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Inside the eigenvalues of certain Hermitian Toeplitz band matrices

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ABSTRACT

While extreme eigenvalues of large Hermitian Toeplitz matrices have been studied in detail for a long time, much less is known about individual inner eigenvalues. This paper explores the behavior of the jth eigenvalue of an n-by-n banded Hermitian Toeplitz matrix as n tends to infinity and provides asymptotic formulas that are uniform in j for $1 \le j \le n$. The real-valued generating function of the matrices is assumed to increase strictly from its minimum to its maximum, and then to decrease strictly back from the maximum to the minimum, having nonzero second derivatives at the minimum and the maximum. The results, which are of interest in numerical analysis, probability theory, or statistical physics, for example, are illustrated and underpinned by numerical examples.

1. Introduction and main results

The $n \times n$ Toeplitz matrix $T_n(a)$ generated by a function a in L^1 on the complex unit circle $\mathbf{T}$ is defined by $T_n(a) = (a_{j-k})_{j,k=1}^n$ where a_ℓ is the ℓth Fourier coefficient of a,

$$a_\ell = \frac{1}{2\pi} \int_0^{2\pi} a(e^{ix}) e^{-i\ell x} dx \quad (\ell \in \mathbf{Z}).$$

The asymptotics of the eigenvalues of $T_n(a)$ as $n \to \infty$ has been thoroughly studied by many authors for almost a century now. See the books [1,2] for more about this topic. We here bound ourselves to the case where a is real-valued, in which case $\overline{a_\ell} = a_{-\ell}$ for all $\ell \in \mathbf{Z}$ and hence the matrices $T_n(a)$ are all Hermitian. The eigenvalues are then real and may be labeled so that

$$\lambda_1^{(n)} \le \lambda_2^{(n)} \le \cdots \le \lambda_n^{(n)}.$$

The first Szegö limit theorem describes the collective behavior of the eigenvalues. It says in particular that, under certain assumptions,

$$\frac{|\{j : \lambda_j^{(n)} \in (\alpha, \beta)\}|}{n} = \frac{|\{t \in \mathbf{T} : a(t) \in (\alpha, \beta)\}|}{2\pi} + o(1) \tag{1}$$

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as $n \to \infty$, where $|E|$ denotes the cardinality of E on the left and the Lebesgue measure of E on the right. Much attention has been paid to the extreme eigenvalues, that is, to the behavior of $\lambda_j^{(n)}$ as $n \to \infty$ and j or $n - j$ remain fixed. The pioneering work on this problem was done in [3–6]. This work is also outlined on pages 256 to 259 of [7]. Recent work on and applications of extreme eigenvalues include the papers [8–15]. The purpose of this paper is to explore the behavior of $\lambda_j^{(n)}$ inside the set of the eigenvalues, for example, the asymptotics of $\lambda_j^{(n)}$ as $n \to \infty$ and $j/n \to x \in (0,1)$.

Throughout the paper we assume the following. The function a is a Laurent polynomial

$$a(t) = \sum_{k=-r}^{r} a_k t^k \quad (t = e^{ix} \in \mathbf{T})$$

with $r \geq 1$, $a_r \neq 0$, and $\overline{a_k} = a_{-k}$ for all k. The last condition means that a is real-valued on $\mathbf{T}$. It may be assumed without loss of generality that $a(\mathbf{T}) = [0, M]$ with $M > 0$ and that $a(1) = 0$ and $a(e^{i\varphi_0}) = M$ for some $\varphi_0 \in (0, 2\pi)$. We require that the generating function $g(x) := a(e^{ix})$ is strictly increasing on $(0, \varphi_0)$ and strictly decreasing on $(\varphi_0, 2\pi)$ and that the second derivatives of g at $x = 0$ and $x = \varphi_0$ are nonzero.

For $\lambda \in (0, M)$ and $t \in \mathbf{T}$, we define the argument of $a(t) - \lambda$ to be 0 if $a(t) > \lambda$ and to be π if $a(t) < \lambda$. Then $\log(a - \lambda)$ is a well-defined function in $L^1(\mathbf{T})$. Let $(\log(a - \lambda))_\ell$ be its ℓth Fourier coefficient and put

$$G(a - \lambda) = \exp(\log(a - \lambda))_0,$$
$$E(a - \lambda) = \exp \sum_{\ell=1}^{\infty} \ell \, (\log(a - \lambda))_\ell (\log(a - \lambda))_{-\ell}.$$

We will show that there are continuous functions

$$\varphi : [0, M] \to [0, \pi], \qquad \theta : [0, M] \to \mathbf{R}$$

such that $\varphi(0) = \theta(0) = 0$, $\varphi(M) = \pi$, $\theta(M) = 0$, and

$$G(a - \lambda) = |G(a - \lambda)| e^{i\varphi(\lambda)}, \tag{2}$$
$$E(a - \lambda) = \frac{1}{i} |E(a - \lambda)| e^{i(\varphi(\lambda) + \theta(\lambda))}. \tag{3}$$

The function φ will turn out to be bijective and to have a well-defined derivative $\varphi'(\lambda) \in (0, \infty]$ for all $\lambda \in (0, M)$. In what follows, O estimates are always uniform, that is, $O(b_n)$ denotes a sequence $\{\xi_n\}$ such that $|\xi_n| \leq C b_n$ for all n with some constant $C < \infty$ that depends only on the function a. Thus, if ξ_n depends on parameters such as $\lambda, j, k, \ldots$, then C is independent of the parameters.

Here are our main results.

Theorem 1.1. *There is a number $\delta > 0$ such that for $\lambda \in (0, M)$,*

$$\det T_n(a - \lambda) = 2\, |E(a - \lambda)|\, |G(a - \lambda)|^n \left(\sin((n+1)\varphi(\lambda) + \theta(\lambda)) + O(e^{-\delta n}) \right).$$

From (2) and (3) we infer that the formula of this theorem may also be written in the form

$$\det T_n(a - \lambda) = E(a - \lambda)\, G(a - \lambda)^n + \overline{E(a - \lambda)}\, \overline{G(a - \lambda)}^n + |E(a - \lambda)|\, |G(a - \lambda)|^n\, O(e^{-\delta n}).$$

Theorem 1.2. *If n is sufficiently large, then the function*

$$[0, M] \to [0, (n+1)\pi], \quad \lambda \mapsto (n+1)\varphi(\lambda) + \theta(\lambda)$$

is bijective and increasing. For $1 \leq j \leq n$, the eigenvalues $\lambda_j^{(n)}$ satisfy

$$(n+1)\varphi(\lambda_j^{(n)}) + \theta(\lambda_j^{(n)}) = \pi j + O(e^{-\delta n}),$$

and if $\lambda_{j,*}^{(n)} \in (0, M)$ is the uniquely determined solution of the equation

$$(n+1)\varphi(\lambda_{j,*}^{(n)}) + \theta(\lambda_{j,*}^{(n)}) = \pi j,$$

then $|\lambda_j^{(n)} - \lambda_{j,*}^{(n)}| = O(e^{-\delta n})$.

In Section 4 we will provide an exponentially fast iteration procedure for solving the equation $(n+1)\varphi(\lambda) + \theta(\lambda) = \pi j$. More importantly, in Sections 4 and 5 we will show how Theorem 1.2 can be employed to derive, at least in principle, an asymptotic expansion of the form

$$\sum_{k=0}^{\infty} \frac{c_k(d)}{(n+1)^k}, \quad d := \frac{\pi j}{n+1} \tag{4}$$

for the jth eigenvalue $\lambda_j^{(n)}$. We consider d as a parameter representing j and n and therefore suppress the dependence on j and n in the notation. The coefficients $c_k(d)$ become more and more complicated as k increases. We limit ourselves to the first few coefficients. Let $\psi : [0, \pi] \to [0, M]$ be the inverse of the bijective and increasing function φ. Clearly, ψ is differentiable in $(0, \pi)$.

Theorem 1.3. *We have*

$$\lambda_j^{(n)} = \psi(d) - \frac{\psi'(d)\theta(\psi(d))}{n+1} + O\left(\frac{(\theta(\psi(d)))^2}{n^2}\right) + O\left(\frac{\psi'(d)\theta(\psi(d))}{n^2}\right).$$

We emphasize once more that the estimate provided by Theorem 1.3 is uniform in $j \in \{1, \dots, n\}$. Since ψ' and θ are bounded on $(0, M)$, we obtain in particular that

$$\lambda_j^{(n)} = \psi(d) - \frac{\psi'(d)\theta(\psi(d))}{n+1} + O\left(\frac{1}{n^2}\right), \tag{5}$$

uniformly in d from compact subsets of $(0, \pi)$. For the inner eigenvalues, Theorem 1.3 implies the following.

Theorem 1.4. *Let $x \in (0, 1)$ and let $\lambda_x \in (0, M)$ be the solution of the equation $\varphi(\lambda_x) = \pi x$. If $n \to \infty$ and $j/n \to x$, then*

$$\lambda_j^{(n)} = \lambda_x + \frac{\pi}{\varphi'(\lambda_x)}\left(\frac{j}{n+1} - x\right) - \frac{\theta(\lambda_x)}{\varphi'(\lambda_x)}\frac{1}{n+1} + O\left(\left(\frac{j}{n+1} - x\right)^2 + \frac{1}{n^2}\right),$$

uniformly in x from compact subsets of $(0, 1)$. This formula may be rewritten using that

$$\lambda_x = \psi(\pi x), \quad 1/\varphi'(\lambda_x) = \psi'(\pi x), \quad \theta(\lambda_x) = \theta(\psi(\pi x)).$$

The last theorem reveals, in particular, that the eigenvalues $\lambda_j^{(n)}$ are scaled according to formula

$$\lambda_{j+1}^{(n)} - \lambda_j^{(n)} = \frac{\pi}{\varphi'(\lambda_x)}\frac{1}{n+1} + O\left(\left(\frac{j}{n+1} - x\right)^2 + \frac{1}{n^2}\right)$$

as $n \to \infty$ and $j/n \to x \in (0, 1)$.

