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Eigenvalues of Toeplitz matrices emerging from finite differences for certain ordinary differential operators

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We consider Hermitian Toeplitz matrices emerging from finite linear combinations with non-negative coefficients of the differential operators $(-1)^k \mathrm{d}^{2k}/\mathrm{d}x^{2k}$ over the interval $(0,1)$ after discretizing them on a uniform grid of step size $1/(n+1)$. The collective distribution in the Szegő–Weyl sense of the eigenvalues of these matrices as n goes to infinity can be described by GLT theory. However, we focus on the asymptotic behavior of the individual eigenvalues, on both the inner eigenvalues in the bulk and on the extreme eigenvalues. The difficulty of the problem is that not only the order of the matrices depends on n but also their so-called symbols. Our main results are third order asymptotic formulas for the eigenvalues in the case $k \leqslant 2$. These results reveal some basic phenomena one should expect when considering the problem in full generality.

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1. Introduction

Independently of whether we really need them or not, the eigenvalues of a Hermitian matrix are something we want to know. Central finite differences over the uniform grid with stepsize $h = 1/(n+1)$ for the differential operators $-\mathrm{d}^2/\mathrm{d}x^2$ and $\mathrm{d}^4/\mathrm{d}x^4$ on the interval $(0,1)$ with appropriate boundary conditions lead to the symmetric tridiagonal and pentadiagonal $n \times n$ Toeplitz matrices

$$\frac{1}{h^2}\begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & -1 \\ & & & -1 & 2 \end{pmatrix}, \qquad \frac{1}{h^4}\begin{pmatrix} 6 & -4 & 1 & & & & \\ -4 & 6 & -4 & 1 & & & \\ 1 & -4 & 6 & -4 & 1 & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \ddots & \ddots & 1 \\ & & & \ddots & \ddots & \ddots & -4 \\ & & & & 1 & -4 & 6 \end{pmatrix},$$

respectively. More generally, for the operator $(-1)^k \mathrm{d}^{2k}/\mathrm{d}x^{2k}$ we obtain the symmetric $n \times n$ Toeplitz matrix whose first row is

$$\frac{1}{h^{2k}}\left(\binom{2k}{k}, -\binom{2k}{k-1}, \binom{2k}{k-2}, \ldots, (-1)^k \binom{2k}{0}, 0, \ldots, 0 \right) \tag{1.1}$$

$(n-k-1$ zeros). This is a banded matrix, and the so-called symbol associated with a banded symmetric Toeplitz matrix having the first row $(c_0, c_1, c_2, \ldots, c_k, 0, \ldots, 0)$ is the function on the complex unit circle $\mathbb{T}$ defined by

$$a(t) = c_0 + \sum_{\ell=1}^{k} c_k (t^\ell + t^{-\ell}) = c_0 + 2\sum_{\ell=1}^{k} c_k \cos(\ell\sigma), \quad t = \mathrm{e}^{\mathrm{i}\sigma} \in \mathbb{T}.$$

The $n \times n$ Toeplitz matrix with the symbol a is denoted by $T_n(a)$. In the case where the first row is (1.1) we get

$$\begin{aligned} h^{2k} a(t) &= \binom{2k}{k} + \sum_{\ell=1}^{k} (-1)^\ell \binom{2k}{k-\ell} (t^{-\ell} + t^\ell) = (-1/t)^k (1-t)^{2k} \\ &= (1-1/t)^k (1-t)^k = (2 - t - 1/t)^k = (2 - 2\cos(\sigma))^k. \end{aligned}$$

Thus, discretizing the operator $(-1)^k \mathrm{d}^{2k}/\mathrm{d}x^{2k}$ gives us the Toeplitz matrix

$$\frac{1}{h^{2k}} T_n((2 - 2\cos(\sigma))^k), \tag{1.2}$$

and for the operator $\sum_{k=0}^{\mu}(-1)^k\alpha_k \mathrm{d}x^{2k}/\mathrm{d}x^{2k}$ with positive numbers α_k the resulting matrix is

$$T_n\left(\sum_{k=0}^{\mu}\frac{\alpha_k}{h^{2k}}(2-2\cos(\sigma))^k\right)=\alpha_0 I+\frac{\alpha_\mu}{h^{2\mu}}T_n\left(\sum_{k=1}^{\mu}\frac{\alpha_k}{\alpha_\mu}h^{2\mu-2k}(2-2\cos(\sigma))^k\right). \quad (1.3)$$

What can be said about the eigenvalues of Toeplitz matrices we encounter in (1.2) and (1.3)? Clearly, this is eventually the question on the eigenvalues of the Toeplitz matrices $T_n(a_n)$ with

$$a_n(\mathrm{e}^{\mathrm{i}\sigma})=(2-2\cos(\sigma))^{\mu}+\frac{\beta_1}{(n+1)^2}(2-2\cos(\sigma))^{\mu-1} + \cdots + \frac{\beta_{\mu-1}}{(n+1)^{2\mu-2}}(2-2\cos(\sigma)) \quad (1.4)$$

with real numbers $\beta_1,\ldots,\beta_{\mu-1}\geqslant 0$. The difficulty is that not only the order of the matrix $T_n(a_n)$ depends on n but also the symbol a_n.

For $\sigma\in\mathbb{R}$, put $g_n(\sigma)=a_n(\mathrm{e}^{\mathrm{i}\sigma})$. The function g_n is strictly monotonically increasing on $[0,\pi]$ from 0 to its maximum M_n. It results that the eigenvalues of $T_n(a_n)$ all belong to the open interval $(0,M_n)$, and Theorem 4 of [1] tells us that the eigenvalues are all simple. Thus, we may label and order them as follows:

$$\lambda_1(T_n(a_n))<\lambda_2(T_n(a_n))<\ldots<\lambda_n(T_n(a_n)).$$

The collective behavior of the eigenvalues of “pure” Hermitian Toeplitz matrices is described by Szegő’s classical limit theorem [2]. See the books [3–5]. In the case of order dependent symbols such as (1.4) we may have recourse to the theory of GLT sequences (Generalized Locally Toeplitz sequences), which has its origin in the work of Tilli [6] and was developed to a powerful machinery by Serra-Capizzano and his students and colleagues in a series of papers. We refer to the book [7] by Garoni and Serra-Capizzano. For the order dependent symbol (1.4), GLT theory gives

$$\lim_{n\to\infty}\sum_{j=1}^{n}\frac{F(\lambda_j(T_n(a_n)))}{n}=\frac{1}{2\pi}\int_{-\pi}^{\pi}F((2-2\cos(\sigma))^{\mu})\mathrm{d}\sigma=\frac{1}{\pi}\int_{0}^{\pi}F((2-2\cos(\sigma))^{\mu})\mathrm{d}\sigma$$

for every continuous function F on $\mathbb{R}$; see [8, Theorem 1.2] and [9,10] for more details. (Note that $F((2-2\cos(\sigma))^{\mu})$ is an even function.) Thus, the collective distribution of the eigenvalues of $T_n(a_n)$ is independent of the constant $\beta_1,\ldots,\beta_{\mu-1}$ in (1.4). We also see that the eigenvalues of $T_n(a_n)$ eventually fill the segment $[0,4^{\mu}]$ densely and are distributed like the values of the function $(2-2\cos(\sigma))^{\mu}$ for $\sigma\in(0,\pi)$. In other terms, as $n\to\infty$, the fraction of the eigenvalues in some interval (c,d) converges to the fraction of the $\sigma\in(0,\pi)$ for which $(2-2\cos(\sigma))^{\mu}\in(c,d)$.

This paper is devoted to the asymptotic behavior of individual eigenvalues. Let first $\beta_1 = \cdots = \beta_{\mu-1} = 0$, that is, consider $a(\mathrm{e}^{\mathrm{i}\sigma}) = (2 - 2\cos(\sigma))^\mu$. In that case the symbol is independent of n. For $\mu = 1$, the eigenvalues are known exactly:

$$\lambda_j(T_n(2 - 2\cos(\sigma))) = 2 - 2\cos\Big(\frac{\pi j}{n+1}\Big) \quad (j = 1, \ldots, n). \tag{1.5}$$

We obtain in particular that

$$\lambda_1(T_n(2 - 2\cos(\sigma))) = 2 - 2\Big(1 - \frac{1}{2}\frac{\pi^2}{(n+1)^2} + O\Big(\frac{1}{n^4}\Big)\Big) = \frac{\pi^2}{(n+1)^2}(1 + o(1)) \tag{1.6}$$

as $n \to \infty$. For general μ we have

$$\lambda_1(T_n((2 - 2\cos(\sigma))^\mu) = \frac{c_\mu}{(n+1)^{2\mu}}(1 + o(1)) \text{ as } n \to \infty \tag{1.7}$$

with certain constants c_μ. This was proved by Parter [11,12]. From (1.6) we infer that $c_1 = \pi^2$, Parter showed that $c_2 = 500.5467\ldots$ is the fourth power of the smallest positive x satisfying $\cos(x) = 1/\cosh(x)$, and in [13] it was observed that $c_3 = (2\pi)^6 \approx 61529$ and that c_μ grows astronomically fast as $\mu \to \infty$:

$$c_\mu = \sqrt{8\pi\mu}\Big(\frac{4\mu}{\mathrm{e}}\Big)^{2\mu}\Big(1 + O\Big(\frac{1}{\sqrt{\mu}}\Big)\Big) \text{ as } \mu \to \infty.$$

See also the second author's contribution to the article [14].

Toeplitz matrices T_n with nonnegative symbols that do not vanish identically are positive definite, i.e., $(T_n f, f) > 0$ for all nonzero $f \in \mathbb{C}^n$. This implies that the smallest eigenvalue of the matrix given by (1.4) is larger than or equal to the smallest eigenvalue of $T_n((2 - 2\cos(\sigma))^\mu)$ and thus, for sufficiently large n,

$$\lambda_1(T_n(a_n)) \geqslant \lambda_1(T_n((2 - 2\cos(\sigma))^\mu)) \geqslant \frac{c_\mu}{2(n+1)^{2\mu}}. \tag{1.8}$$

Finally, one can show that the largest eigenvalue $\lambda_n(T_n(a_n))$ of $T_n(a_n)$ converges to the maximum of $(2 - 2\cos(\sigma))^\mu$, that is, $\lambda_n(T_n(a_n)) \to 4^\mu$ as $n \to \infty$.

Parter [11,12] and Widom [15] studied not only the smallest and largest eigenvalues of $T_n((2 - 2\cos(\sigma))^\mu)$ but also the so-called extreme eigenvalues. They established in particular analogues of (1.7) for $\lambda_j(T_n((2-2\cos(\sigma))^\mu)$ and $4^\mu - \lambda_{n-j+1}(T_n((2-2\cos(\sigma))^\mu)$ if $j \in \{1, 2, 3, \ldots\}$ is a fixed number. See also pages 256 to 259 of [16].

By asymptotic formulas for the individual eigenvalues of the Toeplitz matrices with the symbol (1.4) we mean formulas of the type

$$\lambda_j(T_n(a_n)) = \sum_{k=0}^{m} \frac{q_k(\pi j/(n+1))}{(n+1)^k} + O\Big(\frac{1}{n^{m+1}}\Big) \text{ as } n \to \infty, \tag{1.9}$$

which should hold uniformly for all indexes j in some prescribed sets S_n, for example, $S_n = \{1, 2, \ldots, 100\}$ or $S_n = \{\lfloor\sqrt{n}\rfloor, \ldots, n\}$, and in which $q_0, \ldots, q_k$ are functions depending only on $\mu, \beta_0, \ldots, \beta_{m-1}$. Unfortunately, we are unable to master the task of proving such formulas in full generality. We therefore restrict ourselves to the case $\mu = 2$ and small m, with the conviction and hope that this case may prepare the ground for understanding more general situations.

If $\mu = 1$ (and hence no betas appear), formula (1.5) says that $\lambda_j(T_n(a)) = g(\pi j/(n+1))$ with $g(\sigma) = a(e^{i\sigma})$. Thus, in this case (1.9) holds with $q_0(\sigma) = g(\sigma)$, $q_k(\sigma) = 0$ for all $k \geqslant 1$, and for arbitrarily large m.

Let us consider the case $\mu = 2$ and $\beta_1 = 0$. In that case formulas of the type (1.9) were derived in [17,18]. We want to mention a delicacy of the matter. Namely, in [18] it is shown that there do not exist continuous functions $q_0, \ldots, q_4\colon [0, \pi] \to \mathbb{R}$ and numbers $C > 0, N \in \mathbb{N}$ such that

$$\left|\lambda_j(T_n(2 - 2\cos(\sigma))^2) - \sum_{k=0}^{4} \frac{q_k(\pi j/(n+1))}{(n+1)^k}\right| \leqslant \frac{C}{(n+1)^5}$$

for every $n \geqslant N$ and every $j \in \{1, \ldots, n\}$. On the other hand, it is proved there that for an arbitrary integer $m \geqslant 0$ there are continuous functions $q_0, \ldots, q_m\colon [0, \pi] \to \mathbb{R}$ and a number $C_m > 0$ such that

$$\left|\lambda_j(T_n(2 - 2\cos(\sigma))^2) - \sum_{k=0}^{m} \frac{q_k(\pi j/(n+2))}{(n+2)^k}\right| \leqslant \frac{C_m}{(n+2)^{m+1}} \tag{1.10}$$

whenever $n \geqslant 1$ and $\frac{m}{2}\log(n) \leqslant j \leqslant n$ and that there is a constant $C > 0$ such that, with the same q_0, q_1, q_2, q_3,

$$\left|\lambda_j(T_n(2 - 2\cos(\sigma))^2) - \sum_{k=0}^{3} \frac{q_k(\pi j/(n+2))}{(n+2)^k}\right| \leqslant \frac{C}{(n+2)^4}$$

for all $n \geqslant 1$ and all $j \in \{1, \ldots, n\}$.

