\sin(\frac{s}{2}) f(s)^{n+2}}{\sqrt{h_1(s)h_2(s)}} \mathrm{e}^{\mathrm{i}(\frac{n}{2}+1)s},$$

and satisfies $R_n(s) = O(\mathrm{e}^{-\Delta n})$ and $R_n'(s) = O(n\mathrm{e}^{-\Delta n})$, uniformly in $s \in \Omega_\delta$.

Proof. From Proposition 3.13, we know that $D_n(a - \psi(s))$ can be written as

$$\frac{\mathrm{e}^{\mathrm{i}s(n+\frac{1}{2})} g(s)^n}{2\mathrm{i}\sin(\frac{s}{2}) h_2(s)} - \frac{\mathrm{e}^{-\mathrm{i}\frac{s}{2}} g(s)^n}{2\mathrm{i}\sin(\frac{s}{2}) h_1(s)} + \frac{\mathrm{e}^{\mathrm{i}s(n+1)} f(s)^{n+2} g(s)^n}{h_1(s)h_2(s)},$$

and, thus, it equals

$$\begin{aligned}
&\frac{g(s)^n e^{\frac{i}{2}ns}}{2i\sin(\frac{s}{2})h_1(s)}\Big(\frac{h_1(s)}{h_2(s)}e^{\frac{i}{2}(n+1)s} - e^{-\frac{i}{2}(n+1)s} + \frac{2i\sin(\frac{s}{2})f(s)^{n+2}e^{i(\frac{n}{2}+1)s}}{h_2(s)}\Big)\\
&\quad = \frac{g(s)^n e^{\frac{i}{2}ns}}{2i\sin(\frac{s}{2})h_1(s)}\Big(e^{i\theta(s)}e^{\frac{i}{2}(n+1)s} - e^{-\frac{i}{2}(n+1)s} + 2ie^{\frac{i}{2}\theta(s)}R_n(s)\Big)\\
&\quad = \frac{g(s)^n e^{\frac{i}{2}(ns+\theta(s))}}{\sin(\frac{s}{2})h_1(s)}\Big[\sin\Big(\frac{(n+1)s+\theta(s)}{2}\Big) + R_n(s)\Big],
\end{aligned}$$

where θ is defined in Proposition 3.15.

We are left with finding the order of R_n and its derivative. In the proof of Proposition 3.15 we mentioned that the functions h_j $(j = 1, 2)$ defined in (3.6) are bounded away from zero in Ω_δ, and, moreover, since according to Proposition 3.14 f is analytic there, h_j and, hence, R_n are analytic there too.

Writing

$$f(s)^{n+2}e^{i(\frac{n}{2}+1)} = (f(s)^2 e^{is})^{\frac{n}{2}+1},$$

and using the bound $|f(s)| < e^{-\Delta}$ (see the proof of Proposition 3.14), we can find a sufficiently small $\delta > 0$ such that $|f(s)^2 e^{is}| < 1$ for every $s \in \Omega_\delta$. We thus have

$$|R_n(s)| \leqslant \kappa|f(s)^{n+2}e^{i(\frac{n}{2}+1)s}| = \kappa|f(s)|^{n+2} \leqslant \kappa e^{-\Delta(n+2)} = O(e^{-n\Delta}),$$

as needed. Finally, a similar calculation gives us the required bound for R_n'. ■

4. Proof of the main theorems

A point $\lambda = \psi(s)$ is an eigenvalue of $T_n(a)$ if only if

$$D_n(a - \psi(s)) = 0.$$

Because the functions g, h_1, and h_2, defined in (3.6), do not take the value zero, Theorem 3.17 tells us that the last equation implies

$$\sin\Big(\frac{(n+1)s+\theta(s)}{2}\Big) + R_n(s) = 0,$$

or equivalently

$$(n+1)s + \theta(s) + (-1)^j E_n(s) = 2\pi j, \tag{4.1}$$

where $j \in \mathbb{Z}$, $s \in [0, 2\pi]$, and $E_n(s) \equiv 2\arcsin R_n(s)$. We are going to show that the term $E_n(s)$, being relatively small, plays the role of a remainder suggesting the usage of the reduced equation

$$(n+1)s + \theta(s) = 2\pi j. \tag{4.2}$$

We now introduce the necessary auxiliary ingredients to prove our main results.