Here is what Theorem 1.3 yields for the extreme eigenvalues.

Theorem 1.5. *If $n \to \infty$ and $j/n \to 0$, then*

$$\lambda_j^{(n)} = \sum_{k=0}^{3} (-1)^k \frac{\psi^{(k)}(d)}{k!}\left(\frac{\theta(\psi(d))}{n+1}\right)^k + O\left(\frac{1}{n^4}\right) \tag{6}$$

$$= \frac{g''(0)}{2}\left(\frac{\pi j}{n+1}\right)^2\left(1 + \frac{w_0}{n+1}\right) + O\left(\frac{j^4}{n^4}\right) \tag{7}$$

$$= \frac{g''(0)}{2}\left(\frac{\pi j}{n+1}\right)^2 + O\left(\frac{j^3}{n^3}\right), \tag{8}$$

where

$$w_0 = \frac{1}{\pi}\int_{-\pi}^{\pi}\left(\frac{g'(x)}{g(x)} - \cot\frac{x}{2} - \frac{g'''(0)}{3g''(0)}\right)\cot\frac{x}{2}\,dx. \tag{9}$$

In this theorem, (6) ⇒ (7) ⇒ (8). Note that if the number j remains fixed, then $O\left(j^4/n^4\right) = O\left(1/n^4\right)$. Our proof will also yield (6) to (9) under the sole hypothesis that $n \to \infty$ and $j/n \le C_0$ for some C_0 independent of n; in that case the constants hidden in the O terms depend on C_0 and a but on nothing else. Under the assumption that $g(x) = a(e^{ix})$ is an even function, Widom [4] proved that, for each fixed j,

$$\lambda_j^{(n)} = \frac{g''(0)}{2}\left(\frac{\pi j}{n+1}\right)^2\left(1 + \frac{w_0}{n+1} + o\left(\frac{1}{n}\right)\right).$$

This is slightly weaker than (7).

A result similar to Theorem 1.5 is also valid for $n \to \infty$ and $j/n \to 1$. For instance, the analogue of (8) reads

$$\lambda_j^{(n)} = M - \frac{|g''(\varphi_0)|}{2}\left(\pi - \frac{\pi j}{n+1}\right)^2 + O\left(\left(1 - \frac{j}{n+1}\right)^3\right).$$

In Section 5 we will also show that if $0 \le \alpha < \beta \le M$ then

$$|\{j : \lambda_j^{(n)} \in (\alpha, \beta)\}| = (n+1)\frac{\varphi(\beta) - \varphi(\alpha)}{\pi} + \frac{\theta(\beta) - \theta(\alpha)}{\pi} + \kappa_n(\alpha, \beta)$$

with $|\kappa_n(\alpha, \beta)| < 2$ for all n large enough.

The paper is organized as follows. In Section 2, we phase in the main actors of our approach, such as the functions $\varphi(\lambda)$ and $\theta(\lambda)$, and prove their basic properties. In Section 3, we use a formula by Widom to represent the determinant $\det T_n(a - \lambda)$ in a form that will be convenient for further analysis. There we also prove Theorem 1.1. Section 4 is devoted to the proof of Theorem 1.2 and, in addition, contains a convergence theorem on an iteration method for solving the equation $(n+1)\varphi(\lambda) + \theta(\lambda) = \pi j$. Theorems 1.3–1.5 are proved in Section 5. In that section, we also briefly discuss the asymptotics of $\lambda_{j+1}^{(n)} - \lambda_j^{(n)}$ and improvements of (1). Some examples are provided in Section 6.

2. The main actors

In this section we introduce and study the quantities which occur in our asymptotic formulas. Let a be as in Section 1. For each $\lambda \in [0, M]$, there exist exactly one $\varphi_1(\lambda) \in [0, \varphi_0]$ and exactly one $\varphi_2(\lambda) \in [\varphi_0 - 2\pi, 0]$ such that

$$g(\varphi_1(\lambda)) = g(\varphi_2(\lambda)) = \lambda;$$

recall that $g(x) = a(e^{ix})$. We put

$$\varphi(\lambda) = \frac{\varphi_1(\lambda) - \varphi_2(\lambda)}{2}.$$

Clearly, $\varphi(0) = 0$, $\varphi(M) = \pi$, φ is a continuous and strictly increasing map of $[0, M]$ onto $[0, \pi]$, the derivative $\varphi'(\lambda) \in (0, \infty]$ exists for all $\lambda \in (0, M)$ (with $\varphi'(\lambda) = \infty$ if and only if $g'(\varphi_1(\lambda)) = 0$ or $g'(\varphi_2(\lambda)) = 0$), and

$$\varrho := \inf_{\lambda \in (0,M)} \varphi'(\lambda) > 0. \tag{10}$$

Recall that $\psi : [0, \pi] \to [0, M]$ is the inverse of the function $\varphi : [0, M] \to [0, \pi]$.

Lemma 2.1. *Let $g(x) = g_2x^2 + g_3x^3 + g_4x^4 + \cdots$ be the Taylor series of g at $x = 0$. Then as $\lambda \to 0 + 0$,*

$$\varphi_1(\lambda) = \frac{1}{g_2^{1/2}}\lambda^{1/2} - \frac{g_3}{2g_2^2}\lambda + \frac{5g_3^2 - 4g_2g_4}{8g_2^{7/2}}\lambda^{3/2} + O(\lambda^2),$$

$$\varphi_2(\lambda) = -\frac{1}{g_2^{1/2}}\lambda^{1/2} - \frac{g_3}{2g_2^2}\lambda - \frac{5g_3^2 - 4g_2g_4}{8g_2^{7/2}}\lambda^{3/2} + O(\lambda^2),$$

$$\varphi(\lambda) = \frac{1}{g_2^{1/2}}\lambda^{1/2} + \frac{5g_3^2 - 4g_2g_4}{8g_2^{7/2}}\lambda^{3/2} + O(\lambda^{5/2}),$$

$$\varphi'(\lambda) = \frac{1}{2g_2^{1/2}}\lambda^{-1/2} + \frac{3}{2}\,\frac{5g_3^2 - 4g_2g_4}{8g_2^{7/2}}\lambda^{1/2} + O(\lambda^{3/2}),$$

and as $x \to 0 + 0$,

$$\psi(x) = g_2x^2 + \left(g_4 - \frac{5g_3^2}{4g_2}\right)x^4 + O(x^6),$$

$$\psi'(x) = 2g_2x + \left(4g_4 - \frac{5g_3^2}{g_2}\right)x^3 + O(x^5).$$

The series for $\varphi_1(\lambda)$ and $\varphi_2(\lambda)$ have equal coefficients at even powers of $\lambda^{1/2}$ and opposite coefficients at odd powers of $\lambda^{1/2}$. The series for $\varphi(\lambda)$ contains only odd powers of $\lambda^{1/2}$, while the series for $\psi(x)$ involves only even powers of x.

Proof. The equation $g(\varphi) = \lambda$ has the two solutions $\varphi_1(\lambda) = \Phi(\lambda^{1/2})$ and $\varphi_2(\lambda) = \Phi(-\lambda^{1/2})$ where Φ is analytic in a neighborhood of the origin. Consequently,

$$\varphi_1(\lambda) = \sum_{k=0}^{\infty}\Phi_k\lambda^{k/2}, \qquad \varphi_2(\lambda) = \sum_{k=0}^{\infty}(-1)^k\Phi_k\lambda^{k/2}.$$

The coefficients Φ_k and subsequently the series for ψ and ψ' can be determined by standard computations. □

For $\lambda \in \mathbf{C}$, we write $a - \lambda$ in the form

$$\begin{aligned} a(t) - \lambda &= t^{-r}(a_r t^{2r} + \cdots + (a_0 - \lambda)t^r + \cdots + a_{-r}) \\ &= a_r t^{-r} \prod_{k=1}^{2r} (t - z_k(\lambda)) \end{aligned} \tag{11}$$

with complex numbers $z_k(\lambda)$. We may label the zeros $z_1(\lambda), \ldots, z_{2r}(\lambda)$ so that each z_k is a continuous function of $\lambda \in \mathbf{C}$. Now take $\lambda \in [0, M]$. Then $a - \lambda$ has exactly the two zeros $e^{i\varphi_1(\lambda)}$ and $e^{i\varphi_2(\lambda)}$ on $\mathbf{T}$. We put

$$z_r(\lambda) = e^{i\varphi_1(\lambda)}, \qquad z_{r+1}(\lambda) = e^{i\varphi_2(\lambda)}.$$