Formula (1.10) concerns what we call inner eigenvalues. For the extreme eigenvalues, it was established in [17,18] that, for every fixed $j = 1, 2, \ldots$,

$$\lambda_j(T_n(2 - 2\cos(\sigma))^2) = \frac{\Lambda_j^4}{(n+2)^4} + O\Big(\frac{1}{n^6}\Big) = \frac{\Lambda_j^4}{(n+1)^4} - \frac{4\Lambda_j^4}{(n+1)^5} + O\Big(\frac{1}{n^6}\Big)$$

with certain constants Λ_j that are solutions of explicitly given nonlinear equations.

Last but not least, we want to emphasize that individual eigenvalue asymptotics for Toeplitz matrices with certain order dependent symbols have also been studied in [8,19]. The symbols treated in paper [19] are of the form

$$|\sigma|^2 + \frac{1}{n^{1/n}}|\sigma|^{2-1/n} + \frac{1}{n^{2/n}}|\sigma|^{2-2/n} + \cdots + \frac{1}{n^{(n-1)/n}}|\sigma|^{2-(n-1)/n}.$$

Such matrix sequences arise in the numerical approximation of distributed-order fractional differential equations. Paper [8] deals with symbols $c(\sigma) + \beta_n d(\sigma)$ where β_n is $1/(n+1)$ or $1/(n+1)^{1/(n+1)}$ and both c and d are so-called simple-loop symbols. These are smooth real functions which move strictly monotonically from the minimum to the maximum and then strictly monotonically back from the maximum to the minimum with nonzero second derivatives at the minimum and the maximum. As the second derivative of $(2-2\cos(\sigma))^2$ vanishes at the minimum, this is not a simple-loop symbol. Moreover, paper [8] contains numerical experiments for the symbol (1.4) with $\mu = 2$. The numerical data obtained there anticipate part of the results we will rigorously prove here.

Throughout the following we let $\beta \geqslant 0$ and

$$a_n(\mathrm{e}^{\mathrm{i}\sigma}) = g_n(\sigma) := (2-2\cos(\sigma))^2 + \frac{\beta}{(n+1)^2}(2-2\cos(\sigma)). \tag{1.11}$$

The main results on the asymptotic behavior of the individual eigenvalues of $T_n(a_n)$ will be stated in Section 2. Our proofs of these results occupy much space. The starting point is the representation of $\lambda_{j,n}$ in the form $\lambda_{j,n} = g_n(s_{j,n})$ and the derivation of a manageable equation for $s_{j,n}$. This is done in Section 3. In Section 4 we prepare the proofs, which will then be given in Section 5. Section 6 contains some selected numerical experiments.

2. Main results

Let $a_n(\mathrm{e}^{\mathrm{i}\sigma}) = g_n(\sigma)$ be the symbol (1.11). Thus, we are dealing with the $n \times n$ pentadiagonal symmetric Toeplitz matrix with $6 + 2\beta/(n+1)^2$ on the main diagonal, $-4-\beta/(n+1)^2$ on the two neighboring diagonals, and 1 on the two next-neighbors. We abbreviate $\lambda_j(T_n(a_n))$ to $\lambda_{j,n}$. We already know that

$$0 < \lambda_{1,n} < \lambda_{2,n} < \ldots < \lambda_{n,n} \tag{2.1}$$

for all n, that $\lambda_{1,n} \geqslant c_2/(2(n+1)^4)$ for all sufficiently large n (recall (1.8)), and that $\lambda_{n,n} \to 16$ as $n \to \infty$.

We consider $\lambda_{j,n}$ as $n \to \infty$. This includes that j may also depend on n, that is, we actually study sequences of the form $\lambda_{j_n,n}$. If $j_n/\sqrt{n} \to 0$, we speak of *extreme eigenvalues*. For example, we have this case for $\lambda_{j,n}$ ($j \geqslant 1$ fixed) or $\lambda_{\lfloor \log(n) \rfloor,n}$. If all we know is that $j_n \to \infty$, we say that we are concerned with *inner eigenvalues*. Notice that with this terminology $\lambda_{\lfloor \log(n) \rfloor,n}$ counts as both extreme and inner. If even $j_n/\sqrt{n} \to \infty$, we refer to $\lambda_{j_n,n}$ as *strictly inner eigenvalues*. For instance, the central eigenvalue $\lambda_{\lfloor n/2 \rfloor,n}$ and the upper eigenvalues $\lambda_{n-k,n}$ ($k \geqslant 0$ fixed) are strictly inner eigenvalues. The eigenvalues $\lambda_{\lfloor \sqrt{n} \rfloor,n}$ are inner but neither extreme nor strictly inner. Herewith our main results.

Table 1
The solutions Λ_j of $x = \pi j + \hat{\eta}(x)$ for $\beta = 3$ and $j = 1, \ldots, 12$ obtained in `Mathematica v.14` with 50 precision digits.

j	Λ_j
1	4.6615957921253250704770283809852175762404777989570329941397516124742
2	7.8294357550286280464178485224978660178640330119617839862874945103994
3	10.9833219742053586857558636944919324013825126356233870292544720164376
4	14.1297083866674503605432431142412867774937568040962386988935124151196
5	17.2737576759361830668285878591532490830030757604197293039667440327106
6	20.4167666752780333653448447261680646408376114269524511082439997941392
7	23.5592496662074388344504002956960693389393620185033287471112478472193
8	26.7014380862110537101045668827905284566037755080621804941835825906322
9	29.8434488417154735629659308097877516397130369383543849499314490373543
10	32.9853461256939590010781633627961538946284882867448068757571468688292
11	36.1271675617397123740954961433504885555276833628962867845017802482102
12	39.2689363835010789993399482697496623249078649039256071620370774499135

Theorem 2.1. ***(Extreme eigenvalues)*** *For each fixed j the equation*

$$x = \pi j + \hat{\eta}(x)$$

with

$$\hat{\eta}(x) := 2 \arctan\left(\frac{x(x^2+\beta)^{-1/2} \sinh\sqrt{x^2+\beta} - \sin(x)}{\cosh\sqrt{x^2+\beta} - \cos(x)}\right)$$

possesses a unique solution $x \in \mathbb{R}$. Denote this solution by Λ_j. If $\{j_n\}$ is a sequence satisfying $j_n/\sqrt{n} \to 0$, then

$$\lambda_{j,n} = g_n\left(\frac{\Lambda_j}{n+1}\right) + \hat{R}_{j,n}$$

for all n and $j \leqslant j_n$, where $|\hat{R}_{j,n}| \leqslant Cj^5/n^5$ with some constant C independent of j and n.

We remark that $g_n(\Lambda_j/(n+1))$ is of the order j^4/n^4.

A key point in the previous theorem is that we arrived at an equation not depending on n, namely $x = \pi j + \hat{\eta}(x)$. This technique is reminiscent of the one used in the classical works [11,12,15,20], where the values Λ_j came from the eigenvalues of a certain integral operator. More recently, a similar approach was used in [21].

The equation $x = \pi j + \hat{\eta}(x)$ can easily and almost instantly be solved with any equation solver, for instance `FindRoot` in `Mathematica v.14`. See Table 1. Notice that, for instance, if $j_n = \lfloor \log_{10}(n) \rfloor$, then the first 12 values of Λ_j are sufficient to go up to $n = 10^{12}$.

Theorem 2.2. ***(Inner eigenvalues)*** *For $s, \sigma \in (0, \pi)$, put*

$$\eta_{\text{INN}}(s) := 2\arctan\left(\frac{\sin(s)}{2 - 2\cos(s) + \sqrt{1-\cos(s)}\sqrt{3-\cos(s)}}\right) \tag{2.2}$$

and

$$q_0(\sigma) := 4(1-\cos(\sigma))^2, \quad q_1(\sigma) := 8\sin(\sigma)(1-\cos(\sigma))\eta_{\text{INN}}(\sigma).$$

Let $\{j_n\}$ be a sequence converging to infinity. Then, with $\sigma_{j,n} := \pi j/(n+1)$,

$$\lambda_{j,n} = q_0(\sigma_{j,n}) + \frac{q_1(\sigma_{j,n})}{n+1} + L_{j,n}$$

for all n and $j \geqslant j_n$. We have $L_{j,n} = O(j^2/n^4)$ as $n \to \infty$ uniformly in $j \geqslant j_n$, which means that there is a constant C independent of j and n such that $|L_{j,n}| \leqslant Cj^2/n^4$ for all $j \geqslant j_n$.

Theorem 2.3. ***(Strictly inner eigenvalues)*** *Let η_{INN}, q_0, q_1, $\sigma_{j,n}$ be as in the previous theorem. In addition, put*

$$q_2(\sigma) := 2(1-\cos(\sigma))\{\beta + 4\sin(\sigma)\eta_{\text{INN}}(\sigma)\eta'_{\text{INN}}(\sigma) + 2\eta^2_{\text{INN}}(\sigma)(1+2\cos(\sigma))\}.$$

Let $\{j_n\}$ be a sequence satisfying $j_n/\sqrt{n} \to \infty$. We have

$$\lambda_{j,n} = q_0(\sigma_{j,n}) + \frac{q_1(\sigma_{j,n})}{n+1} + \frac{q_2(\sigma_{j,n})}{(n+1)^2} + K_{j,n}$$

for all n and $j \geqslant j_n$. Given such a sequence $\{j_n\}$, there is a constant C independent of j and n such that $|K_{j,n}| \leqslant Cj/n^4$ for all $j \geqslant j_n$.

When $\beta = 0$, the symbol in (1.11) coincides with the one studied in [17]. We here want in particular to understand the influence of the parameter β on the expansion of $\lambda_{j,n}$. For the inner eigenvalues, the previous two theorems tell us that β is only affecting the term with denominator $(n+1)^2$, and hence we can say that its influence is relatively small in this case. However, for the extreme eigenvalues, Theorem 2.1 reveals that β is affecting Λ_j directly; see Fig. 1. Consequently, its influence is stronger in this case.

3. The equations behind the main results

Recall that we order the eigenvalues of $\lambda_{j,n}$ of $T_n(a_n)$ as in (2.1). These lie all in $(0, M_n)$ with $M_n = 16 + 4\beta/(n+1)^2$. The strict monotony of $g_n\colon (0,\pi) \to (0, M_n)$ implies that the equation $\lambda_{j,n} = g_n(s_{j,n})$ has a unique solution $s_{j,n} \in (0,\pi)$ and that

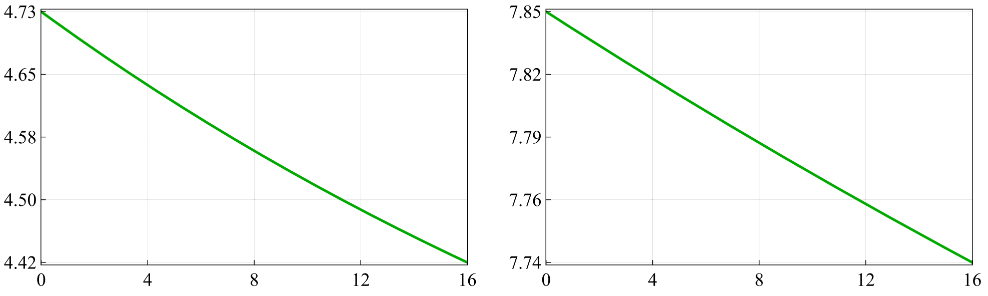

Fig. 1. The variation of the parameter Λ_j in Theorem 2.1, with respect to $\beta \in [0, 16]$ for $j = 1$ (left) and $j = 2$ (right).

$$s_{1,n} < s_{2,n} < \ldots < s_{n,n}.$$

Our goal is to obtain asymptotic expansions for the "abscissas" $s_{j,n}$. These will then give the desired asymptotics for the eigenvalues $\lambda_{j,n}$. We therefore start with studying the equation $\lambda = g_n(s)$.

We define the auxiliary function $b_n \colon [0, 2\pi] \times [0, \pi] \to \mathbb{R}$ by

$$b_n(\mathrm{e}^{\mathrm{i}\sigma}, s) := \frac{g_n(\sigma) - g_n(s)}{\cos(s) - \cos(\sigma)}.$$

As the following lemma shows, this function is much nicer than it appears at the first glance.

Lemma 3.1. *We have*

$$b_n(t, s) = -2t^{-1} + 4 + 2\gamma_n^2(s) - 2t$$

with $\gamma_n(s) = \sqrt{4\sin^2(s/2) + \beta/(n+1)^2}$.