Consider the functions

$$H_{j,n}(s) \equiv \sigma_{j,n} - \frac{\theta(s)}{n+1},$$
$$\widetilde{H}_{j,n}(s) \equiv \sigma_{j,n} - \frac{\theta(s) + (-1)^j E_n(s)}{n+1},$$

where $\sigma_{j,n} = 2\pi j/(n+1)$ and θ is defined in Proposition 3.15. Note that if $s_{j,n}$ and $s^*_{j,n}$ are solutions of equations (4.1) and (4.2), respectively, then we obtain

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

Because θ is analytic on Ω_δ (see Proposition 3.15), we know that both

$$\sup\{|\theta(s)|: s \in \Omega_\delta\} \quad \text{and} \quad \sup\{|\theta'(s)|: s \in \Omega_\delta\}$$

are finite. Lastly, recall the constant $d_{j,n} = \sigma_{j,n} - \theta(\sigma_{j,n})/(n+1)$ and the set $\Theta_{j,n}$ defined in (2.4).

Proposition 4.1. *Let a be the function given by* (2.1)*. For every sufficiently large n and any $j \in \{1,\dots,n\}$, $H_{j,n}(s)$ and $\widetilde{H}_{j,n}(s)$ are contractive maps on $\Theta_{j,n}$ to itself.*

Proof. From the mean value theorem, we know that if f is an analytic function satisfying $|f'(z)| \leqslant M$ in some convex domain G, then

$$|f(z_1) - f(z_2)| \leqslant M|z_1 - z_2|,$$

for $z_1, z_2 \in G$. Take $s \in \Theta_{j,n}$ and let $\|v\|_\infty$ stand for $\sup\{|v(s)|: s \in \Omega_\delta\}$. We start with $\widetilde{H}_{j,n}(s)$,

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

By Theorem 3.17, we know that $R_n(s) = O(\mathrm{e}^{-\Delta n})$. Thus, using the Maclaurin series of arcsin, we obtain $E_n(s) = 2 \arcsin R_n(s) = O(\mathrm{e}^{-\Delta n})$. We now manipulate the last expression in order to include the term $|s - d_{j,n}|$,

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

The very last bound, being strictly smaller than $r_{j,n}$, tells us that $\widetilde{H}_{j,n}(s)$ belongs to $\Theta_{j,n}$ for every sufficiently large n.

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

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

The bound $|E_n'(s)| = O(n\mathrm{e}^{-\Delta n})$, uniformly in $s \in \Theta_{j,n}$, is a consequence of Theorem 3.17, and therefore

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

and, hence, $\widetilde{H}_{j,n}$ is contractive on $\Theta_{j,n}$.

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

$$|H_{j,n}(s) - d_{j,n}| \leqslant r_{j,n}\Big(\frac{1}{3} + \frac{\|\theta'\|_\infty}{n+1}\Big),$$

which tells us that $H_{j,n}(s) \in \Theta_{j,n}$ for every sufficiently large n. Similarly, the inequality

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

shows that $H_{j,n}(s)$ is contractive on $\Theta_{j,n}$ as well, which finishes the proof. ■

With the previous result 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 $\Theta_{j,n}$, satisfying (4.3) and being the solutions of (4.1) and (4.2), respectively.

Proof of Theorem 2.3. As in the previous proof, let $\|v\|_\infty$ stand for $\sup\{|v(s)|: s \in \Omega_\delta\}$. A simple calculation shows that

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

which means that $|d_{j+1,n} - d_{j,n}| = O(1/n)$ while $r_{j,n} = O(1/n^2)$. Therefore, for every sufficiently large n, the domains $\Theta_{j,n}$ are pairwise disjoint. Thus, Proposition 4.1 tells us that, for every $j \in \{1, \ldots, n\}$, $H_{j,n}(s) = s$ has a unique solution $s_{j,n} \in \Theta_{j,n}$ satisfying (4.1), with $E_n(s) = O(\mathrm{e}^{-n\Delta})$. The order of $E_n'(s)$ follows from Theorem 3.17, finishing the proof of the second statement.