For $t \in \mathbf{T}$ we have (11) on the one hand, and since $a(t) - \lambda$ is real, we get

$$\begin{aligned} a(t) - \lambda &= \overline{a(t) - \lambda} = \overline{a_r}\, t^r \prod_{k=1}^{2r} \left(\frac{1}{t} - \bar{z}_k(\lambda) \right) \\ &= \overline{a_r} \left(\prod_{k=1}^{2r} \bar{z}_k(\lambda) \right) t^{-r} \prod_{k=1}^{2r} \left(t - \frac{1}{\bar{z}_k(\lambda)} \right) \end{aligned} \tag{12}$$

on the other. Here and in similar cases that will follow, $\bar{z}_k(\lambda) := \overline{z_k(\lambda)}$. Comparing (11) and (12) we see that the zeros in $\mathbf{C} \setminus \mathbf{T}$ may be relabeled so that they appear in pairs $z_k(\lambda)$, $1/\bar{z}_k(\lambda)$ with $|z_k(\lambda)| > 1$. Put $u_k(\lambda) = z_k(\lambda)$ for $1 \le k \le r - 1$. We relabel $z_{r+2}(\lambda), \ldots, z_{2r}(\lambda)$ to get $z_{2r-k}(\lambda) = 1/\bar{u}_k(\lambda)$ for $1 \le k \le r - 1$. In summary, for $\lambda \in [0, M]$ we have

$$\begin{aligned} \mathcal{Z} &:= \{z_1(\lambda), \ldots, z_{r-1}(\lambda), e^{i\varphi_1(\lambda)}, e^{i\varphi_2(\lambda)}, z_{r+2}(\lambda), \ldots, z_{2r}(\lambda)\} \\ &= \{u_1(\lambda), \ldots, u_{r-1}(\lambda), e^{i\varphi_1(\lambda)}, e^{i\varphi_2(\lambda)}, 1/\bar{u}_{r-1}(\lambda), \ldots, 1/\bar{u}_1(\lambda)\}. \end{aligned} \tag{13}$$

Since all u_k are continuous, it follows that

$$e^{\delta_0} := \min_{\lambda \in [0,M]} \min_{1 \le k \le r-1} |u_k(\lambda)| > 1.$$

Put

$$h_\lambda(z) = \prod_{k=1}^{r-1} \left(1 - \frac{z}{u_k(\lambda)} \right), \qquad \sigma(\lambda) = \frac{\varphi_1(\lambda) + \varphi_2(\lambda)}{2},$$

$$d_0(\lambda) = (-1)^r a_r e^{i\sigma(\lambda)} \prod_{k=1}^{r-1} u_k(\lambda). \tag{14}$$

For $t \in \mathbf{T}$ we then may write

$$\begin{aligned} a(t) - \lambda &= a_r t^{-r} (t - e^{i\varphi_1(\lambda)})(t - e^{i\varphi_2(\lambda)}) \prod_{k=1}^{r-1} (t - u_k(\lambda)) \prod_{k=1}^{r-1} (t - 1/\bar{u}_k(\lambda)) \\ &= a_r t^{-r} (-e^{i\varphi_1(\lambda)}) \left(1 - \frac{t}{e^{i\varphi_1(\lambda)}} \right) t \left(1 - \frac{e^{i\varphi_2(\lambda)}}{t} \right) \prod_{k=1}^{r-1} (-u_k(\lambda)) \\ &\quad \times \prod_{k=1}^{r-1} \left(1 - \frac{t}{u_k(\lambda)} \right) t^{r-1} \prod_{k=1}^{r-1} \left(1 - \frac{\bar{t}}{\bar{u}_k(\lambda)} \right) \\ &= d_0(\lambda) e^{i\varphi(\lambda)} \left(1 - \frac{t}{e^{i\varphi_1(\lambda)}} \right) \left(1 - \frac{e^{i\varphi_2(\lambda)}}{t} \right) h_\lambda(t) \overline{h_\lambda(t)}. \end{aligned} \tag{15}$$

Let

$$\Theta(\lambda) := \frac{h_\lambda(e^{i\varphi_1(\lambda)})}{h_\lambda(e^{i\varphi_2(\lambda)})} = \prod_{k=1}^{r-1} \frac{1 - e^{i\varphi_1(\lambda)}/u_k(\lambda)}{1 - e^{i\varphi_2(\lambda)}/u_k(\lambda)}.$$

Clearly, $\Theta(0) = \Theta(M) = 1$. The function Θ is continuous and nonzero on $[0, M]$. Since $|u_k(\lambda)| > 1$, the real parts of $1 - e^{i\varphi_1(\lambda)}/u_k(\lambda)$ and $1 - e^{i\varphi_2(\lambda)}/u_k(\lambda)$ are positive and hence the closed curve

$$[0, M] \to \mathbf{C} \setminus \{0\}, \qquad \lambda \mapsto \frac{1 - e^{i\varphi_1(\lambda)}/u_k(\lambda)}{1 - e^{i\varphi_2(\lambda)}/u_k(\lambda)} \tag{16}$$

has winding number zero. The winding number of the closed curve

$$[0, M] \to \mathbf{C} \setminus \{0\}, \qquad \lambda \mapsto \Theta(\lambda)$$

is therefore also zero. We define $\theta(\lambda)$ as the continuous argument of $\Theta(\lambda)$ that assumes the value 0 at $\lambda = 0$ and $\lambda = M$.

Lemma 2.2. *The function $\theta(\lambda)$ can be expanded into a power series in $\sqrt{\lambda}$ in some neighborhood of 0, and this decomposition contains only odd powers of $\sqrt{\lambda}$. In particular,*

$$\theta(\lambda) = b_0\,\lambda^{1/2} + O(\lambda^{3/2}), \qquad \theta'(\lambda) = \frac{b_0}{2}\,\lambda^{-1/2} + O(\lambda^{1/2})$$

as $\lambda \to 0+0$. Here

$$b_0 = -\frac{w_0}{\sqrt{2g''(0)}}, \quad w_0 = 4\,\mathrm{Re}\left(\sum_{\nu=1}^{r-1} \frac{1}{u_\nu(0)-1}\right).$$

Proof. We write $\lambda = \mu^2$ and thus have $\theta(\lambda) = \mathrm{Im}\,\xi(\mu)$ where the function ξ is defined as

$$\xi(\mu) = \log \frac{h_{\mu^2}(\mathrm{e}^{\mathrm{i}\varphi_1(\mu^2)})}{h_{\mu^2}(\mathrm{e}^{\mathrm{i}\varphi_2(\mu^2)})}.$$

To prove the lemma we will show that ξ is analytic in some neighborhood of 0, that its Taylor expansion contains only odd powers of μ, and that

$$\xi'(0) = -\frac{4\mathrm{i}}{\sqrt{2g''(0)}} \sum_{\nu=1}^{r-1} \frac{1}{u_\nu(0)-1}. \tag{17}$$

Fix some positive number δ such that $\delta < \delta_0$ and denote by $\mathcal{A}$ the unital Banach algebra consisting of all functions $f \in C(\mathbf{T})$ such that $\|f\|_{\mathcal{A}} < \infty$ where

$$\|f\|_{\mathcal{A}} = \sum_{n\in\mathbf{Z}} |f_n| \mathrm{e}^{-|n|\delta}.$$

For every $\lambda \in [0, M]$, consider the function v_λ defined by

$$v_\lambda(t) = \frac{a(t)-\lambda}{(t-\mathrm{e}^{\mathrm{i}\varphi_1(\lambda)})(t-\mathrm{e}^{\mathrm{i}\varphi_2(\lambda)})}.$$

It follows from our assumptions on a that v_λ is a Laurent polynomial whose zeros are outside the annulus $1-\delta_0 < |z| < 1+\delta_0$. Moreover, the coefficients of odd powers of $\lambda^{1/2}$ in $\mathrm{e}^{\mathrm{i}\varphi_1(\lambda)}$ and $\mathrm{e}^{\mathrm{i}\varphi_2(\lambda)}$ are opposite to each other. Hence the coefficients of the polynomials $t^r(a(t)-\lambda)$ and $(t-\mathrm{e}^{\mathrm{i}\varphi_1(\lambda)})(t-\mathrm{e}^{\mathrm{i}\varphi_2(\lambda)})$ are analytic functions of λ in a neighborhood of 0. Consequently, the Fourier coefficients of v_λ are analytic functions of λ in a neighborhood of 0. Hence $v_\lambda \in \mathcal{A}$ and the $\mathcal{A}$-valued function $\lambda \mapsto v_\lambda$ is analytic in a neighborhood of 0.

We know that v_λ has a logarithm for each $\lambda \in [0, M]$. Denote by $\log v_\lambda$ the logarithm of v_λ which is real-valued at $t = 1$. For each λ, the function $\log v_\lambda$ is analytic in the annulus $1-\delta_0 < |z| < 1+\delta_0$ and therefore belongs to $\mathcal{A}$. Moreover, the function $\lambda \mapsto \log v_\lambda$ is analytic in a neighborhood of 0 because log is analytic on $\exp(\mathcal{A})$. Let $P_+ : \mathcal{A} \to \mathcal{A}$ be the operator acting by the rule $P_+\left(\sum_{n\in\mathbf{Z}} f_n t^n\right) = \sum_{n\geq 0} f_n t^n$. This is a bounded linear operator and $P_+\mathcal{A}$ is a closed subalgebra of $\mathcal{A}$ with the same identity element. Since $\log h_\lambda$ is nothing but $P_+(\log v_\lambda)$, we conclude that $\lambda \mapsto \log h_\lambda$ is a $P_+\mathcal{A}$-valued analytic function in a neighborhood of 0. Thus,

$$\log h_\lambda(t) = \sum_{k=0}^{\infty} c_k(t)\lambda^k \tag{18}$$

with $c_k \in \mathcal{A}$ and $\|c_k\|_\infty \leq \|c_k\|_{\mathcal{A}} \leq r_0^k$ where r_0 is some positive number.