Proof. Taking $t = \mathrm{e}^{\mathrm{i}\sigma}$ we obtain

$$\begin{aligned} b_n(t, s) &= -\frac{g_n(\sigma) - g_n(s)}{\cos(\sigma) - \cos(s)} \\ &= -\frac{(2 - 2\cos(\sigma))^2 - (2 - 2\cos(s))^2}{\cos(\sigma) - \cos(s)} - \frac{\beta}{(n+1)^2} \cdot \frac{(2 - 2\cos(\sigma)) - (2 - 2\cos(s))}{\cos(\sigma) - \cos(s)} \\ &= 4(2 - \cos(\sigma) - \cos(s)) + \frac{2\beta}{(n+1)^2}, \end{aligned}$$

and it remains to notice that $\cos(\sigma) = (t + t^{-1})/2$ and $2 - 2\cos(s) = 4\sin^2(s/2)$. □

Thus, $b_n(\mathrm{e}^{\mathrm{i}\sigma}, s) = b_0 - 4\cos(\sigma)$ with a constant $b_0 \geqslant 4$ (depending on s and n). This implies that, for each s, the symmetric tridiagonal Toeplitz matrix $T_m(b_n(\cdot, s))$ is invertible for every m and n; see, e.g., [16, Sections 2.2 or 10.1]. The inverse of $T_m(b_n(\cdot, s))$ will be denoted by $T_m^{-1}(b_n(\cdot, s))$. We consider $T_{n+2}(b_n(\cdot, s))$ and think of this matrix as acting on the linear space of polynomials $c_0 + c_1 t + \cdots + c_{n+1} t^{n+1}$ $(t \in \mathbb{T})$ in the natural fashion. Let $\chi_k(t) := t^k$. Then

$$\Theta_n(t, s) := [T_{n+2}^{-1}(b_n(\cdot, s))\chi_0](t), \tag{3.1}$$

is a well-defined polynomial of the above form for each s and n. We may write

$$\Theta_n(t, s) = \theta_0(s) + \theta_1(s)t + \cdots + \theta_{n+1}(s)t^{n+1}, \tag{3.2}$$

where the coefficients $\theta_0(s), \ldots, \theta_{n+1}(s)$ are the entries of the first column of the matrix $T_{n+2}^{-1}(b_n(\cdot, s))$, which is real.

Theorem 3.2. *A number $\lambda = g_n(s)$ is an eigenvalue of $T_n(a_n)$ if and only if there is a $j \in \mathbb{Z}$ such that*

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

where $H_n(s) := 2 \arg \Theta_n(\mathrm{e}^{\mathrm{i}s}, s)$.

Proof. Let $P_m \colon L^2(\mathbb{T}) \to L^2(\mathbb{T})$ be the projection defined by

$$P_m \sum_{k=-\infty}^{\infty} f_k t^k := \sum_{k=0}^{m-1} f_k t^k$$

and recall that we may identify the range of P_m with $\mathbb{C}^m$. We are looking for the values $\lambda \in (0, M_n)$ for which $T_n(a_n)X = \lambda X$ has non-zero solutions $X \in P_n L^2(\mathbb{T})$. Using $\lambda = g_n(s)$ and switching to the variable s, the previous equation becomes

$$T_n(a_n - g_n(s))X = 0, \tag{3.3}$$

which can be written in polynomial language as

$$P_n(a_n - g_n(s))X = P_n b_n(\cdot, s)p(\cdot, s)X = 0,$$

where $p(t, s) = p(\mathrm{e}^{\mathrm{i}\sigma}, s) := \cos(s) - \cos(\sigma) = -t^{-1}/2 + \cos(s) - t/2$. Equivalently

$$(P_{n+1} - P_1)b_n(\cdot, s)\chi_1 p(\cdot, s)X = 0. \tag{3.4}$$

The function X is a polynomial of degree $n - 1$ in the variable t, and hence we can write $X(t) = x_0 + x_1 t + \cdots + x_{n-1} t^{n-1}$. The product $b_n(t, s)\chi_1(t)p(t, s)X(t)$ equals

$$x_0 t^{-1} + (x_1 - \beta_n x_0) + \cdots + (x_{n-2} - \beta_n x_{n-1})t^{n+1} + x_{n-1} t^{n+2}, \tag{3.5}$$

where $\beta_n := 4 + \beta/(n+1)^2$. Indeed, we have $b_n(t,s) = -2t^{-1} + 4 + 2\gamma_n^2(s) - 2t$ and $\gamma_n^2(s) = 4\sin^2(s/2) + \beta/(n+1)^2 = 2 - 2\cos(s) + \beta/(n+1)^2$ by Lemma 3.1, and hence $b_n(t,s)\chi_1(t)p(t,s)X(t)$ equals

$$\begin{aligned}
&-2\big(1-(2+\gamma_n^2(s))t+t^2\big)\Big(-\frac{1}{2t}+\cos(s)-\frac{1}{2}t\Big)\big(x_0+x_1t+\cdots+x_{n-1}t^{n-1}\big)\\
&=\big(1-(\beta_n-2\cos(s))t+t^2\big)\Big(\frac{1}{t}-2\cos(s)+t\Big)\big(x_0+x_1t+\cdots+x_{n-1}t^{n-1}\big)\\
&=\frac{x_0}{t}+\big\{-2\cos(s)x_0+x_1-(\beta_n-2\cos(s))x_0\big\}+\cdots\\
&\quad+\big\{-(\beta_n-2\cos(s))x_{n-1}-2\cos(s)x_{n-1}+x_{n-2}\big\}t^{n+1}+x_{n-1}t^{n+2}\\
&=\frac{x_0}{t}+x_1-\beta_nx_0+\cdots+(x_{n-2}-\beta_nx_{n-1})t^{n+1}+x_{n-1}t^{n+2}.
\end{aligned}$$

Equation (3.4) tells us that the coefficients of t^k with $k = 1, \ldots, n$ in (3.5) are zero. We so arrive at the equation

$$b_n(t,s)\chi_1(t)p(t,s)X(t) = x_0t^{-1} + (x_1-\beta_nx_0) + (x_{n-2}-\beta_nx_{n-1})t^{n+1} + x_{n-1}t^{n+2}. \tag{3.6}$$

We are now ready to solve (3.3) for X. Take

$$Y := P_{n+2}b_n(\cdot,s)\chi_1p(\cdot,s)X.$$

Since $P_{n+2}\chi_1p(\cdot,s)X = \chi_1p(\cdot,s)X$, we get $Y = T_{n+2}(b_n(\cdot,s))\chi_1p(\cdot,s)X$ or equivalently, $T_{n+2}^{-1}(b_n(\cdot,s))Y = \chi_1p(\cdot,s)X$. In addition, (3.6) implies that $Y(t) = y_0 + y_{n+1}t^{n+1}$ with $y_0 = x_1 - \beta_nx_0$ and $y_{n+1} = x_{n-2} - \beta_nx_{n-1}$. This gives

$$T_{n+2}^{-1}(b_n(\cdot,s))Y = y_0[T_{n+2}^{-1}(b_n(\cdot,s))\chi_0](t) + y_{n+1}[T_{n+2}^{-1}(b_n(\cdot,s))\chi_{n+1}](t).$$

Therefore

$$tp(t,s)X(t) = y_0[T_{n+2}^{-1}(b_n(\cdot,s))\chi_0](t) + y_{n+1}[T_{n+2}^{-1}(b_n(\cdot,s))\chi_{n+1}](t). \tag{3.7}$$

We now employ the previous expression to derive a relationship between s and the function Θ_n given by (3.1) which does not involve the coefficients y_0 and y_{n+1}. Consider the flip operator W_n given by

$$W_n\sum_{k=0}^{n-1} f_kt^k := \sum_{k=0}^{n-1} f_{n-1-k}t^k.$$

Using the well-known identity $W_{n+2}T_{n+2}(b_n(\cdot,s))W_{n+2} = T_{n+2}(\tilde{b}_n(\cdot,s))$, where $\tilde{b}_n(t,s) := b_n(t^{-1},s)$, we easily obtain

$$[T_{n+2}^{-1}(b_n(\cdot,s))\chi_{n+1}](t) = t^{n+1}\Theta_n(t^{-1},s).$$

Hence (3.7) can be written as

$$tp(t,s)X(t) = y_0\Theta_n(t,s) + y_{n+1}t^{n+1}\Theta_n(t^{-1},s),$$

which combined with $p(\mathrm{e}^{\mathrm{i}s},s) = p(\mathrm{e}^{-\mathrm{i}s},s) = 0$ yields

$$0 = y_0\Theta_n(\mathrm{e}^{\mathrm{i}s},s) + y_{n+1}\mathrm{e}^{\mathrm{i}(n+1)s}\Theta_n(\mathrm{e}^{-\mathrm{i}s},s),$$
$$0 = y_0\Theta_n(\mathrm{e}^{-\mathrm{i}s},s) + y_{n+1}\mathrm{e}^{-\mathrm{i}(n+1)s}\Theta_n(\mathrm{e}^{\mathrm{i}s},s).$$

The previous linear system has non-trivial solutions if and only if its determinant is zero, that is,

$$\mathrm{e}^{\mathrm{i}(n+1)s} = \pm\frac{\Theta_n(\mathrm{e}^{\mathrm{i}s},s)}{\Theta_n(\mathrm{e}^{-\mathrm{i}s},s)}.$$

Finally, the theorem is a direct consequence of the previous equation together with the equality $\Theta_n(t,s) = \overline{\Theta_n(t^{-1},s)}$, which follows from (3.2). □

Theorem 3.2 provides us with an implicit and exact equation for the eigenvalues of $T_n(a_n)$. However, the term $H_n(s)$ is difficult to handle, and hence we expand it to obtain a simpler expression. It turns out that such an expansion depends on the collective behavior of n and s. We will take the argument of $\Theta_n(\mathrm{e}^{\mathrm{i}s},s)$ in $(-\pi,\pi]$, will denote by $s = s^*_{j,n}$ the solution of $(n+1)s = \pi j + H_n(s)$, and Theorem 5.1 will show that $s^*_{j,n}$ coincides with the $s_{j,n}$ introduced above. (Note that in Theorem 3.2 the choice of the argument is not yet specified.) Getting the asymptotics of $s^*_{j,n}$ requires asymptotic analysis of $H_n(s)$ in the cases $sn \to \infty$ and $s^2n \to 0$, which will eventually lead to the following two theorems.

Theorem 3.3. ***(Inner and strictly inner eigenvalues)*** *Denote by $s_{j,n}$ the numbers given by $g_n(s_{j,n}) = \lambda_{j,n}$. Let $\eta_{\text{INN}}(s)$ be the function (2.2), put*

$$p_0(\sigma) := \sigma, \quad p_1(\sigma) := \eta_{\text{INN}}(\sigma), \quad p_2(\sigma) := \eta_{\text{INN}}(\sigma)\eta'_{\text{INN}}(\sigma),$$

and abbreviate $\pi j/(n+1)$ to $\sigma_{j,n}$.

(i) *If $j = j_n \to \infty$, then*

$$(n+1)s_{j,n} = \pi j + \eta_{\text{INN}}(s_{j,n}) + E_{j,n}$$

and there is a constant C independent of n such that $|E_{j_n,n}| \leqslant C/j_n^2$ for all sufficiently large n.

(ii) *If $j = j_n \to \infty$, we have*

$$s_{j,n} = p_0(\sigma_{j,n}) + \frac{p_1(\sigma_{j,n})}{n+1} + F_{j,n}$$

where $|F_{j_n,n}| \leqslant C/n^2$ *for all sufficiently large* n *with a constant* C *independent on* n.

(iii) *If even* $j/\sqrt{n} = j_n/\sqrt{n} \to \infty$, *then*

$$s_{j,n} = p_0(\sigma_{j,n}) + \frac{p_1(\sigma_{j,n})}{n+1} + \frac{p_2(\sigma_{j,n})}{(n+1)^2} + G_{j,n}$$

and there is a constant C *independent of* n *such that* $|G_{j_n,n}| \leqslant C/(j_n^2 n)$ *whenever* $j_n/\sqrt{n}$ *is large enough.*

Theorem 3.4. ***(Extreme eigenvalues)*** *If* $j/\sqrt{n} = j_n/\sqrt{n} \to 0$ *as* $n \to \infty$, *then the numbers* $s_{j,n}$ *given by* $g_n(s_{j,n}) = \lambda_{j,n}$ *satisfy*

$$(n+1)s_{j,n} = \pi j + \eta_{\mathrm{EXT}}(s_{j,n}) + R_{j,n}$$

where

$$\eta_{\mathrm{EXT}}(s) := 2\arctan\left(\frac{\left(1+\frac{\beta}{(n+1)^2s^2}\right)^{-1/2}\sinh\sqrt{(n+1)^2s^2+\beta} - \sin((n+1)s)}{\cosh\sqrt{(n+1)^2s^2+\beta} - \cos((n+1)s)}\right)$$

and there is a constant C *independent of* n *such that* $|R_{j_n,n}| \leqslant Cj_n^2/n$ *whenever* $j_n/\sqrt{n}$ *is sufficiently small.*

We are now going to prove Theorems 3.3, 3.4 and subsequently we will prove Theorems 2.1, 2.2, 2.3. The proofs require some technical preliminaries. These are the subject of the following section.