Theorem 3.17 together with (4.1) tells us that $\lambda_{j,n} = \psi(s_{j,n})$ is an eigenvalue of $T_n(a)$, which obviously belongs to $\psi(\Theta_{j,n})$. Since, by Proposition 3.9, ψ is injective and the sets $\Theta_{j,n}$ $(j = 1, \ldots, n)$ are pairwise disjoint, the same applies to the sets

$\psi(\Theta_{j,n})$ $(j = 1, \ldots, n)$, making the points $\lambda_{j,n}$ $(j = 1, \ldots, n)$ pairwise distinct, and proving the first statement.

We are left with the proof of the third statement. From Proposition 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 $\Theta_{j,n}$. Consider the function

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

and note that

$$\begin{aligned}F_n(s_{j,n}) - F_n(s_{j,n}^*) &= (n+1)(\widetilde{H}_{j,n}(s_{j,n}) - H_{j,n}(s_{j,n}^*))\\ &= (-1)^j E_n(s_{j,n}) = O(\mathrm{e}^{-\Delta n}),\end{aligned}$$

where $E_n(s)$ is given by (4.1). On the other hand,

$$F_n(s_{j,n}) = F_n(s_{j,n}^*) + F_n'(s_{j,n}^*)(s_{j,n} - s_{j,n}^*) + O(|s_{j,n} - s_{j,n}^*|^2),$$

and hence

$$\begin{aligned}|F_n(s_{j,n}) - F_n(s_{j,n}^*)| &= |F_n'(s_{j,n}^*)(s_{j,n} - s_{j,n}^*) + O(|s_{j,n} - s_{j,n}^*|^2)|\\ &= |F_n'(s_{j,n}^*)||s_{j,n} - s_{j,n}^*|\Big[1 + O\Big(\frac{|s_{j,n} - s_{j,n}^*|}{|F_n'(s_{j,n}^*)|}\Big)\Big].\end{aligned}$$

Solving the previous equation for $|s_{j,n}^* - s_{j,n}|$, we obtain

$$|s_{j,n}^* - s_{j,n}| = \frac{|F_n(s_{j,n}) - F_n(s_{j,n}^*)|}{|F_n'(s_{j,n}^*)|}\Big[1 + O\Big(\frac{|s_{j,n} - s_{j,n}^*|}{|F_n'(s_{j,n}^*)|}\Big)\Big]^{-1}.$$

The bound $|F_n(s_{j,n}) - F_n(s_{j,n}^*)| = O(\mathrm{e}^{-\Delta n})$, together with

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

produces the estimation $|s_{j,n}^* - s_{j,n}| = O(\mathrm{e}^{-\Delta n}/n)$.

To finish the proof we merge $\|\psi'\|_\infty < \infty$ (see Proposition 3.11) with

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

to obtain

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

where $E(s_{j,n}^*) = O(\mathrm{e}^{-\Delta n}/n)$ uniformly in j. ∎

Proof of Theorem 2.4. As in the previous proof, let $\|v\|_\infty$ stand for $\sup\{|v(s)|: s \in \Omega_\delta\}$. Since $H_{j,n}(s)$ is contractive on $\Theta_{j,n}$ (see Proposition 4.1), the Banach fixed-point theorem tells us that $H_{j,n}(s)$ admits a unique fixed-point, namely $s^*_{j,n}$. Furthermore, the recursive sequence

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

converges to $s^*_{j,n}$ as $\ell \to \infty$.

A simple recursive calculation shows that

$$|s^{(\ell)}_{j,n} - s^*_{j,n}| \leqslant \frac{q^{\ell-1}}{1-q}|s^{(1)}_{j,n} - s^{(2)}_{j,n}|, \tag{4.4}$$

where $q \equiv \|\theta'\|_\infty/(n+1)$. Consider the second term in the sequence $s^{(\ell)}_{j,n}$ $(\ell \geqslant 1)$, and write