Putting $\lambda = \mu^2$ and $t = \mathrm{e}^{\mathrm{i}\varphi_1(\mu^2)}$ or $t = \mathrm{e}^{\mathrm{i}\varphi_2(\mu^2)}$ in (18), we obtain a series of analytic functions on the right-hand side. The inequality $\|c_k\|_\infty \leq r_0^k$ guarantees that the series converge absolutely in some neighborhood of 0. Therefore the functions $\mu \mapsto h_{\mu^2}(\mathrm{e}^{\mathrm{i}\varphi_1(\mu^2)})$ and $\mu \mapsto h_{\mu^2}(\mathrm{e}^{\mathrm{i}\varphi_2(\mu^2)})$ are analytic in some neighborhood of 0. Further, the common value of these functions at $\mu = 0$ is $h_0(1)$. It follows that ξ is analytic in some neighborhood of 0 and $\xi(0) = 0$.

By virtue of (18), the function $\log h_\lambda(t)$ may be expanded into a double series converging for $|t| < 1+\delta$ and $0 \leq \lambda < 1/(2r_1)$,

$$\log h_\lambda(t) = \sum_{j=0}^{\infty}\sum_{k=0}^{\infty} A_{j,k}\lambda^j t^k = \log h_0(t) + \sum_{j=1}^{\infty}\sum_{k=0}^{\infty} A_{j,k}\lambda^j t^k.$$

Accordingly,

$$\xi(\mu) = \sum_{j=0}^{\infty}\sum_{k=0}^{\infty} A_{j,k}\mu^{2j}\left(\mathrm{e}^{k\mathrm{i}\varphi_1(\mu^2)} - \mathrm{e}^{k\mathrm{i}\varphi_2(\mu^2)}\right).$$

From Lemma 2.1 we infer that the expansions of $e^{ki\varphi_1(\mu^2)}$ and $e^{ki\varphi_2(\mu^2)}$ have the same coefficients at even powers of μ. Thus the expansion of $\xi(\mu)$ contains only odd powers of μ.

We finally calculate $\xi'(0)$, that is, the coefficient of μ in the series for $\xi(\mu)$. Lemma 2.1 yields

$$e^{i\varphi_{1,2}(\mu^2)} = 1 \pm \frac{i}{g_2^{1/2}}\mu - \frac{g_2 + ig_3}{g_2^2}\mu^2 + O(\mu^3).$$

Therefore

$$\begin{aligned}
\xi(\mu) &= \log \frac{h_{\mu^2}(e^{i\varphi_1(\mu^2)})}{h_{\mu^2}(e^{i\varphi_2(\mu^2)})} = \log \frac{h_0(e^{i\varphi_1(\mu^2)})}{h_0(e^{i\varphi_2(\mu^2)})} + \mu^2 \cdot O(e^{i\varphi_1(\mu^2)} - e^{i\varphi_2(\mu^2)}) \\
&= \sum_{\nu=1}^{r-1}\left(\log\left(1 - \frac{e^{i\varphi_1(\mu^2)}}{u_\nu(0)}\right) - \log\left(1 - \frac{e^{i\varphi_2(\mu^2)}}{u_\nu(0)}\right)\right) + O(\mu^3) \\
&= \sum_{\nu=1}^{r-1}\left(\log\left(1 - \frac{e^{i\varphi_1(\mu^2)} - 1}{u_\nu(0) - 1}\right) - \log\left(1 - \frac{e^{i\varphi_2(\mu^2)} - 1}{u_\nu(0) - 1}\right)\right) + O(\mu^3) \\
&= -\sum_{\nu=1}^{r-1}\sum_{k=1}^{\infty} \frac{\left(e^{i\varphi_1(\mu^2)} - 1\right)^k - \left(e^{i\varphi_2(\mu^2)} - 1\right)^k}{k(u_\nu(0) - 1)^k} + O(\mu^3) \\
&= -\frac{2i}{g_2^{1/2}}\left(\sum_{\nu=1}^{r-1}\frac{1}{u_\nu(0) - 1}\right)\mu + O(\mu^3) \\
&= -\frac{4i}{\sqrt{2g''(0)}}\left(\sum_{\nu=1}^{r-1}\frac{1}{u_\nu(0) - 1}\right)\mu + O(\mu^3),
\end{aligned}$$

which implies (17). □

The following lemma shows that the constant w_0 from Lemma 2.2 is just the constant (9). We remark that our integral formula (9) is a little simpler than the original integral formula established by Widom [4] in the case of symmetric matrices.

Lemma 2.3. *We have*

$$w_0 = \frac{1}{\pi}\int_{-\pi}^{\pi}\left(\frac{g'(x)}{g(x)} - \cot\frac{x}{2} - \frac{g'''(0)}{3g''(0)}\right)\cot\frac{x}{2}\,dx.$$

Proof. By Lemma 2.2, $w_0 = 4\,\mathrm{Re}\,\alpha$ where

$$\alpha = \sum_{j=1}^{r-1}\frac{1}{u_j(0) - 1} = -\sum_{j=1}^{r-1}\frac{1}{1 - u_j(0)}.$$

Recall that $\{u_j(0) : 1 \le j \le r-1\}$ is the complete set of the roots of a outside the closed unit disk, counted with multiplicities. If for some j the root $u_j(0)$ has multiplicity m then its contribution to the sum may be written as

$$\frac{m}{1 - u_j(0)} = \mathrm{Res}_{z=u_j(0)}\frac{a'(z)}{a(z)(1 - z)}.$$

Thus, α is the sum of the residues of $a'(z)/(a(z)(1-z))$ outside the closed unit disk. The residue theorem therefore implies that

$$\alpha = -\frac{1}{2\pi i}\int_{|z|=R}\frac{a'(z)\,dz}{a(z)(1 - z)} + \frac{1}{2\pi i}\int_{|z|=\rho}\frac{a'(z)\,dz}{a(z)(1 - z)}$$

where $R > \max(|u_1(0)|, \ldots, |u_{r-1}(0)|)$ and $1 < \rho < \min(|u_1(0)|, \ldots, |u_{r-1}(0)|)$. The first integral tends to 0 as $R \to \infty$ and hence

$$\alpha = \frac{1}{2\pi i}\int_{|z|=\rho}\frac{a'(z)\,dz}{a(z)(1 - z)}. \qquad (19)$$

The integrand in (19) has a double pole at $z = 1$. It is easy to see that, for z near 1,

$$\frac{a'(z)}{a(z)} = \frac{2}{z - 1} + \frac{a'''(1)}{3a''(1)} + O(z - 1).$$

Since

$$\frac{1}{2\pi \mathrm{i}}\int_{|z|=\rho}\frac{\mathrm{d}z}{(1-z)^2}=0, \qquad \frac{1}{2\pi \mathrm{i}}\int_{|z|=\rho}\frac{\mathrm{d}z}{1-z}=-1,$$

we may write

$$\alpha=-\frac{a'''(1)}{3a''(1)}+\frac{1}{2\pi \mathrm{i}}\int_{|z|=\rho}\left(\frac{a'(z)}{a(z)}-\frac{2}{z-1}-\frac{a'''(1)}{3a''(1)}\right)\frac{\mathrm{d}z}{1-z}.$$

The integrand is now regular at $z=1$. Deforming the integration contour to the unit circle, we get

$$\alpha=-\frac{a'''(1)}{3a''(1)}+\frac{1}{2\pi \mathrm{i}}\int_{|z|=1}\left(\frac{a'(z)}{a(z)}-\frac{2}{z-1}-\frac{a'''(1)}{3a''(1)}\right)\frac{\mathrm{d}z}{1-z}. \tag{20}$$

To transform the contour integral into a real integral, we make the change of variables $z=\mathrm{e}^{\mathrm{i}x}$. Taking into account the formula

$$\mathrm{i}\mathrm{e}^{\mathrm{i}x}\,\frac{a'(\mathrm{e}^{\mathrm{i}x})}{a(\mathrm{e}^{\mathrm{i}x})}=\frac{g'(x)}{g(x)},$$

we obtain

$$\begin{aligned}\alpha &= -\frac{a'''(1)}{3a''(1)}+\frac{1}{2\pi \mathrm{i}}\int_{-\pi}^{\pi}\left(\frac{g'(x)}{g(x)i\mathrm{e}^{\mathrm{i}x}}-\frac{2}{\mathrm{e}^{\mathrm{i}x}-1}-\frac{a'''(1)}{3a''(1)}\right)\frac{i\mathrm{e}^{\mathrm{i}x}\,\mathrm{d}x}{1-\mathrm{e}^{\mathrm{i}x}}\\ &= -\frac{a'''(1)}{3a''(1)}+\frac{1}{4\pi}\int_{-\pi}^{\pi}\left(\frac{g'(x)\mathrm{e}^{-\mathrm{i}x/2}}{g(x)}-\frac{2\mathrm{i}\mathrm{e}^{\mathrm{i}x/2}}{\mathrm{e}^{\mathrm{i}x}-1}-\frac{a'''(1)i\mathrm{e}^{\mathrm{i}x/2}}{3a''(1)}\right)\frac{2\mathrm{i}\mathrm{e}^{\mathrm{i}x/2}}{\mathrm{e}^{\mathrm{i}x}-1}\,\mathrm{d}x\\ &= -\frac{a'''(1)}{3a''(1)}+\frac{1}{4\pi}\int_{-\pi}^{\pi}\left(\frac{g'(x)\mathrm{e}^{-\mathrm{i}x/2}}{g(x)}-\frac{1}{\sin\frac{x}{2}}-\frac{a'''(1)i\mathrm{e}^{\mathrm{i}x/2}}{3a''(1)}\right)\frac{\mathrm{d}x}{\sin\frac{x}{2}}.\end{aligned}$$