4. Technical matters

According to (3.1), $\Theta_n(t,s)$ is the solution of

$$T_{n+2}(b_n(\cdot,s))\Theta_n(\cdot,s) = \chi_0,$$

that is, $P_{n+2}b_n(t,s)P_{n+2}\Theta_n(t,s) = P_{n+2}b_n(t,s)\Theta_n(t,s) = 1$. In addition, Lemma 3.1 and (3.2) tell us that $b_n(t,s)\Theta_n(t,s)$ is the polynomial $-2\theta_0(s)t^{-1} + \cdots - 2\theta_{n+1}(s)t^{n+2}$. Consequently, we may actually write

$$b_n(t,s)\Theta_n(t,s) = -u_0(s)t^{-1} + 1 - u_{n+2}(s)t^{n+2},$$

where $u_0(s) = 2\theta_0(s)$ and $u_{n+2}(s) = 2\theta_{n+1}(s)$. Since b_n is bounded away from zero, we can solve the previous equation for Θ_n, obtaining

$$\Theta_n(t,s) = \frac{-u_0(s)t^{-1} + 1 - u_{n+2}(s)t^{n+2}}{b_n(t,s)} = \frac{-u_0(s)t^{-1} + 1 - u_{n+2}(s)t^{n+2}}{-2t^{-1} + 4 + 2\gamma_n^2(s) - 2t}.$$

Thus, $H_n(s) = 2\arg\Theta_n(\mathrm{e}^{\mathrm{i}s}, s)$ equals

$$H_n(s) = 2\arg\left(\frac{1 - u_0(s)\mathrm{e}^{-\mathrm{i}s} - u_{n+2}(s)\mathrm{e}^{\mathrm{i}(n+2)s}}{b_n(t,s)}\right). \tag{4.1}$$

Notice now that $\Theta_n(t,s)$ is a polynomial of degree $n+2$ in the variable t. This implies that the zeros of the denominator above must be zeros of the numerator also. Since the zeros of the denominator are

$$t_{1,2} = 1 + \frac{1}{2}\gamma_n^2(s) \pm \gamma_n(s)\sqrt{1 + \frac{1}{4}\gamma_n^2(s)}, \tag{4.2}$$

we arrive at the system

$$\begin{aligned} t_1^{-1}u_0(s) + t_1^{n+2}u_{n+2}(s) &= 1, \\ t_2^{-1}u_0(s) + t_2^{n+2}u_{n+2}(s) &= 1, \end{aligned}$$

which, by Cramer's rule together with the equality $t_1 t_2 = 1$, gives

$$\begin{aligned} u_0(s) &= \frac{t_1^{n+2} - t_2^{n+2}}{t_1^{-1}t_2^{-1}(t_1^{n+3} - t_2^{n+3})} = \frac{t_1^{n+2} - t_2^{n+2}}{t_1^{n+3} - t_2^{n+3}}, \\ u_{n+2}(s) &= \frac{t_2^{-1} - t_1^{-1}}{t_1^{-1}t_2^{-1}(t_1^{n+3} - t_2^{n+3})} = \frac{t_1 - t_2}{t_1^{n+3} - t_2^{n+3}}. \end{aligned} \tag{4.3}$$

We can now simplify (4.1) further. From (4.2) we know that t_1 and t_2 are real, and hence by (4.3), so are u_0 and u_{n+2}. In addition, Lemma 3.1 tells us that for each $s \in [0, \pi]$, the function $b_n(\cdot, s)$ is positive. This shows that the real part of the term in parentheses in (4.1) is

$$\{1 - u_0(s)\cos(s) - u_{n+2}(s)\cos((n+2)s)\}/b_n(t,s),$$

while its imaginary part equals

$$\{u_0(s)\sin(s) - u_{n+2}(s)\sin((n+2)s)\}/b_n(t,s).$$

Hence, we may take

$$H_n(s) = 2\arctan\left(\frac{u_0(s)\sin(s) - u_{n+2}(s)\sin((n+2)s)}{1 - u_0(s)\cos(s) - u_{n+2}(s)\cos((n+2)s)}\right), \tag{4.4}$$

and we will work with this choice of the argument throughout the following. See Fig. 2.

Our next goal is to expand H_n in such a way that the main term is independent of n. It turns out that such an expansion depends on the joint behavior of n and s. We therefore split the task. The following Lemmas 4.2 and 4.3 show the resulting asymptotic expressions for H_n in different cases. But first we need the following technical result.

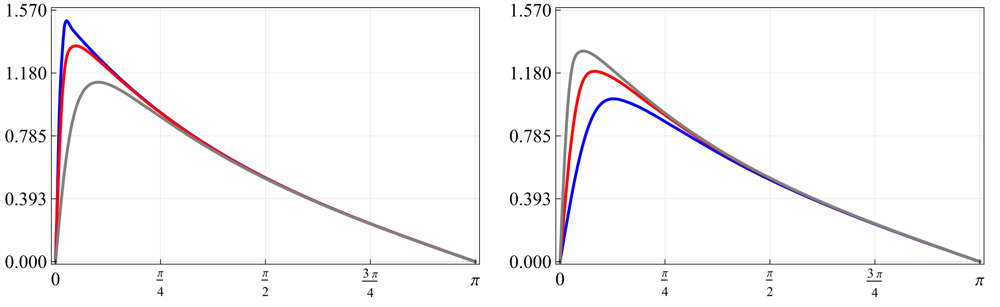

Fig. 2. The function H_n in (4.4). Left: for $n = 50$ and $\beta = 0$ (blue), $\beta = 10$ (red), and $\beta = 100$ (gray). Right: for $\beta = 10$ and $n = 10$ (blue), $n = 20$ (red), and $n = 40$ (gray). (For interpretation of the colors in the figure, the reader is referred to the web version of this article.)

Lemma 4.1. *As $sn \to \infty$, we have*

$$t_{1,2} = \kappa_{\pm}(s) + O\Big(\frac{1}{sn^2}\Big),$$

where $t_{1,2}$ is given by (4.2) and

$$\kappa_{\pm}(s) := 1 + 2\sin^2(s/2) \pm 2\sin(s/2)\sqrt{1+\sin^2(s/2)}.$$

In addition, $t_2 < 1 - s/8$ for all sufficiently large n.

Proof. Note that

$$\begin{aligned} t_{1,2} &= 1 + \frac{1}{2}\gamma_n^2(s) \pm \gamma_n(s)\sqrt{1+\frac{1}{4}\gamma_n^2(s)} \\ &= 1 + 2\sin^2\left(\frac{s}{2}\right) + O\Big(\frac{1}{n^2}\Big) \pm \sqrt{\Big\{4\sin^2\left(\frac{s}{2}\right) + O\Big(\frac{1}{n^2}\Big)\Big\}\Big\{1+\sin^2\left(\frac{s}{2}\right) + O\Big(\frac{1}{n^2}\Big)\Big\}}, \end{aligned}$$

and use $1+\sin^2(s/2) \geqslant 1$ and $4\sin^2(s/2) \geqslant (4/\pi^2)s^2$ to get

$$\begin{aligned} t_{1,2} &= 1 + 2\sin^2\left(\frac{s}{2}\right) \pm 2\sin\left(\frac{s}{2}\right)\sqrt{1+O\Big(\frac{1}{s^2n^2}\Big)}\sqrt{1+\sin^2\left(\frac{s}{2}\right)}\sqrt{1+O\Big(\frac{1}{n^2}\Big)} + O\Big(\frac{1}{n^2}\Big) \\ &= 1 + 2\sin^2\left(\frac{s}{2}\right) \pm 2\sin\left(\frac{s}{2}\right)\sqrt{1+\sin^2\left(\frac{s}{2}\right)}\Big\{1+O\Big(\frac{1}{s^2n^2}\Big)\Big\} + O\Big(\frac{1}{n^2}\Big) \\ &= \kappa_{\pm}(s) + O\Big(\frac{1}{sn^2}\Big), \end{aligned}$$

where $\kappa_{\pm}(s) = 1 + 2\sin^2(s/2) \pm 2\sin(s/2)\sqrt{1+\sin^2(s/2)}$, proving the first assertion.

To prove the second assertion, take the minus sign above and write

$$t_2 - 1 < -2\sin\left(\frac{s}{2}\right)\Big\{\sqrt{1+\sin^2\left(\frac{s}{2}\right)} - \sin\left(\frac{s}{2}\right)\Big\} + O\Big(\frac{1}{sn^2}\Big)$$

$$< -2\sin\left(\frac{s}{2}\right)\left\{\sqrt{1+\sin^2\left(\frac{s}{2}\right)}+\sin\left(\frac{s}{2}\right)\right\}^{-1}+O\Big(\frac{1}{sn^2}\Big),$$

which in combination with $\sqrt{1+\sin^2(s/2)}+\sin(s/2) < \sqrt{2}+1 < 4$ and $\sin(s/2) > s/\pi$ for $s \in [0,\pi]$, produces

$$t_2 - 1 < -\frac{1}{2}\sin\left(\frac{s}{2}\right)+O\Big(\frac{1}{sn^2}\Big) < -\frac{s}{2\pi}+O\Big(\frac{1}{sn^2}\Big).$$

Since $sn \to \infty$, the error term is arbitrarily small, hence the proof is finished after noticing that $-s/(2\pi) < -s/8$. □

Lemma 4.2. *We have $H_n(s) = \eta_{\text{INN}}(s) + O(1/(s^2n^2))$ as $sn \to \infty$, where $\eta_{\text{INN}}(s)$ is given by (2.2).*

Proof. We use (4.4), which is an exact equation for H_n. But first, we need to expand the involved terms u_0 and u_{n+2}. Note that $t_1t_2 = 1$ to obtain $t_2/t_1 = t_2^2$. From (4.3) we can write

$$u_0(s) = \frac{1}{t_1}\cdot\frac{1-(t_2/t_1)^{n+2}}{1-(t_2/t_1)^{n+3}} = t_2\cdot\frac{1-t_2^{2(n+2)}}{1-t_2^{2(n+3)}}.$$

Because $s \in (0,\pi]$, we have $\gamma_n(s) \in (0,\sqrt{4+\beta/2})$ for every $n \geqslant 1$. Then from basic calculus and (4.2), we know that t_2 is a decreasing function of $\gamma_n(s)$ such that $t_2 \in (9/100,1)$ for every $n \geqslant 1$. Consequently, $\lim_{n\to\infty} u_0(s) = t_2$, but this is not enough for our purposes. We need to obtain an accurate bound for $u_0(s)-t_2$ and proceed as follows. Notice that $\log(1-x) < -x$ for $x \in (0,1)$. From Lemma 4.1 we know that $t_2 < 1-s/8$. Hence

$$t_2^{2(n+2)} = t_2^4 \mathrm{e}^{2n\log(t_2)} = O(\mathrm{e}^{2n\log(1-s/8)}) = O(\mathrm{e}^{-sn/4}),$$

that is, $t_2^{2(n+2)} = O(\mathrm{e}^{-sn/4})$.

We are ready to estimate u_0. Using that $t_2 < 1$ for every $n \geqslant 1$ and $s \in (0,\pi]$, we can write

$$u_0(s) = t_2\cdot\{1+O(\mathrm{e}^{-sn/4})\} = t_2 + O(\mathrm{e}^{-sn/4}). \tag{4.5}$$

A similar calculation produces

$$u_{n+2}(s) = O(\mathrm{e}^{-sn/8}) \quad \text{as} \quad sn \to \infty, \tag{4.6}$$

and we have what it is necessary to prove the lemma. Combining (4.5) and (4.6) with (4.4) we obtain

$$\begin{aligned} H_n(s) &= 2\arctan\left(\frac{\{t_2 + O(\mathrm{e}^{-sn/4})\}\sin(s) - O(\mathrm{e}^{-sn/8})}{1 - \{t_2 + O(\mathrm{e}^{-sn/4})\}\cos(s) - O(\mathrm{e}^{-sn/8})}\right) \\ &= 2\arctan\left(\frac{t_2\sin(s) + O(\mathrm{e}^{-sn/8})}{1 - t_2\cos(s) + O(\mathrm{e}^{-sn/8})}\right) \\ &= 2\arctan\left(\frac{t_2\sin(s)}{1 - t_2\cos(s)} + O\Big(\frac{1}{s\mathrm{e}^{sn/8}}\Big)\right) \\ &= 2\arctan\left(\frac{\sin(s)}{t_1 - \cos(s)} + O\Big(\frac{1}{s\mathrm{e}^{sn/8}}\Big)\right). \end{aligned} \tag{4.7}$$

From Lemma 4.1 we know that $t_1 = \kappa_+(s) + O(1/(sn^2))$ where

$$\begin{aligned} \kappa_+(s) &= 1 + 2\sin^2\left(\frac{s}{2}\right) + 2\sin\left(\frac{s}{2}\right)\sqrt{1 + \sin^2\left(\frac{s}{2}\right)}, \\ &= 2 - \cos(s) + \sqrt{1 - \cos(s)}\sqrt{3 - \cos(s)}. \end{aligned} \tag{4.8}$$

Hence, it is easy to see that $\kappa_+(s) - \cos(s)$ is bounded away from zero and has order $O(s)$. Consequently,

$$\begin{aligned} \frac{\sin(s)}{t_1 - \cos(s)} &= \frac{\sin(s)}{\kappa_+(s) - \cos(s) + O(1/(sn^2))} \\ &= \frac{\sin(s)}{\{\kappa_+(s) - \cos(s)\}\{1 + O(1/(s^2n^2))\}} \\ &= \frac{\sin(s)}{\kappa_+(s) - \cos(s)}\left\{1 + O\Big(\frac{1}{s^2n^2}\Big)\right\} \\ &= \frac{\sin(s)}{\kappa_+(s) - \cos(s)} + O\Big(\frac{1}{s^2n^2}\Big). \end{aligned} \tag{4.9}$$

Finally, combining (4.7) with (4.9), we obtain

$$\begin{aligned} H_n(s) &= 2\arctan\left(\frac{\sin(s)}{\kappa_+(s) - \cos(s)} + O\Big(\frac{1}{s^2n^2}\Big)\right) \\ &= 2\arctan\left(\frac{\sin(s)}{\kappa_+(s) - \cos(s)}\right) + O\Big(\frac{1}{s^2n^2}\Big). \end{aligned}$$