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

Therefore, $|s^{(1)}_{j,n} - s^{(2)}_{j,n}| = O(\theta(\sigma_{j,n})\theta'(\sigma_{j,n})/n^2) = O(\theta(\sigma_{j,n})/n^2)$, which combined with (4.4), produces

$$s^*_{j,n} = s^{(2)}_{j,n} + O\Big(\frac{\theta(\sigma_{j,n})}{n^3}\Big).$$

Because of Proposition 3.16, we know that $\theta(\sigma_{j,n}) = O(\sigma_{j,n}(\sigma_{j,n} - 2\pi))$, resulting in the important expansion

$$s^*_{j,n} = \sigma_{j,n} - \frac{\theta(\sigma_{j,n})}{n+1} + \frac{\theta'(\sigma_{j,n})\theta(\sigma_{j,n})}{(n+1)^2} + O\Big(\frac{\sigma_{j,n}(\sigma_{j,n} - 2\pi)}{n^3}\Big). \tag{4.5}$$

By Theorem 2.3, we know that

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

and we are ready to obtain the required expression for $\lambda_{j,n}$. Apply ψ to the point $s^*_{j,n}$ expanded as in (4.5). This gives

$$\psi(s^*_{j,n}) = \psi(\sigma_{j,n}) + \frac{\mathbf{r}_1(\sigma_{j,n})}{n+1} + \frac{\mathbf{r}_2(\sigma_{j,n})}{(n+1)^2} + E(\sigma_{j,n}),$$

where $E(\sigma_{j,n})$ plays the role of a remainder term and satisfies

$$\begin{aligned}E(\sigma_{j,n}) &= O\Big(\frac{\psi'(\sigma_{j,n})\sigma_{j,n}(\sigma_{j,n}-2\pi)}{n^3}\Big)\\ &\qquad + O\Big(\frac{\psi''(\sigma_{j,n})\theta'(\sigma_{j,n})\theta(\sigma_{j,n}^2)}{n^3}\Big) + O\Big(\frac{\psi'''(\sigma_{j,n})\theta(\sigma_{j,n})^3}{n^3}\Big)\\ &= O\Big(\frac{\sigma_{j,n}^2(\sigma_{j,n}-2\pi)^2}{n^3}\Big),\end{aligned}$$

while the coefficients $\mathbf{r}_k(s)$ $(k=1,2)$ are given by

$$\mathbf{r}_1(s) \equiv -\psi'(s)\theta(s), \quad \mathbf{r}_2(s) \equiv \frac{1}{2}\psi''(s)\theta(s)^2 + \psi'(s)\theta(s)\theta'(s),$$

finishing the proof. ∎

Proof of Theorem 2.5. Let (j_n) be a sequence with $j_n^2/n \to 0$ and take $j \in \{1,\dots, j_n\}$. For simplicity, we write ν_k instead of $\nu_{k,1}$. From Propositions 3.11 and 3.16, we know that as $s \to 0$, we have

$$\begin{aligned}\psi'(s) &= 2\nu_1 s + 4\nu_2 s^3 + O(s^5),\\ \psi''(s) &= 2\nu_1 + 12\nu_2 s^2 + O(s^4),\\ \theta'(s) &= \varkappa_1 + O(s^2).\end{aligned}$$

Then, as $s \to 0$,

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

Take $s = \sigma_{j,n}$ and use the second statement in Theorem 2.4 to obtain

$$\begin{aligned}\lambda_{j,n} &= \rho_1 + \nu_1\sigma_{j,n}^2 + \nu_2\sigma_{j,n}^4 - 2\varkappa_1\nu_1\frac{\sigma_{j,n}^2}{n+1} + 3\nu_1\varkappa_1^2\frac{\sigma_{j,n}^2}{(n+1)^2}\\ &\quad + O(\sigma_{j,n}^6) + O\Big(\frac{\sigma_{j,n}^4}{n^2}\Big) + O\Big(\frac{\sigma_{j,n}^4}{n}\Big) + O\Big(\frac{\sigma_{j,n}^2(\pi-\sigma_{j,n})^2}{n^3}\Big),\end{aligned}$$

which combined with $O(\sigma_{j,n}^2(\pi-\sigma_{j,n})^2 n^{-3}) = O(j^2 n^{-5})$, gives us the first statement of the theorem. The second statement can be similarly proved. ∎

5. Numerical experiments

In this section we test the asymptotic expansions in Theorems 2.4 for the Toeplitz matrices $T_n(a)$ with generating function

$$a(z) = z^2 + (2+3\mathrm{i})z + (2+3\mathrm{i})z^{-1},$$

that is, the function a in (2.1) with $c = 2+3\mathrm{i}$. See Figure 8.