Finally, using the formulas $a'''(1)/a''(1)=-1-ig'''(0)/3g''(0)$ and

$$\begin{aligned}-\frac{\mathrm{i}\mathrm{e}^{\mathrm{i}x}}{\sin\frac{x}{2}}\frac{a'''(1)}{3a''(1)} &= \mathrm{i}\left(\cot\frac{x}{2}+\mathrm{i}\right)\left(1+\frac{\mathrm{i}g'''(0)}{3g''(0)}\right)\\ &= -1-\frac{g'''(0)\cot\frac{x}{2}}{3g''(0)}+\mathrm{i}\left(\cot\frac{x}{2}-\frac{g'''(0)}{3g''(0)}\right)\end{aligned}$$

and taking the real part, we arrive at

$$\begin{aligned}\operatorname{Re}\alpha &= 1+\frac{1}{4\pi}\int_{-\pi}^{\pi}\left(\frac{g'(x)\cot\frac{x}{2}}{g(x)}-\frac{1}{\sin^2\frac{x}{2}}-1-\frac{g'''(0)\cot\frac{x}{2}}{3g''(0)}\right)\mathrm{d}x\\ &= \frac{1}{4\pi}\int_{-\pi}^{\pi}\left(\frac{g'(x)}{g(x)}-\cot\frac{x}{2}-\frac{g'''(0)}{3g''(0)}\right)\cot\frac{x}{2}\,\mathrm{d}x. \quad \square\end{aligned}$$

In addition to the function $d_0(\lambda)$ given by (14) we need the function $d_1(\lambda)$ defined by

$$d_1(\lambda)=\frac{1}{|h_\lambda(\mathrm{e}^{\mathrm{i}\varphi_1(\lambda)})h_\lambda(\mathrm{e}^{\mathrm{i}\varphi_2(\lambda)})|}\prod_{k,s=1}^{r-1}\left(1-\frac{1}{u_k(\lambda)\overline{u}_s(\lambda)}\right)^{-1}. \tag{21}$$

Lemma 2.4. *The functions d_0 and d_1 are real-valued, bounded and bounded away from zero on* $[0, M]$.

In what follows, we frequently suppress the dependence on λ.

Proof. For d_1, the assertion follows from the equality

$$\prod_{k,s=1}^{r-1}\left(1-\frac{1}{u_k\overline{u}_s}\right)=\prod_{k=1}^{r-1}\left(1-\frac{1}{|u_k|^2}\right)\prod_{s<k}\left|1-\frac{1}{u_k\overline{u}_s}\right|^2.$$

As for d_0, it is evident that $|d_0|$ is bounded and bounded away from zero on $[0, M]$. To see that $d_0>0$, note first that comparison of (11) and (12) gives

$$a_r=\overline{a}_r\prod_{k=1}^{2r}\overline{z}_k=\overline{a}_r\mathrm{e}^{-\mathrm{i}\varphi_1}\mathrm{e}^{-\mathrm{i}\varphi_2}\prod_{k=1}^{r-1}\frac{\overline{u}_k}{u_k},$$

whence

$$2\ \arg a_r + 2\ \arg\sigma + 2\sum_{k=1}^{r-1}\arg u_k = 0 \pmod{2\pi}.$$

Consequently,

$$\arg d_0 = r\pi + \arg a_r + \arg\sigma + \sum_{k=1}^{r-1}\arg u_k = 0 \pmod{\pi},$$

which shows that $d_0(\lambda)$ is real. By (15),

$$a(t) = d_0(0)|1-t|^2\,|h_0(t)|^2$$

and thus $d_0(0) > 0$. As $d_0(\lambda)$ is never zero and depends continuously on λ on $[0, M]$, it results that $d_0(\lambda) > 0$ for all $\lambda \in [0, M]$. □

We finally relate $\varphi(\lambda)$ and $\theta(\lambda)$ to the terms $G(a-\lambda)$ and $E(a-\lambda)$.

Proposition 2.5. *For every* $\lambda \in (0, M)$,

$$|G(a-\lambda)| = d_0(\lambda), \quad G(a-\lambda) = d_0(\lambda)\mathrm{e}^{\mathrm{i}\varphi(\lambda)},$$
$$|E(a-\lambda)| = \frac{d_1(\lambda)}{2\ \sin\varphi(\lambda)}, \quad E(a-\lambda) = \frac{d_1(\lambda)}{2\mathrm{i}\ \sin\varphi(\lambda)}\mathrm{e}^{\mathrm{i}(\varphi(\lambda)+\theta(\lambda))}.$$

Proof. We start with the Fourier series

$$\log\left(1-\frac{t}{\mathrm{e}^{\mathrm{i}\varphi_1}}\right) = -\sum_{\ell=1}^{\infty}\frac{t^\ell}{\ell\mathrm{e}^{\mathrm{i}\ell\varphi_1}}, \qquad \log\left(1-\frac{\mathrm{e}^{\mathrm{i}\varphi_2}}{t}\right) = -\sum_{\ell=1}^{\infty}\frac{\mathrm{e}^{\mathrm{i}\ell\varphi_2}}{\ell t^\ell},$$
$$\log h(t) = \sum_{k=1}^{r-1}\log\left(1-\frac{t}{u_k}\right) = -\sum_{k=1}^{r-1}\sum_{\ell=1}^{\infty}\frac{t^\ell}{\ell u_k^\ell},$$
$$\log\overline{h}(t) = \sum_{k=1}^{r-1}\log\left(1-\frac{1}{t\overline{u}_k}\right) = -\sum_{k=1}^{r-1}\sum_{\ell=1}^{\infty}\frac{1}{\ell\overline{u}_k^\ell t^\ell}.$$

From (15) we therefore obtain that

$$(\log(a-\lambda))_0 = \log d_0 + \mathrm{i}\varphi + 2\mu\pi\mathrm{i} \quad (\mu\in\mathbf{Z})$$

and hence $|G(a-\lambda)| = d_0$ (by Lemma 2.4) and $G(a-\lambda) = d_0\mathrm{e}^{\mathrm{i}\varphi}$. Furthermore, from (15) we also infer that

$$\begin{aligned}\sum_{\ell=1}^{\infty}\ell(\log(a-\lambda))_\ell(\log(a-\lambda))_{-\ell} &= \sum_{\ell=1}^{\infty}\ell\left(\frac{1}{\ell\mathrm{e}^{\mathrm{i}\ell\varphi_1}}+\sum_{k=1}^{r-1}\frac{1}{\ell u_k^\ell}\right)\left(\frac{\mathrm{e}^{\mathrm{i}\ell\varphi_2}}{\ell}+\sum_{k=1}^{r-1}\frac{1}{\ell\overline{u}_k^\ell}\right)\\
&= \sum_{\ell=1}^{\infty}\frac{\mathrm{e}^{-2\mathrm{i}\ell\varphi}}{\ell} + \sum_{k=1}^{r-1}\sum_{\ell=1}^{\infty}\frac{1}{\ell}\frac{1}{\overline{u}_k^\ell}\frac{1}{\mathrm{e}^{\mathrm{i}\ell\varphi_1}} + \sum_{k=1}^{r-1}\sum_{\ell=1}^{\infty}\frac{1}{\ell}\frac{\mathrm{e}^{\mathrm{i}\ell\varphi_2}}{u_k^\ell} + \sum_{k=1}^{r-1}\sum_{s=1}^{r-1}\sum_{\ell=1}^{\infty}\frac{1}{\ell}\frac{1}{u_k^\ell\overline{u}_s^\ell}\\
&= -\log(1-\mathrm{e}^{-2\mathrm{i}\varphi}) - \sum_{k=1}^{r-1}\log\left(1-\frac{\mathrm{e}^{-\mathrm{i}\varphi_1}}{\overline{u}_k}\right)\\
&\quad - \sum_{k=1}^{r-1}\log\left(1-\frac{\mathrm{e}^{\mathrm{i}\varphi_2}}{u_k}\right) - \sum_{k=1}^{r-1}\sum_{s=1}^{r-1}\log\left(1-\frac{1}{u_k\overline{u}_s}\right)\\
&= -\log(\mathrm{e}^{-\mathrm{i}\varphi}\,2\mathrm{i}\sin\varphi) - \log\overline{h}(\mathrm{e}^{\mathrm{i}\varphi_1}) - \log h(\mathrm{e}^{\mathrm{i}\varphi_1}) - \sum_{k=1}^{r-1}\sum_{s=1}^{r-1}\log\left(1-\frac{1}{u_k\overline{u}_s}\right).\end{aligned}$$

Thus,

$$E(a-\lambda) = \frac{\mathrm{e}^{\mathrm{i}\varphi}}{2\mathrm{i}\sin\varphi}\,\frac{1}{\overline{h(\mathrm{e}^{\mathrm{i}\varphi_1})}h(\mathrm{e}^{\mathrm{i}\varphi_2})}\prod_{k,s=1}^{r-1}\left(1-\frac{1}{u_k\overline{u}_s}\right)^{-1}.$$

Since

$$\overline{h(e^{i\varphi_1})}h(e^{i\varphi_2}) = \frac{\overline{h(e^{i\varphi_1})}}{\overline{h(e^{i\varphi_2})}}\,|h(e^{i\varphi_2})|^2$$
$$= e^{-i\theta}\left|\frac{h(e^{i\varphi_1})}{h(e^{i\varphi_2})}\right|\,|h(e^{i\varphi_2})|^2 = e^{-i\theta}|h(e^{i\varphi_1})h(e^{i\varphi_2})|, \tag{22}$$

we get from (21) that

$$E(a-\lambda) = \frac{d_1}{2i\sin\varphi}e^{i(\varphi+\theta)}.$$

Lemma 2.4 tells us that $d_1 > 0$, and we know that $\varphi \in (0,\pi)$. This gives the asserted formula for the modulus of $E(a-\lambda)$. □

3. Determinants

The purpose of this section is to establish a formula for the Toeplitz determinant $\det T_n(a-\lambda)$ that will allow us to analyze the asymptotics of the eigenvalues of $T_n(a)$ as $n\to\infty$. This section also contains the proof of Theorem 1.1.