This together with (4.8) finishes the proof. □

Lemma 4.3. *Assume $s \geqslant \varepsilon/n$ for some $\varepsilon > 0$. Then $H_n(s) = \eta_{\mathrm{EXT}}(s) + O(s^2 n)$ as $s^2 n \to 0$ with $\eta_{\mathrm{EXT}}(s)$ as in Theorem 3.4.*

Proof. The assumption $s \geqslant \varepsilon/n$ implies $1/n^2 = O(s^2)$ and hence

$$\gamma_n(s) = \sqrt{4\sin^2\left(\frac{s}{2}\right) + \frac{\beta}{(n+1)^2}} = \sqrt{s^2 + O(s^4) + O(s^2)} = O(s),$$

as $s \to 0$. We begin by expanding $t_{1,2}$. Due to (4.2) we can write

$$
\begin{aligned}
t_{1,2} &= 1 \pm \gamma_n(s) + \frac{1}{2}\gamma_n^2(s) + O(\gamma_n^3(s)) \\
&= 1 \pm \gamma_n(s) + \frac{1}{2}\gamma_n^2(s) + O(s^3),
\end{aligned}
$$

as $s \to 0$, which implies that $\log(t_{1,2}) = \pm\gamma_n(s) + O(s^3)$. We then have

$$
\begin{aligned}
t_{1,2}^{n+2} &= t_{1,2} t_{1,2}^{n+1} \\
&= t_{1,2} \exp\{(n+1)\log(t_{1,2})\} \\
&= \{1 \pm \gamma_n(s) + O(s^2)\} \exp\left\{\pm (n+1)\gamma_n(s) + O(s^3 n)\right\} \\
&= \{1 \pm \gamma_n(s) + O(s^2)\} \mathrm{e}^{\pm(n+1)\gamma_n(s)} \mathrm{e}^{O(s^3 n)} \\
&= \{1 \pm \gamma_n(s) + O(s^2)\} \mathrm{e}^{\pm(n+1)\gamma_n(s)} (1 + O(s^3 n)),
\end{aligned} \tag{4.10}
$$

as $s \to 0$. A similar calculation produces

$$
t_{1,2}^{n+3} = (1 \pm 2\gamma_n(s)) \mathrm{e}^{\pm(n+1)\gamma_n(s)} + O(s^3 n). \tag{4.11}
$$

We now use (4.3) to derive asymptotic expressions for u_0 and u_{n+2}. By (4.10) and (4.11), we can write

$$
\begin{aligned}
u_0(s) &= \frac{(1+\gamma_n(s))\mathrm{e}^{(n+1)\gamma_n(s)} - (1-\gamma_n(s))\mathrm{e}^{-(n+1)\gamma_n(s)} + O(s^3 n)}{(1+2\gamma_n(s))\mathrm{e}^{(n+1)\gamma_n(s)} - (1-2\gamma_n(s))\mathrm{e}^{-(n+1)\gamma_n(s)} + O(s^3 n)} \\
&= \frac{\tanh((n+1)\gamma_n(s)) + \gamma_n(s)}{\tanh((n+1)\gamma_n(s)) + 2\gamma_n(s)} + O(s^3 n) \\
&= 1 - \frac{\gamma_n(s)}{\tanh((n+1)\gamma_n(s)) + 2\gamma_n(s)} + O(s^3 n) \\
&= 1 - \frac{\gamma_n(s)}{\tanh((n+1)\gamma_n(s))} + O(s^3 n).
\end{aligned}
$$

Similarly, using that

$$
\cosh((n+1)\gamma_n(s)) = O(\mathrm{e}^{sn}), \quad O(s) + O(s^3 n) = s\{O(1) + O(s^2 n)\} = O(s),
$$

and $\sinh((n+1)\gamma_n(s)) = O(\mathrm{e}^{sn})$, we get

$$
\begin{aligned}
u_{n+2}(s) &= \frac{2\gamma_n(s) + O(s^3 n)}{2\sinh((n+1)\gamma_n(s)) + 4\gamma_n(s)\cosh((n+1)\gamma_n(s)) + O(s^3 n)} \\
&= \frac{\gamma_n(s) + O(s^3 n)}{\sinh((n+1)\gamma_n(s)) + O(s)}
\end{aligned}
$$

$$= \frac{\gamma_n(s)\{1 + O(s^2 n)\}}{\sinh((n+1)\gamma_n(s))\{1 + O(s)\}}$$
$$= \frac{\gamma_n(s)}{\sinh((n+1)\gamma_n(s))}\{1 + O(s^2 n)\},$$

which because of $\gamma_n(s)/\sinh((n+1)\gamma_n(s)) = O(1/n) = O(s)$ can be simplified to

$$u_{n+2}(s) = \frac{\gamma_n(s)}{\sinh((n+1)\gamma_n(s))} + O(s^3 n).$$

Note again that $b_n(\cdot, s)$ is positive for each $s \in (0, \pi]$. Combining the previous expressions with (4.1) this time, we obtain

$$\begin{aligned} H_n(s) &= 2\arg\{1 - u_0(s)\mathrm{e}^{-\mathrm{i}s} - u_{n+2}(s)\mathrm{e}^{\mathrm{i}(n+2)s}\} \\ &= 2\arg\{1 - u_0(s)(1 - \mathrm{i}s + O(s^2)) - u_{n+2}(s)(1 + \mathrm{i}s + O(s^2))\mathrm{e}^{\mathrm{i}(n+1)s}\} \\ &= 2\arg\left\{\frac{\gamma_n(s)}{\tanh((n+1)\gamma_n(s))} - \frac{\gamma_n(s)\cos((n+1)s)}{\sinh((n+1)\gamma_n(s))}\right. \\ &\quad \left. +\mathrm{i}\left(s - \frac{\gamma_n(s)\sin((n+1)s)}{\sinh((n+1)\gamma_n(s))}\right) + O(s^3 n)\right\}. \end{aligned}$$

Since $s \leqslant \gamma_n(s)$ for sufficiently small s, this can be simplified to

$$\begin{aligned} H_n(s) &= 2\arctan\left(\frac{\frac{s}{\gamma_n(s)}\sinh((n+1)\gamma_n(s)) - \sin((n+1)s) + O(s^2 n)}{\cosh((n+1)\gamma_n(s)) - \cos((n+1)s) + O(s^2 n)}\right) \\ &= 2\arctan\left(\frac{\left\{\frac{s}{\gamma_n(s)}\sinh((n+1)\gamma_n(s)) - \sin((n+1)s)\right\}\{1 + O(s^2 n)\}}{\left\{\cosh((n+1)\gamma_n(s)) - \cos((n+1)s)\right\}\{1 + O(s^2 n)\}}\right) \\ &= 2\arctan\left(\frac{\frac{s}{\gamma_n(s)}\sinh((n+1)\gamma_n(s)) - \sin((n+1)s)}{\cosh((n+1)\gamma_n(s)) - \cos((n+1)s)}\right) + O(s^2 n). \end{aligned}$$

Finally, we need to get rid of the term $\gamma_n(s)$. Taking into account that

$$\frac{s}{\gamma_n(s)} = \left(1 + \frac{\beta}{(n+1)^2 s^2}\right)^{-1/2} + O(s^2)$$
$$(n+1)\gamma_n(s) = \sqrt{(n+1)^2 s^2 + \beta} + O(s^2),$$

we arrive at

$$H_n(s) = 2\arctan\left(\frac{\left(1 + \frac{\beta}{(n+1)^2 s^2}\right)^{-1/2}\sinh\sqrt{(n+1)^2 s^2 + \beta} - \sin((n+1)s)}{\cosh\sqrt{(n+1)^2 s^2 + \beta} - \cos((n+1)s)}\right) + O(s^2 n),$$

which gives us the lemma. $\square$

5. Proofs of the main results

We have $\lambda_{j,n} = g_n(s_{j,n})$ with $s_{1,n} < s_{2,n} < \ldots < s_{n,n}$ and Theorem 3.2 implies that $(n+1)s_{j,n} - \pi j = H_n(s_{j,n})$ for an appropriate choice of the argument in $H_n(s_{j,n}) = 2\arg\Theta(\mathrm{e}^{\mathrm{i}s_{j,n}}, s_{j,n})$. In (4.4) we specified $H_n(s)$ to take values in $(-\pi, \pi]$. The following theorem shows that this is the right choice.

Theorem 5.1. *Let $H_n(s)$ be given by (4.4). Then the equation $(n+1)s - \pi j = H_n(s)$ has a unique solution $s = s^*_{j,n}$ for all n and all $j \in \{1, 2, \ldots, n\}$. If n is large enough, we have $s^*_{j,n} = s_{j,n}$ for all $j \in \{1, 2, \ldots, n\}$.*

Proof. Put $F_n(s) := (n+1)s - H_n(s)$. Then our equation reads

$$F_n(s) = \pi j. \tag{5.1}$$

From (4.4) we infer that H_n is continuous on $[0, \pi]$ and that $H_n(0) = H_n(\pi) = 0$; recall Fig. 2. For $1 \leqslant j \leqslant n$, we have $F_n(0) = 0 < j\pi$ and $F_n(\pi) = (n+1)\pi > j\pi$. The intermediate value theorem therefore tells us that (5.1) has a solution $s^*_{j,n} \in (0, \pi)$. It is obvious that $s^*_{j,n} \neq s^*_{k,n}$ for $j \neq k$. Thus, we get at least n different solutions as j changes from 1 to n. By Theorem 3.2, each solution gives an eigenvalue $g_n(s^*_{j,n})$, and hence there cannot be more than n solutions. It follows that $s^*_{j,n}$ is the unique solution to (5.1).

It remains to show that $s^*_{j,n} = s_{j,n}$. Recall that g_n is strictly monotonically increasing on $[0, \pi]$. Because $g_n(s^*_{j,n})$ is an eigenvalue, we must have $s^*_{j,n} = s_{k,n}$ for some $k \in \{1, \ldots, n\}$. Thus we only need to show the ordering $s^*_{1,n} < s^*_{2,n} < \ldots < s^*_{n,n}$.

From (1.8) with $\mu = 2$ we deduce that $\lambda_{1,n} \geqslant C/(n+1)^4$ with some constant C for all n. Thus, for all j, n we have $g_n(s^*_{j,n}) \geqslant \lambda_{1,n} \geqslant C/(n+1)^4$. If K is large enough, then

$$K\Big((s^*_{j,n})^4 + \frac{1}{(n+1)^2}(s^*_{j,n})^2\Big) \geqslant g_n(s^*_{j,n}) \geqslant \frac{C}{(n+1)^4},$$

and writing $s^*_{j,n} = \tau_{j,n}/(n+1)$, we get $\tau^4_{j,n} + \tau^2_{j,n} \geqslant C/K$. This shows that there is a constant $\varepsilon > 0$ such that $\tau_{j,n} \geqslant \varepsilon$ for all j, n. In summary, $s^*_{j,n} \geqslant \varepsilon/n$ for all j, n.

Consider the set $\Omega_\varepsilon := \{(s, n)\colon s \in (0, \pi),\ n \in \mathbb{N},\ sn \geqslant \varepsilon\}$. We want to show that there is an n such that $H_n(s) \in [0, \pi]$ for all $(s, n) \in \Omega_\varepsilon$ with $n > N$.

Let first $sn \to \infty$ with $s \in (0, \pi)$. From Lemma 4.2 we know that

$$H_n(s) = \eta_{\text{INN}}(s) + O\Big(\frac{1}{s^2 n^2}\Big),$$

where $\eta_{\text{INN}}(s) = 2\arctan(\sin(s)/\{\kappa_+(s) - \cos(s)\})$. Because $\sin(s)/\{\kappa_+(s) - \cos(s)\} > 0$ for $s \in (0, \pi)$, there is a sufficiently large M such that $H_n(s) \in [0, \pi]$ for every (s, n) with $s \in (0, \pi)$ and $sn > M$.

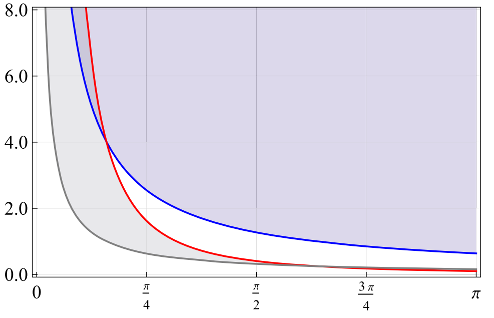

Fig. 3. The region Ω_ε for $\varepsilon = 1/2$, $M = 2$, and $\delta = 1$. The blue, red, and gray curves are the hyperbolas $n = M/s$, $n = \delta/s^2$, and $n = \varepsilon/s$, respectively. The light-blue and light-gray shaded regions correspond to the (s, n) with $sn > M$ and $s^2 n < \delta$, respectively. In this case $M^2/\delta = 4$. (For interpretation of the colors in the figure, the reader is referred to the web version of this article.)

Assume now that $s^2 n \to 0$ with $s > \varepsilon/n$. Lemma 4.3 shows that

$$H_n(s) = \eta_{\text{EXT}}(s) + O(s^2 n)$$

with $\eta_{\text{EXT}}(s)$ as in Theorem 3.4. To simplify the calculation, consider the new variable $x = (n+1)s$ and write $\eta_{\text{EXT}}(s) = \hat{\eta}(x)$ with

$$\hat{\eta}(x) := 2\arctan\left(\frac{x(x^2+\beta)^{-1/2}\sinh\sqrt{x^2+\beta} - \sin(x)}{\cosh\sqrt{x^2+\beta} - \cos(x)}\right). \tag{5.2}$$

Since $\cosh(x) > \cos(x)$ for $x > 0$, the denominator in (5.2) is positive. Because $\sinh(x)/x$ is a strictly increasing function on $(0, \pi)$ and $\sinh(x) > \sin(x)$ for $x > 0$, we obtain

$$\frac{\sinh\sqrt{x^2+\beta}}{\sqrt{x^2+\beta}} > \frac{\sinh(x)}{x} > \frac{\sin(x)}{x}$$

for $x > 0$, which implies that the numerator in (5.2) is also positive. Therefore $\hat{\eta}(x) \in (0, \pi)$ for $x > 0$, and we conclude that $H_n(s) \in [0, \pi]$ for every (s, n) with $s \in (0, \pi)$ and $s^2 n < \delta$ for some sufficiently small $\delta > 0$.