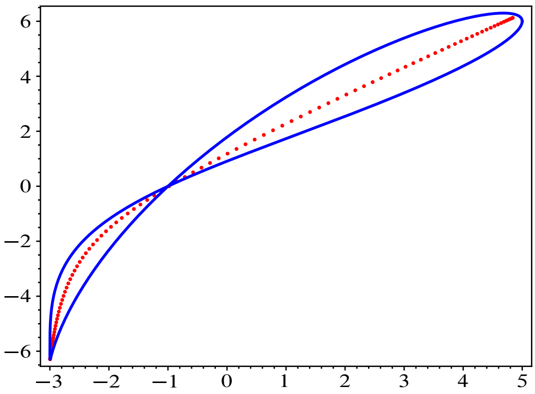


Figure 8. The range of the generating function a (blue curve) and the set $\mathrm{sp}_{128}(T_n(a))$ (red points), for $a(z) = z^2 + cz + cz^{-1}$ with $c = 2 + 3\mathrm{i} \in \mathbb{C} \setminus \Omega$.

5.1. General eigenvalues

We introduce the following term-by-term approximations of $\lambda_{j,n}$ given by our expansion in Theorem 2.4:

$$\begin{aligned}
\lambda_{j,n}^{\mathrm{SL}(1)} &\equiv \mathbf{r}_0(\sigma_{j,n}),\\
\lambda_{j,n}^{\mathrm{SL}(2)} &\equiv \mathbf{r}_0(\sigma_{j,n}) + \frac{\mathbf{r}_1(\sigma_{j,n})}{n+1},\\
\lambda_{j,n}^{\mathrm{SL}(3)} &\equiv \mathbf{r}_0(\sigma_{j,n}) + \frac{\mathbf{r}_1(\sigma_{j,n})}{n+1} + \frac{\mathbf{r}_2(\sigma_{j,n})}{(n+1)^2},
\end{aligned}$$

where

$$\begin{aligned}
\mathbf{r}_0(s) &= \psi(s),\\
\mathbf{r}_1(s) &= -\psi'(s)\theta(s),\\
\mathbf{r}_2(s) &= \frac{1}{2}\psi''(s)\theta^2(s) + \psi'(s)\theta(s)\theta'(s).
\end{aligned}$$

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

$$\mathrm{RE}_{j,n}^{\mathrm{SL}(k)} \equiv \frac{|\lambda_{j,n} - \lambda_{j,n}^{\mathrm{SL}(k)}|}{|\lambda_{j,n}|}, \quad \mathrm{RE}_{n}^{\mathrm{SL}(k)} \equiv \max_{1\leqslant j\leqslant n} \mathrm{RE}_{j,n}^{\mathrm{SL}(k)}.$$

Additionally, we consider the respective normalized error,

$$\mathrm{NE}_{n}^{\mathrm{SL}(k)} \equiv (n+1)^k\, \mathrm{RE}_{n}^{\mathrm{SL}(k)}.$$