Widom [4] proved that if $\lambda \in \mathbf{C}$ and the points $z_1(\lambda),\ldots,z_{2r}(\lambda)$ are pairwise distinct, then the determinant of $T_n(a-\lambda)$ is

$$\det T_n(a-\lambda) = \sum_{J\subset\mathcal{Z},|J|=r} C_J W_J^n \tag{23}$$

where the sum is over all subsets J of cardinality r of the set $\mathcal{Z}$ given by (13) and, with $\bar{J} := \mathcal{Z}\setminus J$,

$$C_J = \prod_{z\in J} z^r \prod_{z\in J,w\in\bar{J}} \frac{1}{z-w}, \qquad W_J = (-1)^r a_r \prod_{z\in J} z.$$

Lemma 3.1. *Let $\lambda \in (0,M)$ and put*

$$J_1 = \{u_1,\ldots,u_{r-1},e^{i\varphi_1}\}, \qquad J_2 = \{u_1,\ldots,u_{r-1},e^{i\varphi_2}\}.$$

Then

$$W_{J_1} = d_0 e^{i\varphi}, \qquad C_{J_1} = \frac{d_1 e^{i(\varphi+\theta)}}{2i\,\sin\varphi},$$
$$W_{J_2} = d_0 e^{-i\varphi}, \qquad C_{J_2} = -\frac{d_1 e^{-i(\varphi+\theta)}}{2i\,\sin\varphi}.$$

Proof. We henceforth abbreviate $\prod_{k=1}^{r-1}$ to $\prod_k$. Obviously,

$$W_{J_1} = (-1)^r a_r\Big(\prod_k u_k\Big)e^{i\varphi_1} = (-1)^r a_r\Big(\prod_k u_k\Big)e^{i\sigma}e^{i\varphi} = d_0 e^{i\varphi}.$$

Further, C_{J_1} equals

$$\frac{\Big(\prod_k u_k^r\Big)e^{ir\varphi_1}}{(e^{i\varphi_1}-e^{i\varphi_2})\prod_k\prod_s\Big(u_k-\frac{1}{\bar{u}_s}\Big)\prod_k(u_k-e^{i\varphi_2})\prod_k\Big(e^{i\varphi_1}-\frac{1}{\bar{u}_k}\Big)}$$
$$= \frac{e^{ir\varphi_1}}{e^{i\sigma}(e^{i\varphi}-e^{-i\varphi})\prod_k\prod_s\Big(1-\frac{1}{u_k\bar{u}_s}\Big)\prod_k(1-\frac{e^{i\varphi_2}}{u_k})e^{i(r-1)\varphi_1}\prod_k\Big(1-\frac{e^{-i\varphi_1}}{\bar{u}_k}\Big)}$$
$$= \frac{e^{i\varphi}}{2i\,\sin\varphi\prod_k\prod_s\Big(1-\frac{1}{u_k\bar{u}_s}\Big)h(e^{i\varphi_2})\overline{h(e^{i\varphi_1})}},$$

which in conjunction with (21) and (22) gives the asserted formula for C_{J_1}. The proof for J_2 is analogous. □

Theorem 3.2. *For every $\lambda \in (0,M)$ and every $\delta < \delta_0$,*

$$\det T_n(a-\lambda) = \frac{d_1(\lambda)d_0^n(\lambda)}{\sin\varphi(\lambda)}\Big[\sin\Big((n+1)\varphi(\lambda)+\theta(\lambda)\Big)+O(e^{-\delta n})\Big].$$

Proof. Fix sufficiently small numbers $\alpha > 0$ and $\beta > 0$. Given a neighborhood $U \subset \mathbf{C}$ of $[0, M]$ and $\lambda \in U$, we denote by $z_1(\lambda), \dots, z_{2r}(\lambda)$ the zeros defined by (11). If $\lambda \in [0, M]$, the zeros are listed in (13). Since the zeros depend continuously on λ, we conclude that if U is sufficiently small, then $r-1$ zeros $z_1(\lambda), \dots, z_{r-1}(\lambda)$ satisfy $|z_k(\lambda)| > e^{\delta_0-\alpha}$, two zeros $z_r(\lambda)$ and $z_{r+1}(\lambda)$ are located in the annulus $\{z \in \mathbf{C} : e^{-\beta} < |z| < e^{\beta}\}$, while for the remaining zeros $z_{r+2}(\lambda), \dots, z_{2r}(\lambda)$ we have $|z_s(\lambda)| < e^{\alpha-\delta_0}$.

We denote by $D_r(z_0)$ the disk $\{z \in \mathbf{C} : |z - z_0| < r\}$ and by $\partial D_r(z_0)$ the boundary circle. A point $\lambda_0 \in \mathbf{C}$ is called a branch point if two of the zeros $z_1(\lambda_0), \dots, z_{2r}(\lambda_0)$ coincide. Pick $\lambda_0 \in [0, M]$. If λ_0 is not a branch point, then the zeros are all analytic functions of λ in a neighborhood of λ_0. In case λ_0 is a branch point, there are a natural number $m \geq 2$, an $\varepsilon > 0$, and a uniformization parameter ζ such that for $\zeta \in D_0(2\varepsilon)$ we may write $\lambda = \lambda_0 + \zeta^m$ and $z_k(\lambda) = \Phi_k(\zeta)$ $(1 \leq k \leq 2r)$ with analytic functions Φ_k in $D_0(2\varepsilon)$. The case where λ_0 is not a branch point can be included into this setting by choosing $m = 1$. As the number of branch points in all of $\mathbf{C}$ is finite, we may assume that $V_{\lambda_0} := \{\lambda_0 + \zeta^m : |\zeta| < 2\varepsilon\}$ does not contain a branch point different from λ_0 itself and that V_{λ_0} is contained in U. If $\zeta \in \partial D_0(\varepsilon)$, then $z_1(\lambda), \dots, z_{2r}(\lambda)$ are pairwise distinct and we can employ Widom's formula. Let

$$J_1 = \{z_1(\lambda), \dots, z_{r-1}(\lambda), z_r(\lambda)\}, \qquad J_2 = \{z_1(\lambda), \dots, z_{r-1}(\lambda), z_{r+1}(\lambda)\}.$$

Suppose $J \subset \mathcal{Z} = \mathcal{Z}(\lambda)$, $|J| = r$, $J \neq J_1$, $J \neq J_2$. If J contains both $z_r(\lambda)$ and $z_{r+1}(\lambda)$, then one of the numbers $z_k(\lambda)$ with $1 \leq k \leq r-1$ is missing and hence

$$\frac{|W_J^n|}{|W_{J_1}^n|} \leq \left|\frac{z_{r+1}(\lambda)}{z_k(\lambda)}\right|^n \leq \left(\frac{e^{\beta}}{e^{\delta_0-\alpha}}\right)^n = e^{-(\delta_0-\alpha-\beta)n}.$$

In the case where neither $z_r(\lambda)$ nor $z_{r+1}(\lambda)$ belong to J, the set J contains a number $z_s(\lambda)$ with $r+2 \leq s \leq 2r$. This implies that

$$\frac{|W_J^n|}{|W_{J_1}^n|} \leq \left|\frac{z_s(\lambda)}{z_r(\lambda)}\right|^n \leq \left(\frac{e^{\alpha-\delta_0}}{e^{-\beta}}\right)^n = e^{-(\delta_0-\alpha-\beta)n}.$$

Obviously,

$$\frac{|W_{J_2}^n|}{|W_{J_1}^n|} = \left|\frac{z_{r+1}(\lambda)}{z_r(\lambda)}\right|^n \leq e^{2\beta n}.$$

Since $z_1(\lambda), \dots, z_{2r}(\lambda)$ are pairwise distinct, we have

$$\min_{|\zeta|=\varepsilon} \min_{j \neq \ell} |z_j(\lambda) - z_\ell(\lambda)| > 0.$$

Thus, $\max\{|C_J| : |\zeta| = \varepsilon\} < \infty$. In summary, there is a constant $K_0 < \infty$ such that $|g_n(\zeta)| \leq K_0 e^{-(\delta_0-\alpha-3\beta)n}$ for all $\zeta \in \partial D_0(\varepsilon)$ where

$$g_n(\zeta) = \frac{1}{W_{J_1}(\lambda)} \left(\det T_n(a-\lambda) - C_{J_1}(\lambda) W_{J_1}^n(\lambda) - C_{J_2}(\lambda) W_{J_2}^n(\lambda)\right)\Big|_{\lambda=\lambda_0+\zeta^m}.$$

The function g_n is obviously analytic in $D_0(2\varepsilon) \setminus \{0\}$. However, due to the term $z_r(\zeta^m) - z_{r+1}(\zeta^m)$ in the denominators of $C_{J_1}(\zeta^m)$ and $C_{J_2}(\zeta^m)$, it need not be analytic at $\zeta = 0$. So let us consider

$$G_n(\zeta) = (z_r(\zeta^m) - z_{r+1}(\zeta^m)) g_n(\zeta).$$

This is an analytic function in $D_0(2\varepsilon)$ that results from g_n by multiplication by a bounded function. Hence

$$|G_n(\zeta)| \leq K e^{-(\delta_0-\alpha-3\beta)n} \tag{24}$$

with some constant $K < \infty$ for all $\zeta \in \partial D_0(\varepsilon)$. The maximum modulus principle now guarantees (24) for all $\zeta \in D_0(\varepsilon)$. We may choose $\alpha > 0$ and $\beta > 0$ so that $\delta_0 - \alpha - 3\beta = \delta$. It follows that

$$|\det T_n(a-\lambda) - C_{J_1}(\lambda) W_{J_1}^n(\lambda) - C_{J_2}(\lambda) W_{J_2}^n(\lambda)| \leq K \frac{|W_{J_1}(\lambda)|^n}{|z_r(\lambda) - z_{r+1}(\lambda)|} e^{-\delta n} \tag{25}$$

for all $\lambda \in U_{\lambda_0} := \{\lambda_0 + \zeta^m : |\zeta| < \varepsilon\}$.