We just proved that $H_n(s) \in [0, \pi]$ for the (s, n) satisfying $sn > M$ or $s^2 n < \delta$ with $s > \varepsilon/n$, that is, for the $(s, n) \in \Omega_\varepsilon$ lying above the hyperbola $n = M/s$ or between the hyperbolas $n = \varepsilon/s$ and $n = \delta/s^2$. This is either the entire Ω_ε, in which case $H_n(s) \in [0, \pi]$ on all of Ω_ε, or the hyperbolas $n = M/s$ and $n = \delta/s^2$ intersect. In the latter case, $H_n(s) \in [0, \pi]$ on the $(s, n) \in \Omega_\varepsilon$ with $n > M^2/\delta$. See Fig. 3.

We are now ready to finish the proof. We know that $(n+1)s^*_{j,n} - H_n(s^*_{j,n}) = \pi j$ and $(n+1)s^*_{j+1,n} - H_n(s^*_{j+1,n}) = \pi(j+1)$. It follows that

$$s^*_{j+1,n} - s^*_{j,n} = \frac{\pi + H_n(s^*_{j+1,n}) - H_n(s^*_{j,n})}{n+1},$$

and since $H_n(s^*_{j+1,n}) - H_n(s^*_{j,n}) \in [-\pi, \pi]$, we get that $s^*_{j+1,n} \geqslant s^*_{j,n}$. Since they must be different, we actually obtain $s^*_{j+1,n} > s^*_{j,n}$ for all sufficiently large n and all $j = 1, \dots, n-1$. $\square$

Proof of Theorem 3.3. Theorem 5.1 tells us that $(n+1)s_{j,n} = \pi j + H_n(s_{j,n})$ with $H_n(s_{j,n})$ in $(-\pi, \pi)$ (and actually in $(0, \pi)$). It follows that $ns_{j,n} \to \infty$ and $s_{j,n} \geqslant cj/n$ with some constant c independent of j and n. We can therefore apply Lemma 4.2 to conclude that

$$(n+1)s_{j,n} = \pi j + \eta_{\text{INN}}(s_{j,n}) + O\left(\frac{1}{n^2 s_{j,n}^2}\right) = \pi j + \eta_{\text{INN}}(s_{j,n}) + O\left(\frac{1}{j^2}\right),$$

which proves part (i).

To prove parts (ii) and (iii), consider the function $U_n(s) := (n+1)s - \eta_{\text{INN}}(s)$. Basic calculus shows that this is a strictly increasing and infinitely differentiable function on $(0, \pi]$. Moreover, $\lim_{s \to 0+} U_n(s) < 2 < \pi j$ and $U_n(\pi) = (n+1)\pi > \pi j$. Hence, the intermediate value theorem implies that $U_n(s) = j\pi$ has a unique solution $\hat{s}_{j,n}$ in $(0, \pi)$.

Intuitively, the points $s_{j,n}$ and $\hat{s}_{j,n}$ must be "close" to each other. To estimate the distance between them, we proceed as follows. We have

$$(n+1)s_{j,n} - H_n(s_{j,n}) = \pi j, \quad (n+1)\hat{s}_{j,n} - \eta_{\text{INN}}(\hat{s}_{j,n}) = \pi j, \tag{5.3}$$

and hence $(n+1)|s_{j,n} - \hat{s}_{j,n}| = |H_n(s_{j,n}) - \eta_{\text{INN}}(\hat{s}_{j,n})|$. Since $H_n(s) = \eta_{\text{INN}}(s) + O(1/(s^2 n^2))$ by Lemma 4.2 and since $\eta_{\text{INN}}(s_{j,n}) - \eta_{\text{INN}}(\hat{s}_{j,n}) = \eta'_{\text{INN}}(\xi)(s_{j,n} - \hat{s}_{j,n})$, for some ξ between $s_{j,n}$ and $\hat{s}_{j,n}$, we get

$$(n+1)|s_{j,n} - \hat{s}_{j,n}| \leqslant M|s_{j,n} - \hat{s}_{j,n}| + O\left(\frac{1}{s_{j,n}^2 n^2}\right)$$

with some constant M, which implies that

$$|s_{j,n} - \hat{s}_{j,n}| = O\left(\frac{1}{s_{j,n}^2 n^3}\right) = O\left(\frac{1}{j^2 n}\right). \tag{5.4}$$

To simplify the writing, we now use the abbreviation $h = 1/(n+1)$. From the second equation in (5.3) we obtain that $\hat{s}_{j,n} = \sigma_{j,n} + \eta_{\text{INN}}(\hat{s}_{j,n})h$, where $\sigma_{j,n} = \pi j h$, and this equation can be solved by iteration as follows. We first write $\hat{s}_{j,n} = \sigma_{j,n} + O(h)$ and iterate to get

$$\begin{aligned} \hat{s}_{j,n} &= \sigma_{j,n} + \eta_{\text{INN}}\{\sigma_{j,n} + O(h)\}h \\ &= \sigma_{j,n} + \eta_{\text{INN}}(\sigma_{j,n})h + O(h^2). \end{aligned}$$

The latter equality together with (5.4) completes the proof of part (ii). A second iteration yields

$$\begin{aligned}\hat{s}_{j,n} &= \sigma_{j,n} + \eta_{\text{INN}}\{\sigma_{j,n} + \eta_{\text{INN}}(\sigma_{j,n})h + O(h^2)\}h \\ &= \sigma_{j,n} + \eta_{\text{INN}}(\sigma_{j,n})h + \eta_{\text{INN}}(\sigma_{j,n})\eta'_{\text{INN}}(\sigma_{j,n})h^2 + O(h^3).\end{aligned}$$

If $j/\sqrt{n} \to \infty$, then

$$O\Big(\frac{1}{j^2 n}\Big) + O(h^3) = O\Big(\frac{1}{j^2 n}\Big) + O\Big(\frac{1}{n^3}\Big) = O\Big(\frac{1}{j^2 n}\Big),$$

which in combination with (5.4) completes the prof of part (iii). (Notice that a third iteration is pointless because it will produce a new term of order $O(h^3)$.) □

Proof of Theorem 2.2. We have $\lambda_{j,n} = g_n(s_{j,n})$. Thus, with $h := 1/(n+1)$ the asymptotics of Theorem 3.3(ii) gives

$$\begin{aligned}\lambda_{j,n} &= g_n\{\sigma_{j,n} + \eta_{\text{INN}}(\sigma_{j,n})h + O(1/(j^2 n)) + O(1/n^2)\} \\ &= g_n(\sigma_{j,n}) + g'_n(\sigma_{j,n})\{\eta_{\text{INN}}(\sigma_{j,n})h + O(1/(j^2 n)) + O(1/n^2)\} + O(g''_n(\sigma_{j,n})/n^2),\end{aligned}$$

and as

$$\begin{aligned}g_n(\sigma_{j,n}) &= 4(1-\cos(\sigma_{j,n}))^2 + O(j^2/n^4) = O(j^4/n^4), \\ g'_n(\sigma_{j,n}) &= 2\sin(\sigma_{j,n})\{\beta h^2 + 4(1-\cos(\sigma_{j,n}))\} = O(j^3/n^3), \\ g''_n(\sigma_{j,n}) &= 2(\beta h^2 + 4)\cos(\sigma_{j,n}) + 8(1 - 2\cos^2(\sigma_{j,n})) = O(j^2/n^2),\end{aligned}$$

we arrive at the assertion. □

Proof of Theorem 2.3. Proceeding as in the previous proof but this time with the asymptotic expansion provided by Theorem 3.3(iii), we obtain

$$\begin{aligned}\lambda_{j,n} &= g_n\{\sigma_{j,n} + \eta_{\text{INN}}(\sigma_{j,n})h + \eta_{\text{INN}}(\sigma_{j,n})\eta'_{\text{INN}}(\sigma_{j,n})h^2 + O(h^3)\} \\ &= g_n(\sigma_{j,n}) + g'_n(\sigma_{j,n})\{\eta_{\text{INN}}(\sigma_{j,n})h + \eta_{\text{INN}}(\sigma_{j,n})\eta'_{\text{INN}}(\sigma_{j,n})h^2\} \\ &\quad + \frac{g''_n(\sigma_{j,n})}{2}\eta_{\text{INN}}(\sigma_{j,n})^2 h^2 + O(g'''_n(\sigma_{j,n})h^3),\end{aligned}$$

which after noticing that $g'''_n(\sigma_{j,n}) = 2\sin(\sigma_{j,n})\{4 - \beta h^2 - 16\cos(\sigma_{j,n})\} = O(j/n)$ and some straightforward computation gives the assertion. □

Proof of Theorem 3.4. From Theorem 5.1 we infer that there are positive constants ε and C such that $\varepsilon/n \leqslant s_{1,n} \leqslant s_{j,n} \leqslant Cj/n$ for all sufficiently large n and all $j \in \{1, 2, \ldots, n\}$. If $j/\sqrt{n} \to 0$, this implies in particular that $s^2_{j,n} n = O(j^2/n)$ converges to 0. We can therefore have recourse to Lemma 4.3 to obtain that

$$(n+1)s_{j,n} = \pi j + \eta_{\text{EXT}}(s_{j,n}) + O(s^2_{j,n} n) = \pi j + \eta_{\text{EXT}}(s_{j,n}) + O(j^2/n),$$

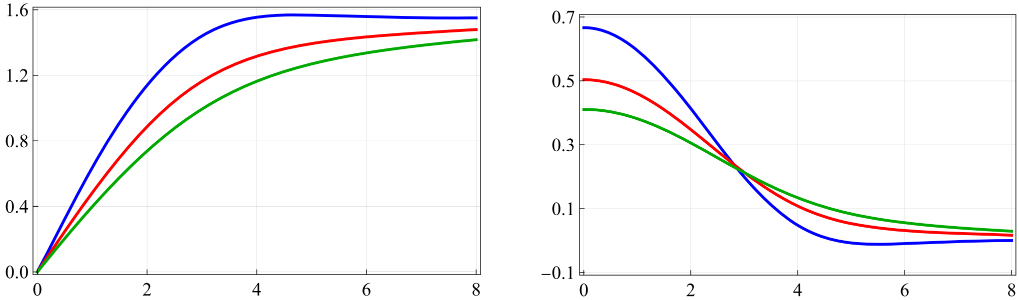

Fig. 4. Left: The function $\hat{\eta}$ for $\beta = 0$ (blue), $\beta = 10$ (red), and $\beta = 20$ (green). Right: The same for $\hat{\eta}'$. (For interpretation of the colors in the figure, the reader is referred to the web version of this article.)

as desired. □

Proof of Theorem 2.1. We proceed following the idea of [21]. As in the proof of Theorem 5.1, consider the variable $x_j = (n+1)s_{j,n}$. Theorem 3.4 says

$$x_j = \pi j + \hat{\eta}(x_j) + O(j^2/n). \tag{5.5}$$

Recall that $j \leqslant j_n$ and that $\{j_n\}$ is a sequence satisfying $j_n/\sqrt{n} \to 0$. Consider equation (5.5) without the error term, that is,

$$x = \pi j + \hat{\eta}(x). \tag{5.6}$$

One can show that the function $\hat{\eta}$ is in C^∞, strictly increasing with $0 < \hat{\eta}'(x) \leqslant 1 - \delta < 1$, and bounded for $x \geqslant 0$. See Fig. 4. Since $\hat{\eta}(0) = 0$ and $\lim_{x\to\infty} \hat{\eta}(x) = \pi/2$, the intermediate value theorem implies that for each $j \geqslant 0$ the equation (5.6) has a unique solution Λ_j.