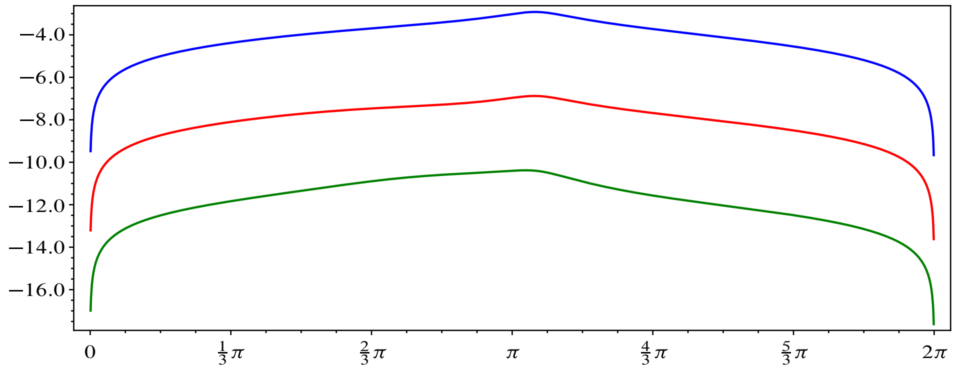


Figure 9. The 10-base logarithm of the individual relative error $\mathrm{RE}_{j,n}^{\mathrm{SL}(k)}$ for $n = 2048$ and different values of k: $k = 1$ (blue), $k = 2$ (red), and $k = 3$ (green). For the eigenvalue $\lambda_{j,n} = \psi(s_{j,n})$ we took as independent variable $s_{j,n}$ and plotted the errors over the grid $j\pi/(n+1)$ for $j \in \{1, \ldots, n\}$.

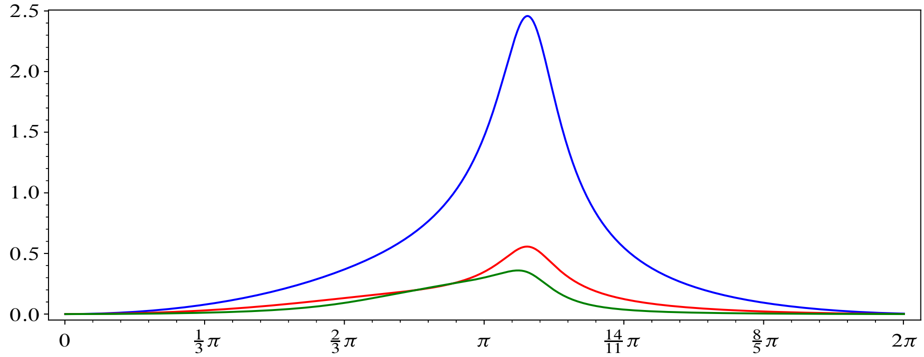


Figure 10. The absolute value of the individual normal error $\mathrm{NE}_{j,n}^{\mathrm{SL}(k)}$ for $n = 2048$ and different values of k: $k = 1$ (blue), $k = 2$ (red), and $k = 3$ (green). For the eigenvalue $\lambda_{j,n} = \psi(s_{j,n})$ we took as independent variable $s_{j,n}$ and plotted the errors over the grid $j\pi/(n+1)$ for $j \in \{1, \ldots, n\}$.

According to our results, the maximum normalized error $\mathrm{NE}_n^{\mathrm{SL}(k)}$ should have a bounded behavior. As a matter of fact, our experiments show that it even has an almost constant behavior. Figures 9 and 10 and Table 2 show the data.

n	$\mathrm{RE}_n^{\mathrm{SL}(1)}$	$\mathrm{NE}_n^{\mathrm{SL}(1)}$	$\mathrm{RE}_n^{\mathrm{SL}(2)}$	$\mathrm{NE}_n^{\mathrm{SL}(2)}$	$\mathrm{RE}_n^{\mathrm{SL}(3)}$	$\mathrm{NE}_n^{\mathrm{SL}(3)}$
25	9.355×10^{-2}	2.432	8.185×10^{-4}	0.553	2.128×10^{-5}	0.350
64	3.882×10^{-2}	2.523	1.360×10^{-4}	0.574	1.337×10^{-6}	0.346
128	1.933×10^{-2}	2.494	3.400×10^{-5}	0.565	1.701×10^{-7}	0.341
256	9.623×10^{-3}	2.473	8.493×10^{-6}	0.560	2.137×10^{-8}	0.339
512	4.805×10^{-3}	2.465	2.122×10^{-6}	0.558	2.675×10^{-9}	0.338
1024	2.400×10^{-3}	2.460	5.305×10^{-7}	0.557	3.346×10^{-10}	0.337
2048	1.199×10^{-3}	2.458	1.326×10^{-7}	0.556	4.184×10^{-11}	0.359

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

5.2. Extreme eigenvalues

Theorem 2.3 tells us, in particular, that for every sufficiently large n, ψ is the spectral symbol of $T_n(a)$, that is, there exists a sequence of points $\{s_{j,n}\}_{j=1}^n$ such that $\operatorname{sp} T_n(a) = \{\lambda_{j,n}\}_{j=1}^n$ where $\lambda_{j,n} \equiv \psi(s_{j,n})$.