Since $[0, M]$ is compact, we get (25) for all $\lambda \in [0, M]$. But if $\lambda \in (0, M)$, then, by Lemmas 3.1 and 2.4, $|W_{J_1}|^n = d_0^n$,

$$C_{J_1} W_{J_1}^n + C_{J_2} W_{J_2}^n = \frac{d_1 d_0^n}{\sin\varphi} \sin((n+1)\varphi + \theta),$$

$$|z_r - z_{r+1}| = |e^{i\varphi_1} - e^{i\varphi_2}| = 2 \sin\frac{\varphi_1 - \varphi_2}{2} = 2 \sin\varphi.$$

Thus, again by Lemma 2.4 and for $\lambda \in (0, M)$,

$$\left|\det T_n(a-\lambda) - \frac{d_1 d_0^n}{\sin\varphi}\,\sin((n+1)\varphi+\theta)\right| = O\left(\frac{d_0^n}{\sin\varphi}\mathrm{e}^{-\delta n}\right) = O\left(\frac{d_1 d_0^n}{\sin\varphi}\mathrm{e}^{-\delta n}\right). \quad \square$$

Proof of Theorem 1.1. This theorem is now almost immediate. Indeed, from Proposition 2.5 we know that

$$E(a-\lambda)\,G(a-\lambda)^n + \overline{E(a-\lambda)G(a-\lambda)}^{\,n} = \frac{d_1 d_0^n}{\sin\varphi}\sin((n+1)\varphi+\theta),$$

$$2\,|E(a-\lambda)|\,|G(a-\lambda)|^n = \frac{d_1 d_0^n}{\sin\varphi},$$

and hence Theorem 1.1 is nothing but Theorem 3.2 in other terms. $\square$

4. Approximations for the eigenvalues

In this section we prove Theorem 1.2 and prepare the proofs of Theorems 1.4 and 1.5.

Lemma 4.1. *There is a natural number $n_0 = n_0(a)$ such that if $n \ge n_0$, then the function*

$$f_n : [0, M] \to [0, (n+1)\pi], \quad f_n(\lambda) = (n+1)\varphi(\lambda) + \theta(\lambda)$$

is bijective and increasing.

Proof. We have

$$f_n'(\lambda) = \varphi'(\lambda)\left(n + 1 - \frac{\theta'(\lambda)}{\varphi'(\lambda)}\right)$$

for $\lambda \in (0, M)$. From Lemmas 2.1 and 2.2 we infer that $|\theta'(\lambda)/\varphi'(\lambda)|$ has a finite limit as $\lambda \to 0+0$. The analogs of Lemmas 2.1 and 2.2 for $\lambda \to M-0$ are also true. Thus, $|\theta'(\lambda)/\varphi'(\lambda)|$ approaches a finite limit as $\lambda \to M-0$. It follows that $|\theta'(\lambda)/\varphi'(\lambda)|$ is bounded on $(0, M)$. This in conjunction with (10) shows that there is an n_0 such that

$$f_n'(\lambda) \ge \varphi'(\lambda)\frac{n}{2} \ge \frac{\varrho n}{2} > 0 \tag{26}$$

for all $n \ge n_0$ and all $\lambda \in (0, M)$. Since $\varphi(0) = \theta(0) = 0$, $\varphi(M) = \pi$, and $\theta(M) = 0$, we arrive at the assertion. $\square$

Proof of Theorem 1.2. The first part of the theorem is just Lemma 4.1, which also implies that there are uniquely determined $\lambda_{j,*}^{(n)} \in (0, M)$ such that $f_n(\lambda_{j,*}^{(n)}) = \pi j$. We have $0 < \lambda_j^{(n)} < M$ for the eigenvalues of $T_n(a)$. Since $d_0, d_1, \sin\varphi$ do not vanish on $(0, M)$, we deduce from Theorem 3.2 that $\sin f_n(\lambda_j^{(n)}) = O(\mathrm{e}^{-\delta n})$. Again using Lemma 4.1, we conclude that $f(\lambda_j^{(n)}) = \pi j + O(\mathrm{e}^{-\delta n})$. Clearly,

$$f_n(\lambda_j^{(n)}) - f_n(\lambda_{j,*}^{(n)}) = f_n'(\xi_{j,n})(\lambda_j^{(n)} - \lambda_{j,*}^{(n)})$$

with some $\xi_{j,n}$ between $\lambda_j^{(n)}$ and $\lambda_{j,*}^{(n)}$. Taking into account (26) and the estimate

$$|f_n(\lambda_j^{(n)}) - f_n(\lambda_{j,*}^{(n)})| = |\pi j + O(\mathrm{e}^{-\delta n}) - \pi j| = O(\mathrm{e}^{-\delta n}),$$

we obtain that $|\lambda_j^{(n)} - \lambda_{j,*}^{(n)}| = O(\mathrm{e}^{-\delta n})$, which completes the proof. $\square$

Here is an iteration procedure for approximating the numbers $\lambda_{j,*}^{(n)}$ and thus the eigenvalues $\lambda_j^{(n)}$. We know that the function $\varphi : [0, M] \to [0, \pi]$ is bijective and increasing. Let $\psi : [0, \pi] \to [0, M]$ be the inverse function. The equation

$$(n+1)\varphi(\lambda) + \theta(\lambda) = \pi j$$

is equivalent to the equation

$$\lambda = \psi\left(\frac{\pi j - \theta(\lambda)}{n+1}\right).$$

We define $\lambda_{j,0}^{(n)}, \lambda_{j,1}^{(n)}, \lambda_{j,2}^{(n)}, \ldots$ iteratively by

$$\lambda_{j,0}^{(n)} = \psi\left(\frac{\pi j}{n+1}\right), \qquad \lambda_{j,k+1}^{(n)} = \psi\left(\frac{\pi j - \theta(\lambda_{j,k}^{(n)})}{n+1}\right) \quad \text{for } k = 0, 1, 2, \ldots.$$

Recall that ϱ is defined by (10) and put

$$\gamma = \sup_{\lambda \in (0,M)} \left| \frac{\theta'(\lambda)}{\varphi'(\lambda)} \right|.$$

Theorem 4.2. *If $n \geq \gamma$ and $1 \leq j \leq n$, then $\lambda_{j,k}^{(n)} \to \lambda_{j,*}^{(n)}$ as $k \to \infty$ and*

$$|\lambda_{j,k}^{(n)} - \lambda_{j,*}^{(n)}| \leq \frac{1}{\varrho} \frac{n+1}{n+1-\gamma} \left(\frac{\gamma}{n+1} \right)^k \frac{|\theta(\lambda_{j,0}^{(n)})|}{n+1}$$

for all $k \geq 0$.

Proof. Fix n and j and put $\varphi_k = \varphi(\lambda_{j,k}^{(n)})$. Then

$$\varphi_0 = \frac{\pi j}{n+1}, \qquad \varphi_{k+1} = \frac{\pi j - \theta(\psi(\varphi_k))}{n+1} \quad \text{for } k = 0, 1, 2, \ldots.$$

We have

$$\varphi_{k+1} - \varphi_k = \frac{\theta'(\psi(\xi_k))\psi'(\xi_k)}{n+1} (\varphi_k - \varphi_{k-1})$$

with some ξ_k between φ_{k-1} and φ_k. Since

$$|\theta'(\psi(\xi))\psi'(\xi)| = \left| \frac{\theta'(\psi(\xi))}{\varphi'(\psi(\xi))} \right| \leq \gamma$$

for $\xi \in (0, \pi)$, we get

$$|\varphi_{k+1} - \varphi_k| \leq \left(\frac{\gamma}{n+1} \right)^k |\varphi_1 - \varphi_0| = \left(\frac{\gamma}{n+1} \right)^k \frac{|\theta(\lambda_{j,0}^{(n)})|}{n+1}$$

and thus, by summing up a geometric series,

$$|\varphi_{k+m} - \varphi_k| \leq \frac{n+1}{n+1-\gamma} \left(\frac{\gamma}{n+1} \right)^k \frac{|\theta(\lambda_{j,0}^{(n)})|}{n+1}$$

for all $m \geq 1$. It follows that φ_k converges to the solution of the equation

$$y_j = \frac{\pi j - \theta(\psi(y_j))}{n+1}$$

and that

$$|\varphi_k - y_j| \leq \frac{n+1}{n+1-\gamma} \left(\frac{\gamma}{n+1} \right)^k \frac{|\theta(\lambda_{j,0}^{(n)})|}{n+1}. \tag{27}$$

Because $y_j = \varphi(\lambda_{j,*}^{(n)})$ and $\varphi_k = \varphi(\lambda_{j,k}^{(n)})$, we obtain that

$$|\varphi_k - y_j| = |\varphi'(\eta)| \, |\lambda_{j,k}^{(n)} - \lambda_{j,*}^{(n)}| \tag{28}$$

with some η between $\lambda_{j,k}^{(n)}$ and $\lambda_{j,*}^{(n)}$. Combining (27) and (28) we arrive at the assertion. □

To establish asymptotic formulas for the eigenvalues, we need the following modification of Theorem 4.2.