Combining (5.5) with (5.6) we obtain

$$|x_j - \Lambda_j| \leqslant |\hat{\eta}(x_j) - \hat{\eta}(\Lambda_j)| + O(j^2/n) = |\hat{\eta}'(\zeta_j)||x_j - \Lambda_j| + O(j^2/n),$$

for some ζ_j between x_j and Λ_j. Since $0 < \hat{\eta}'(x) \leqslant 1 - \delta < 1$, we conclude that

$$|x_j - \Lambda_j| \leqslant (1/\delta)O(j^2/n) = O(j^2/n).$$

Taking into account that $x_j = (n+1)s_{j,n}$ we have $\lambda_{j,n} = g_n(s_{j,n}) = g_n(x_j/(n+1))$. Let $\lambda^*_{j,n} = g_n(\Lambda_j/(n+1))$ and note that

$$|\lambda_{j,n} - \lambda^*_{j,n}| = \left|g_n\Big(\frac{x_j}{n+1}\Big) - g_n\Big(\frac{\Lambda_j}{n+1}\Big)\right| = \left|g_n'\Big(\frac{\xi_j}{n+1}\Big)\right|\frac{|x_j - \Lambda_j|}{n+1}$$

for some ξ_j between x_j and Λ_j. Since $g_n'(s) = O(s^3) + O(s/n^2)$ as $s \to 0$ and $O(\xi_j) = O(\Lambda_j) = O(j)$ we arrive at

$$|\lambda_{j,n} - \lambda^*_{j,n}| = O\Big(\frac{\xi_j^3}{n^3}\Big)O\Big(\frac{j^2}{n^2}\Big) = O\Big(\frac{j^5}{n^5}\Big).$$

Thus, $\lambda_{j,n} = \lambda^*_{j,n} + O(j^5/n^5) = g_n(\Lambda_j/(n+1)) + O(j^5/n^5)$. □

6. Numerical experiments

6.1. Inner eigenvalues

The choice $j_n = \lfloor\sqrt{n}\rfloor$ is the critical case because it is neither extreme nor strictly inner. Theorem 2.2 provides us only with a second order asymptotics. Let us nevertheless try the third order asymptotics of Theorem 2.3 with the function q_2 given there. Thus, for $m = 1, 2, 3$ and $j \geqslant j_n = \lfloor\sqrt{n}\rfloor$, let $\lambda^{\text{INN}(m)}_{j,n}$ be the m-term approximation.

$$\lambda^{\text{INN}(m)}_{j,n} := \sum_{k=0}^{m-1} \frac{q_k(\sigma_{j,n})}{(n+1)^k}.$$

As for the errors, we consider the individual absolute error

$$\text{AE}^{\text{INN}(m)}_{j,n} := |\lambda_{j,n} - \lambda^{\text{INN}(m)}_{j,n}|,$$

which according to Theorem 2.2 is $O(j^3/n^4)$ for $m = 1$ and $O(j^2/n^4)$ for $m = 2$, while Theorem 2.3 suggests that it should be $O(j/n^4)$ for $m = 3$. We also consider the individual normalized errors

$$\text{NE}^{\text{INN}(1)}_{j,n} := \text{AE}^{\text{INN}(1)}_{j,n}\,\frac{n^4}{j^3}, \quad \text{NE}^{\text{INN}(2)}_{j,n} := \text{AE}^{\text{INN}(2)}_{j,n}\,\frac{n^4}{j^2}, \quad \text{NE}^{\text{INN}(3)}_{j,n} := \text{AE}^{\text{INN}(3)}_{j,n}\,\frac{n^4}{j}$$

and the individual relative errors

$$\text{RE}^{\text{INN}(m)}_{j,n} := \frac{|\lambda_{j,n} - \lambda^{\text{INN}(m)}_{j,n}|}{|\lambda_{j,n}|} = \frac{\text{AE}^{\text{INN}(m)}_{j,n}}{|\lambda_{j,n}|}. \tag{6.1}$$

Finally, we compute the respective maximum errors

$$\text{AE}^{\text{INN}(m)}_{n} := \max\{\text{AE}^{\text{INN}(m)}_{j,n} : j \geqslant j_n\},$$
$$\text{NE}^{\text{INN}(m)}_{n} := \max\{\text{NE}^{\text{INN}(m)}_{j,n} : j \geqslant j_n\},$$
$$\text{RE}^{\text{INN}(m)}_{n} := \max\{\text{RE}^{\text{INN}(m)}_{j,n} : j \geqslant j_n\},$$

Figs. 5 and 6, and Table 2 show the data.

Fig. 6 tells us that the approximation $\lambda^{\text{INN}(m)}_{j,n}$ is indeed good for the eigenvalues with $j \geqslant j_n$ but not acceptable for smaller j. This figure confirms Theorem 2.2 numerically and reveals that the range of eigenvalues with an asymptotics as in Theorem 2.3 is probably larger than what we call strictly inner eigenvalues.

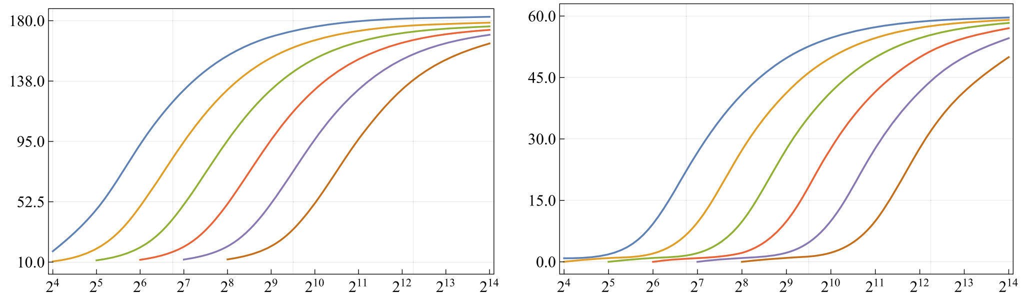

Fig. 5. The individual normalized inner errors $\mathrm{NE}_{j,n}^{\mathrm{INN}(m)}$ for selected values of j and $n = 2^4$–2^{14}. In each figure, from left to right $j = 8, 16, 32, 64, 128, 256$. The left and right figures show the case $m = 2$ and $m = 3$, respectively.

Table 2
The maximum relative, absolute, and normalized errors $\mathrm{RE}_n^{\mathrm{INN}(m)}$, $\mathrm{AE}_n^{\mathrm{INN}(m)}$, and $\mathrm{NE}_n^{\mathrm{INN}(m)}$, respectively, for the eigenvalues of $T_n(a_n)$, $m = 1, 2, 3$, $\beta = 3$, and different values of n.

n	$\mathrm{RE}_n^{\mathrm{INN}(1)}$	$\mathrm{AE}_n^{\mathrm{INN}(1)}$	$\mathrm{NE}_n^{\mathrm{INN}(1)}$	$\mathrm{RE}_n^{\mathrm{INN}(2)}$	$\mathrm{AE}_n^{\mathrm{INN}(2)}$	$\mathrm{NE}_n^{\mathrm{INN}(2)}$	$\mathrm{RE}_n^{\mathrm{INN}(3)}$	$\mathrm{AE}_n^{\mathrm{INN}(3)}$	$\mathrm{NE}_n^{\mathrm{INN}(3)}$
16	2.49×10^{-1}	2.68×10^{-1}	9.23×10^{1}	2.90×10^{-2}	4.09×10^{-2}	4.31×10^{1}	2.53×10^{-4}	1.83×10^{-4}	2.21×10^{0}
32	2.45×10^{-1}	1.33×10^{-1}	1.34×10^{2}	2.75×10^{-2}	1.10×10^{-2}	7.56×10^{1}	3.07×10^{-4}	2.61×10^{-5}	4.21×10^{0}
64	1.72×10^{-1}	6.63×10^{-2}	1.49×10^{2}	1.35×10^{-2}	2.84×10^{-3}	9.29×10^{1}	1.68×10^{-4}	4.42×10^{-6}	9.28×10^{0}
128	1.40×10^{-1}	3.31×10^{-2}	1.66×10^{2}	8.83×10^{-3}	7.21×10^{-4}	1.16×10^{2}	1.32×10^{-4}	7.78×10^{-7}	1.90×10^{1}
256	1.03×10^{-1}	1.65×10^{-2}	1.76×10^{2}	4.83×10^{-3}	1.82×10^{-4}	1.31×10^{2}	6.26×10^{-5}	1.02×10^{-7}	2.72×10^{1}
512	7.95×10^{-2}	8.25×10^{-3}	1.83×10^{2}	2.86×10^{-3}	4.56×10^{-5}	1.45×10^{2}	3.20×10^{-5}	1.29×10^{-8}	3.56×10^{1}
1024	5.68×10^{-2}	4.13×10^{-3}	1.87×10^{2}	1.46×10^{-3}	1.14×10^{-5}	1.53×10^{2}	1.23×10^{-5}	1.62×10^{-9}	4.14×10^{1}
2048	4.15×10^{-2}	2.06×10^{-3}	1.89×10^{2}	7.79×10^{-4}	2.86×10^{-6}	1.60×10^{2}	5.02×10^{-6}	2.03×10^{-10}	4.64×10^{1}
4096	2.98×10^{-2}	1.03×10^{-3}	1.91×10^{2}	4.00×10^{-4}	7.15×10^{-7}	1.64×10^{2}	1.90×10^{-6}	2.55×10^{-11}	4.99×10^{1}
8192	2.15×10^{-2}	5.16×10^{-4}	1.92×10^{2}	2.08×10^{-4}	1.79×10^{-7}	1.68×10^{2}	7.26×10^{-7}	3.19×10^{-12}	5.27×10^{1}
16384	1.53×10^{-2}	2.58×10^{-4}	1.93×10^{2}	1.05×10^{-4}	4.47×10^{-8}	1.70×10^{2}	2.63×10^{-7}	3.98×10^{-13}	5.46×10^{1}

6.2. *Extreme eigenvalues*

To employ the results in Theorem 2.1, we need the numbers Λ_j. Table 1 shows the first 12 of them. Let $\lambda_{j,n}^{\mathrm{EXT}}$ be the approximation of $\lambda_{j,n}$ given by Theorem 2.1, that is,

$$\lambda_{j,n}^{\mathrm{EXT}} := g_n\Big(\frac{\Lambda_j}{n+1}\Big),$$

and for the errors consider the individual absolute error

$$\mathrm{AE}_{j,n}^{\mathrm{EXT}} := |\lambda_{j,n} - \lambda_{j,n}^{\mathrm{EXT}}|,$$

which according to Theorem 2.1 is $O(j^5/n^5)$ when $n \to \infty$. As above, we also consider the individual normalized and relative errors,

$$\mathrm{NE}_{j,n}^{\mathrm{EXT}} := \mathrm{AE}_{j,n}^{\mathrm{EXT}}\,\frac{n^5}{j^5}, \quad \mathrm{RE}_{j,n}^{\mathrm{EXT}} := \frac{\mathrm{AE}_{j,n}^{\mathrm{EXT}}}{|\lambda_{j,n}|}. \tag{6.2}$$

Fig. 7 and Table 3 show the data. In Fig. 7 we plotted the relative errors for the first 17 extreme eigenvalues when using the approximation given by Theorem 2.1 and, moreover,

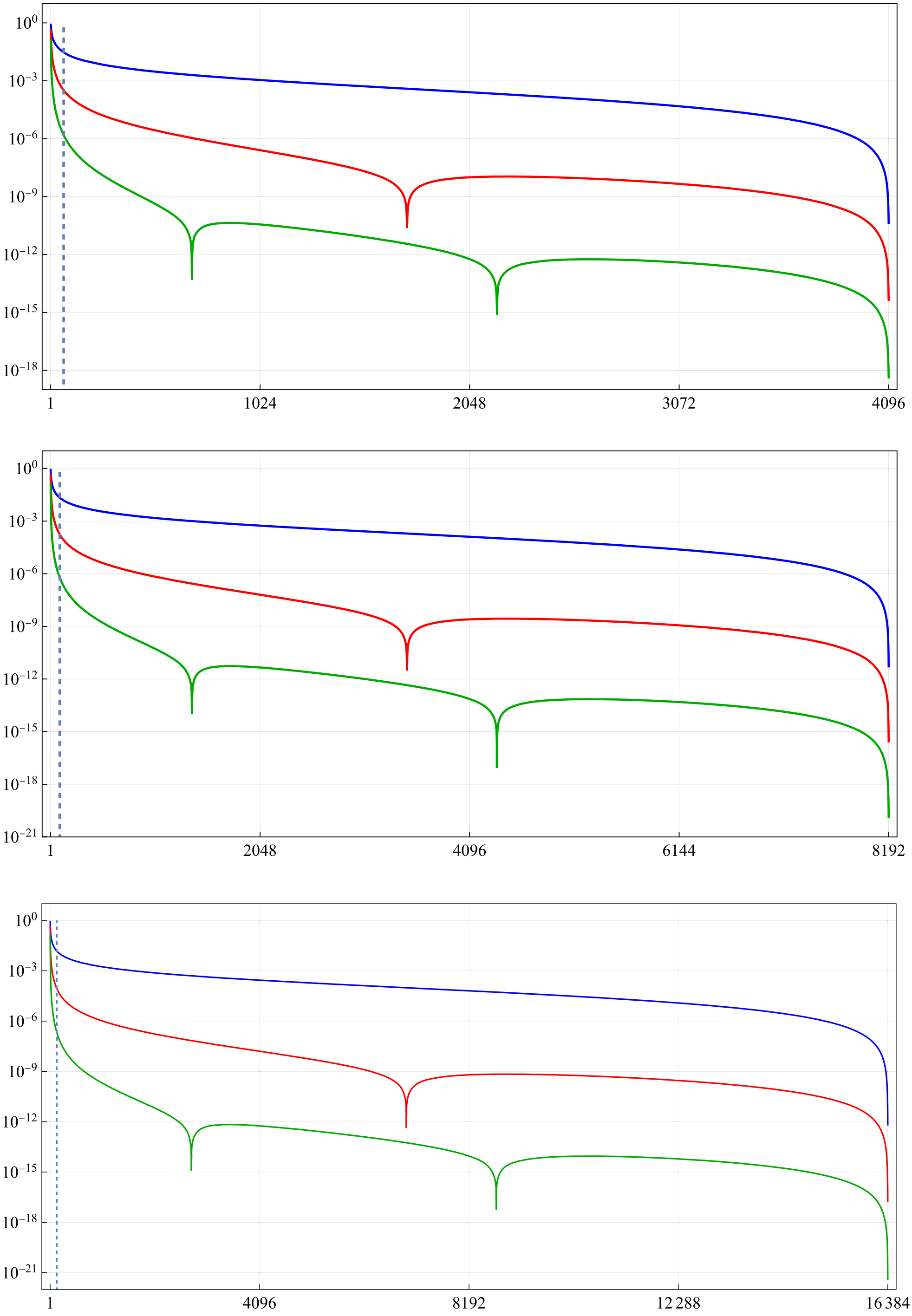

Fig. 6. The log scale of the relative individual errors $\mathrm{RE}_{j,n}^{\mathrm{INN}(m)}$, see (6.1), for $\beta = 3$, $m = 1$ (blue), $m = 2$ (red), and $m = 3$ (green). The top, middle, and bottom figures correspond to $n = 4096$, 8192, and 16384, respectively. In all cases, the dashed vertical line indicates the index $j_n = \lfloor\sqrt{n}\rfloor$. (For interpretation of the colors in the figure, the reader is referred to the web version of this article.)