By Theorem 2.5, we know that there are eigenvalues approaching the extremes of the limiting set $\Lambda(a)$, ρ_1 and ρ_2. We start by analyzing the eigenvalues $\lambda_{j,n}$ arbitrarily close to ρ_1. Take $j_n = \lceil \sqrt{n}\, \rceil$. For $j \in \{1, \ldots, j_n\}$, we define

$$
\begin{aligned}
\lambda_{j,n}^{\mathrm{EXT}(1)} &\equiv \rho_1 + \frac{\mathbf{u}_{1,1} j^2}{(n+1)^2},\\
\lambda_{j,n}^{\mathrm{EXT}(2)} &\equiv \rho_1 + \frac{\mathbf{u}_{1,1} j^2}{(n+1)^2} + \frac{\mathbf{u}_{2,1} j^2}{(n+1)^3},\\
\lambda_{j,n}^{\mathrm{EXT}(3)} &\equiv \rho_1 + \frac{\mathbf{u}_{1,1} j^2}{(n+1)^2} + \frac{\mathbf{u}_{2,1} j^2}{(n+1)^3} + \frac{\mathbf{u}_{3,1} j^4 + \mathbf{u}_{4,1} j^2}{(n+1)^4};
\end{aligned}
\tag{5.1}
$$

where

$$
\mathbf{u}_{1,1} \equiv -\frac{(t_1\pi)^2}{2} a^{(2)}(t_1), \quad \mathbf{u}_{2,1} \equiv \frac{t_1^5\pi^2}{c + t_1^3} a^{(2)}(t_1), \quad \mathbf{u}_{3,1} \equiv -\frac{3t_1^8\pi^2}{2(c+t_1^3)^2} a^{(2)}(t_1),
$$

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

and t_1 is the multiple zero of $a(z) - \rho_1$. Similarly, define the individual relative and normalized relative errors by

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

The reason behind this 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, and 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 $|\lambda_{j,n} - \lambda_{j,n}^{\mathrm{EXT}(k)}|$, which is the absolute error. Moreover, a value of $\mathrm{RE}_{j,n}^{\mathrm{EXT}(k)}$ close to 1 says that the measured object and the approximation are comparable.

Now, we study the eigenvalues $\lambda_{j,n}$ which are arbitrarily close to the point ρ_2. Take $j_n = n - \lceil \sqrt{n} \rceil$. For $j \in \{j_n, \ldots, n\}$ we introduce the approximations

$$\lambda_{j,n}^{\mathrm{EXT}(1)} \equiv \rho_2 + \frac{\mathbf{u}_{1,2}(n+1-j)^2}{(n+1)^2}, \tag{5.2a}$$

$$\lambda_{j,n}^{\mathrm{EXT}(2)} \equiv \rho_2 + \frac{\mathbf{u}_{1,2}(n+1-j)^2}{(n+1)^2} + \frac{\mathbf{u}_{2,2}(n+1-j)^2}{(n+1)^3}, \tag{5.2b}$$

$$\lambda_{j,n}^{\mathrm{EXT}(3)} \equiv \rho_2 + \frac{\mathbf{u}_{1,2}(n+1-j)^2}{(n+1)^2} + \frac{\mathbf{u}_{2,2}(n+1-j)^2}{(n+1)^3} \tag{5.2c}$$

$$+ \frac{\mathbf{u}_{3,2}(n+1-j)^2 + \mathbf{u}_4(n+1-j)^4}{(n+1)^4}; \tag{5.2d}$$

where

$$\mathbf{u}_{1,1} \equiv -\frac{(t_2\pi)^2}{2} a^{(2)}(t_2),$$

$$\mathbf{u}_{2,1} \equiv \frac{t_2^5\pi^2}{c+t_2^3} a^{(2)}(t_2),$$

$$\mathbf{u}_{3,1} \equiv -\frac{3t_2^8\pi^2}{2(c+t_2^3)^2} a^{(2)}(t_2),$$

$$\mathbf{u}_{4,1} \equiv \Big(\frac{t_2^4}{24} a^{(4)}(t_2) - \frac{t_2^3}{6} a^{(3)}(t_2) - \frac{5t_2^4}{72}\frac{a^{(3)}(t_2)^2}{a^{(2)}(t_2)} - \frac{t_2^2}{3} a^{(2)}(t_2)\Big)\pi^4,$$

and t_1 is the multiple zero of $a(z) - \rho_1$. In this case, the individual relative error is given by

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

Tables 3, 4, and Figure 11 show the data.