Table 3
The absolute, relative, and normalized individual extreme errors $\mathrm{AE}^{\mathrm{EXT}}_{j,n}$, $\mathrm{RE}^{\mathrm{EXT}}_{j,n}$, and $\mathrm{NE}^{\mathrm{EXT}}_{j,n}$, respectively, for $j = 1, 2, 10$ with $\beta = 3$.

n	$\mathrm{RE}^{\mathrm{EXT}}_{1,n}$	$\mathrm{AE}^{\mathrm{EXT}}_{1,n}$	$\mathrm{NE}^{\mathrm{EXT}}_{1,n}$	$\mathrm{RE}^{\mathrm{EXT}}_{2,n}$	$\mathrm{AE}^{\mathrm{EXT}}_{2,n}$	$\mathrm{NE}^{\mathrm{EXT}}_{2,n}$	$\mathrm{RE}^{\mathrm{EXT}}_{10,n}$	$\mathrm{AE}^{\mathrm{EXT}}_{10,n}$	$\mathrm{NE}^{\mathrm{EXT}}_{10,n}$
16	2.27×10^{-1}	1.18×10^{-3}	1.23×10^{3}	2.18×10^{-1}	8.15×10^{-3}	5.34×10^{2}	1.02×10^{-1}	6.90×10^{-1}	7.23×10^{1}
32	1.17×10^{-1}	4.74×10^{-5}	1.59×10^{3}	1.16×10^{-1}	3.43×10^{-4}	7.19×10^{2}	8.85×10^{-2}	6.88×10^{-2}	2.31×10^{2}
64	5.95×10^{-2}	1.69×10^{-6}	1.82×10^{3}	5.98×10^{-2}	1.24×10^{-5}	8.35×10^{2}	5.38×10^{-2}	3.25×10^{-3}	3.49×10^{2}
128	3.00×10^{-2}	5.65×10^{-8}	1.94×10^{3}	3.03×10^{-2}	4.19×10^{-7}	8.99×10^{2}	2.92×10^{-2}	1.20×10^{-4}	4.13×10^{2}
256	1.50×10^{-2}	1.83×10^{-9}	2.01×10^{3}	1.53×10^{-2}	1.36×10^{-8}	9.33×10^{2}	1.51×10^{-2}	4.04×10^{-6}	4.44×10^{2}
512	7.53×10^{-3}	5.80×10^{-11}	2.04×10^{3}	7.65×10^{-3}	4.32×10^{-10}	9.50×10^{2}	7.68×10^{-3}	1.31×10^{-7}	4.59×10^{2}
1024	3.77×10^{-3}	1.83×10^{-12}	2.06×10^{3}	3.83×10^{-3}	1.36×10^{-11}	9.59×10^{2}	3.87×10^{-3}	4.15×10^{-9}	4.67×10^{2}
2048	1.89×10^{-3}	5.74×10^{-14}	2.07×10^{3}	1.92×10^{-3}	4.28×10^{-13}	9.64×10^{2}	1.94×10^{-3}	1.31×10^{-10}	4.71×10^{2}
4096	9.43×10^{-4}	1.80×10^{-15}	2.07×10^{3}	9.59×10^{-4}	1.34×10^{-14}	9.66×10^{2}	9.73×10^{-4}	4.10×10^{-12}	4.72×10^{2}
8192	4.72×10^{-4}	5.62×10^{-17}	2.07×10^{3}	4.80×10^{-4}	4.19×10^{-16}	9.67×10^{2}	4.87×10^{-4}	1.28×10^{-13}	4.73×10^{2}
16384	2.36×10^{-4}	1.76×10^{-18}	2.07×10^{3}	2.40×10^{-4}	1.31×10^{-17}	9.68×10^{2}	2.44×10^{-4}	4.01×10^{-15}	4.74×10^{2}

also when using the approximations provided by Theorems 2.2 and 2.3 (although the latter two are for inner eigenvalues only). Interestingly, except for the first two or three eigenvalues, Theorems 2.2 and 2.3 deliver much better approximations than one would expect. This indicates again that the range of applicability of these two theorems is probably larger than supposed.

6.3. Comparison with a formula by Parter

When $\beta = 0$, our symbol a_n given by (1.11) does not depend on n and coincides with the symbol studied in [17]. There the authors used a classical theorem of Parter [11], which states that if $a(\mathrm{e}^{\mathrm{i}\sigma}) = (2 - 2\cos(\sigma))^2$ and $\lambda_{j,n}$ are the eigenvalues of $T_n(a)$ listed in non-decreasing order, then for a fixed $j = 1, 2, \ldots$,

$$\lambda_{j,n} = \Big(\frac{(2j+1)\pi + E_j}{2(n+3)}\Big)^4 + o\Big(\frac{1}{n^4}\Big) \text{ as } n \to \infty, \tag{6.3}$$

where E_j is determined by the equation

$$\tan\Big(\frac{1}{4}\{(2j+1)\pi + E_j\}\Big) = (-1)^j \tanh\Big(\frac{1}{4}\{(2j+1)\pi + E_j\}\Big). \tag{6.4}$$

Numerical experiments reveal that (6.3) and Theorem 2.1 (with $\beta = 0$) indeed deliver comparable results. Here is a proof that (6.3) can in fact be derived from Theorem 2.1. Take $\beta = 0$ and note that $g_n(s) = s^4 + O(s^6)$ as $s \to 0$. Thus, by Theorem 2.1, we can write

$$\lambda_{j,n} = g_n\Big(\frac{\Lambda_j}{n+1}\Big) + O\Big(\frac{1}{n^5}\Big) = \Big(\frac{\Lambda_j}{n+1}\Big)^4 + O\Big(\frac{1}{n^5}\Big),$$

and since $1/(n+3) = 1/(n+1) + O(1/n^2)$, formula (6.3) is equivalent to

$$\lambda_{j,n} = \Big(\frac{\Lambda_j}{n+1}\Big)^4 + O\Big(\frac{1}{n^5}\Big) + o\Big(\frac{1}{n^4}\Big) = \Big(\frac{(2j+1)\pi + E_j}{2(n+1)}\Big)^4 + o\Big(\frac{1}{n^4}\Big).$$

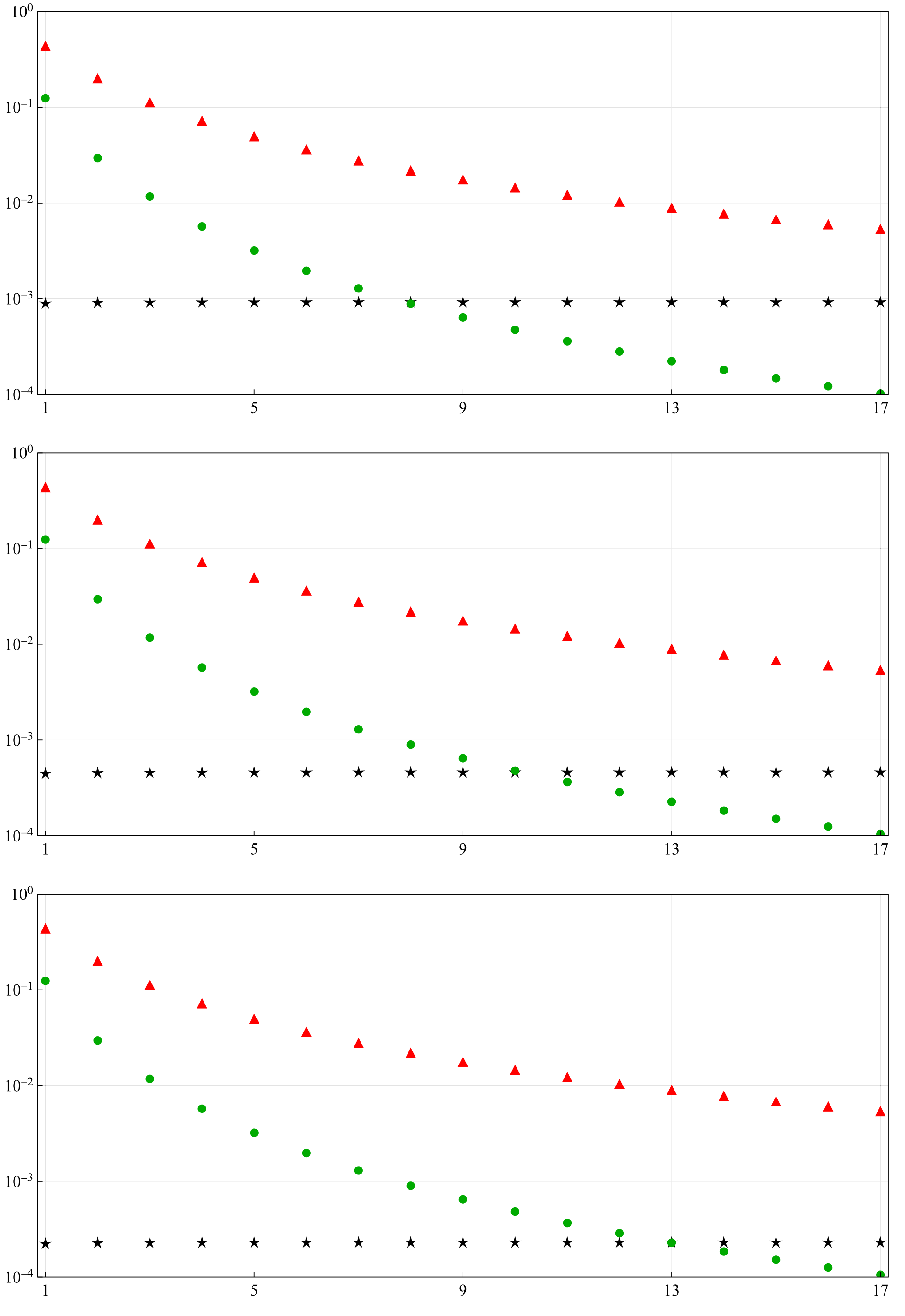

Fig. 7. For $\beta = 3$, the black stars are the log scale for the relative individual extreme errors $\mathrm{RE}^{\mathrm{EXT}}_{j,n}$, see (6.2), for $j = 1, \ldots, 17$. The red triangles and green dots are the relative individual inner errors $\mathrm{RE}^{\mathrm{INN}(m)}_{j,n}$ obtained with $m = 2$ and $m = 3$, respectively. The top, middle, and bottom figures correspond to $n = 4096$, 8192, and 16384, respectively. (For interpretation of the colors in the figure, the reader is referred to the web version of this article.)

Consequently, to show that the main terms in the two approximations coincide, it remains to prove that

$$\Lambda_j = \frac{1}{2}\big((2j+1)\pi + E_j\big). \tag{6.5}$$

This can be done as follows. For even $j = 2k$, equality (6.4) reads $\tan(u/2) = \tanh(u/2)$ with $u = \{(2j+1)\pi + E_j\}/2$. For arbitrary v the identity

$$v = \frac{\dfrac{2v}{1-v^2} - \dfrac{2v}{1+v^2}}{\dfrac{1+v^2}{1-v^2} - \dfrac{1-v^2}{1+v^2}}$$

holds. Taking $v = \tan(u/2) = \tanh(u/2)$ and using the half-angle identities

$$\sin(u) = \frac{2\tan(u/2)}{1+\tan^2(u/2)}, \qquad \cos(u) = \frac{1-\tan^2(u/2)}{1+\tan^2(u/2)},$$
$$\sinh(u) = \frac{2\tanh(u/2)}{1-\tanh^2(u/2)}, \qquad \cosh(u) = \frac{1+\tanh^2(u/2)}{1-\tanh^2(u/2)},$$

we obtain

$$\tan(u/2) = \frac{\dfrac{2\tanh(u/2)}{1-\tanh^2(u/2)} - \dfrac{2\tan(u/2)}{1+\tan^2(u/2)}}{\dfrac{1+\tanh^2(u/2)}{1-\tanh^2(u/2)} - \dfrac{1-\tan^2(u/2)}{1+\tan^2(u/2)}} = \frac{\sinh(u)-\sin(u)}{\cosh(u)-\cos(u)}.$$

Applying the arctan function we arrive at

$$\frac{u}{2} = \pi k + \arctan\left(\frac{\sinh(u)-\sin(u)}{\cosh(u)-\cos(u)}\right)$$

for some $k \in \mathbb{Z}$. The last equation can be written in terms of $\hat{\eta}$ as $u = 2\pi k + \hat{\eta}(u)$, that is, $u = \Lambda_{2k}$. Comparing magnitudes we finally get $\Lambda_{2k} = \Lambda_j$, which proves (6.5) for even j. The case where j is odd can be disposed of analogously.

Declaration of competing interest

The authors declare that they have no conflict of interest.

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Data availability

No data was used for the research described in the article.

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