Acknowledgments. Part of the numerical computations were performed in the computer center Jürgen Tischer of the mathematics department at Universidad del Valle, Cali-Colombia.

Funding. The research of S.M. Grudsky was supported by CONACYT (Mexico) project "Ciencia de Frontera" FORDECYT-PRONACES/61517/2020 and by Regional Mathematical Center of the Southern Federal University with the support of the Ministry of Science and Higher Education of Russia, Agreement 075-02-2024-1427.

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	2.229×10^{-2}	0.378	4.421×10^{-3}	1.277	1.358×10^{-4}	0.667
32	1.036×10^{-2}	0.341	1.178×10^{-3}	1.283	1.802×10^{-5}	0.647
64	4.969×10^{-3}	0.322	3.045×10^{-4}	1.286	2.322×10^{-6}	0.637
128	2.429×10^{-3}	0.313	7.743×10^{-5}	1.288	2.948×10^{-7}	0.632
256	1.200×10^{-3}	0.308	1.952×10^{-5}	1.289	3.714×10^{-8}	0.630
512	5.968×10^{-4}	0.306	4.902×10^{-6}	1.290	4.661×10^{-9}	0.629
1024	2.975×10^{-4}	0.304	1.228×10^{-6}	1.290	5.837×10^{-10}	0.628
2048	1.485×10^{-4}	0.304	3.073×10^{-7}	1.289	7.304×10^{-11}	0.627

Table 3. The relative and normalized 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	3.492×10^{-2}	0.523	6.599×10^{-3}	1.484	3.604×10^{-4}	1.216
32	1.669×10^{-2}	0.550	1.776×10^{-3}	1.934	4.963×10^{-5}	1.783
64	8.152×10^{-3}	0.529	4.617×10^{-4}	1.950	6.533×10^{-6}	1.794
128	4.027×10^{-3}	0.519	1.177×10^{-4}	1.959	8.388×10^{-7}	1.800
256	2.001×10^{-3}	0.514	2.974×10^{-5}	1.964	1.062×10^{-7}	1.804
512	9.977×10^{-4}	0.511	7.475×10^{-6}	1.967	1.337×10^{-8}	1.806
1024	4.981×10^{-4}	0.510	1.873×10^{-6}	1.968	1.677×10^{-9}	1.807
2048	2.488×10^{-4}	0.509	4.690×10^{-7}	1.969	2.101×10^{-10}	1.807

Table 4. The relative and normalized 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.

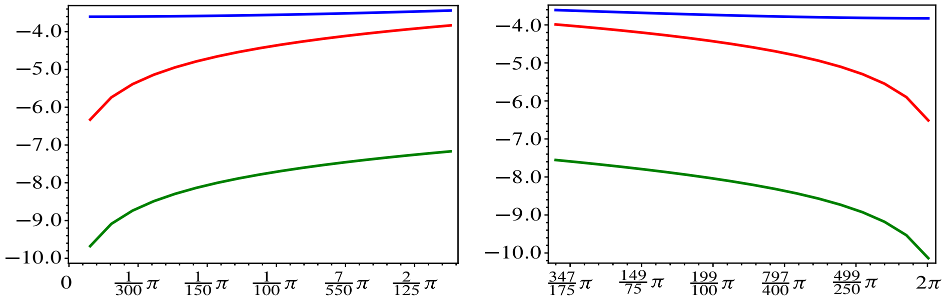


Figure 11. The 10-base logarithm of the individual relative error $\mathrm{RE}_{j,n}^{\mathrm{EXT}(k)}$ for $n = 2048$, using the approximations (5.1) and (5.2) for different values of k: $k = 1$ (blue), $k = 2$ (red), and $k = 3$ (green). The left and right panels show the errors corresponding to the extreme eigenvalues $\lambda_{j,n} = \psi(s_{j,n})$ such that $s_{j,n}$ approaches 0 and 2π, respectively.

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Received 14 August 2024; revised 7 November 2024.

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