Theorem 4.3. *There is a constant γ_0 depending only on a such that if n is sufficiently large, then*

$$|\lambda_{j,k}^{(n)} - \lambda_{j,*}^{(n)}| \leq \gamma_0 \left(\frac{\gamma}{n+1} \right)^k \frac{1}{n+1} \frac{|\theta(\lambda_{j,0}^{(n)})|}{\varphi'(\lambda_{j,0}^{(n)})}$$

for all $1 \leq j \leq n$ and all $k \geq 0$.

Proof. Let $n+1 > 2\gamma$. Then $(n+1)/(n+1-\gamma) < 2$. Combining (27) and (28) we get

$$|\lambda_{j,k}^{(n)} - \lambda_{j,*}^{(n)}| \leq \frac{2}{\varphi'(\eta_0)} \left(\frac{\gamma}{n+1} \right)^k \frac{|\theta(\lambda_{j,0}^{(n)})|}{n+1}$$

where η_0 is the point in the segment between $\lambda_{j,k}^{(n)}$ and $\lambda_{j,*}^{(n)}$ at which $\varphi'(\eta)$ attains its minimum. Thus, we have to show that

$$\frac{1}{\varphi'(\eta_0)} \le \frac{\gamma_0}{\varphi'(\lambda_{j,0}^{(n)})}.$$

Suppose $j/(n+1) \le 1/2$. The case where $j/(n+1) \ge 1/2$ can be disposed of analogously. We have

$$\lambda_{j,0}^{(n)} = \psi\left(\frac{\pi j}{n+1}\right) \le \psi\left(\frac{\pi}{2}\right) < \psi\left(\frac{2\pi}{3}\right).$$

Theorem 4.2 tells us that

$$|\lambda_{j,*}^{(n)} - \lambda_{j,0}^{(n)}| \le \frac{2}{\varrho}\,\frac{|\theta(\lambda_{j,0}^{(n)})|}{n+1} \le \frac{2}{\varrho}\,\frac{\|\theta\|_\infty}{n+1}, \tag{29}$$

where $\|\theta\|_\infty$ is the maximum of θ on $[0, M]$. Consequently, $\lambda_{j,*}^{(n)} < \psi(2\pi/3)$ for all $n \ge n_1$. Since, again by Theorem 4.2,

$$|\lambda_{j,k}^{(n)} - \lambda_{j,*}^{(n)}| \le \frac{2}{\varrho}\,\frac{|\theta(\lambda_{j,0}^{(n)})|}{n+1} \le \frac{2}{\varrho}\,\frac{\|\theta\|_\infty}{n+1}, \tag{30}$$

it follows that $\lambda_{j,k}^{(n)} < \psi(3\pi/4) =: M_0$ for all $n \ge n_2 \ge n_1$ and all $k \ge 0$. By Lemma 2.1, there are constants $0 < \gamma_1 < \gamma_2 < \infty$ such that

$$\gamma_1\,\lambda^{-1/2} \le \varphi'(\lambda) \le \gamma_2\,\lambda^{-1/2}$$

for all $\lambda \in (0, M_0)$. We have

$$\frac{1}{\varphi'(\eta_0)} = \frac{1}{\varphi'(\lambda_{j,0}^{(n)})}\,\frac{\varphi'(\lambda_{j,0}^{(n)})}{\varphi'(\eta_0)}$$

and as $\lambda_{j,0}^{(n)} < M_0$ and $\eta_0 < M_0$, we conclude that

$$\frac{\varphi'(\lambda_{j,0}^{(n)})}{\varphi'(\eta_0)} \le \frac{\gamma_2}{\gamma_1}\,\frac{\eta_0^{1/2}}{(\lambda_{j,0}^{(n)})^{1/2}} \le \frac{\gamma_2}{\gamma_1}\left(\max\left(\frac{\lambda_{j,k}^{(n)}}{\lambda_{j,0}^{(n)}}, \frac{\lambda_{j,*}^{(n)}}{\lambda_{j,0}^{(n)}}\right)\right)^{1/2}. \tag{31}$$

There exist constants $0 < \gamma_3 < \gamma_4 < \infty$ such that

$$\gamma_3 x^2 \le \psi(x) \le \gamma_4 x^2$$

for all $x \in [0, \pi]$. Lemma 2.2 shows that $\theta(\lambda) \le \gamma_5 \lambda^{1/2}$ for all $\lambda \in [0, M]$. Thus,

$$\begin{aligned}\frac{|\theta(\lambda_{j,0}^{(n)})|}{n+1} &\le \gamma_5\,\frac{(\lambda_{j,0}^{(n)})^{1/2}}{n+1} = \gamma_5\,\frac{(\psi(\pi j/(n+1)))^{1/2}}{n+1} \le \gamma_5\gamma_4^{1/2}\,\frac{\pi j}{(n+1)^2}\\ &\le \gamma_5\gamma_4^{1/2}\,\frac{\pi^2 j^2}{(n+1)^2} \le \gamma_5\gamma_4^{1/2}\gamma_3^{-1}\,\psi\left(\frac{\pi j}{n+1}\right) = \gamma_5\gamma_4^{1/2}\gamma_3^{-1}\,\lambda_{j,0}^{(n)}.\end{aligned}$$

Inserting this in (29) and (30) we get

$$\lambda_{j,*}^{(n)} \le \lambda_{j,0}^{(n)} + \frac{2}{\varrho}\,\gamma_5\gamma_4^{1/2}\gamma_3^{-1}\,\lambda_{j,0}^{(n)}, \qquad \lambda_{j,k}^{(n)} \le \lambda_{j,0}^{(n)} + 2\cdot\frac{2}{\varrho}\,\gamma_5\gamma_4^{1/2}\gamma_3^{-1}\,\lambda_{j,0}^{(n)}.$$

This proves that (31) does not exceed

$$\gamma_0 := \frac{\gamma_2}{\gamma_1}\left(1 + 2\cdot\frac{2}{\varrho}\,\gamma_5\gamma_4^{1/2}\gamma_3^{-1}\right)^{1/2}. \quad \square$$

5. Asymptotics of the eigenvalues

This section is devoted to the proofs of Theorems 1.3–1.5. It also contains some consequences of our main results.

Proof of Theorem 1.3. From Theorem 1.2 we know that $\lambda_j^{(n)} = \lambda_{j,*}^{(n)} + O(e^{-\delta n})$. Theorem 4.3 gives

$$\lambda_{j,*}^{(n)} = \lambda_{j,1}^{(n)} + O\left(\frac{|\theta(\lambda_{j,0}^{(n)})|}{\varphi'(\lambda_{j,0}^{(n)})n^2}\right)$$

with $\lambda_{j,0}^{(n)} = \psi(d)$. Since $1/\varphi'(\psi(d)) = \psi'(d)$, we obtain that

$$\lambda_j^{(n)} = \lambda_{j,1}^{(n)} + O\left(\frac{\psi'(d)\theta(\psi(d))}{n^2}\right).$$

Finally,

$$\lambda_{j,1}^{(n)} = \psi\left(d - \frac{\theta(\psi(d))}{n+1}\right) = \psi(d) - \frac{\psi'(d)\theta(\psi(d))}{n+1} + \frac{\psi''(\xi)}{2}\left(\frac{\theta(\psi(d))}{n+1}\right)^2$$

and ψ'' is bounded on $(0, \pi)$. This completes the proof. □

Proof of Theorem 1.4. If $j/n \to x$, then $d \to \pi x$. Consequently,

$$\psi(d) = \psi(\pi x) + \psi'(\pi x)(d - \pi x) + O((d - \pi x)^2),$$
$$\psi'(d) = \psi'(\pi x) + O(d - \pi x),$$
$$\theta(\psi(d)) = \theta(\psi(\pi x)) + \theta'(\psi(\pi x))\psi'(\pi x)(d - \pi x) + O((d - \pi x)^2).$$

These expansions in conjunction with (5) imply that

$$\lambda_j^{(n)} = \psi(\pi x) + \psi'(\pi x)(d - \pi x) - \frac{\psi'(\pi x)\theta(\psi(\pi x))}{n+1} + O((d - \pi x)^2) + O\left(\frac{1}{n^2}\right) + O\left((d - \pi x)\frac{1}{n}\right).$$

Because $|d - \pi x|(1/n) \le 2(d - \pi x)^2 + 2/n^2$, $\psi(\pi x) = \lambda_x$, and $\psi'(\pi x) = 1/\varphi'(\lambda_x)$, this completes the proof. □

Proof of Theorem 1.5. Again $\lambda_j^{(n)} = \lambda_{j,*}^{(n)} + O(e^{-\delta n})$ due to Theorem 1.2. From Theorem 4.3 we therefore get

$$\lambda_j^{(n)} = \lambda_{j,1}^{(n)} + O\left(\frac{|\theta(\lambda_{j,0}^{(n)})|}{\varphi'(\lambda_{j,0}^{(n)})\, n^2}\right) = \lambda_{j,1}^{(n)} + O\left(\frac{\psi'(d)|\theta(\psi(d))|}{n^2}\right);$$

recall that $\lambda_{j,0}^{(n)} = \psi(d)$ and $\varphi'(\psi(d))\psi'(d) = 1$. Since

$$\lambda_{j,1}^{(n)} = \psi\left(d - \frac{\theta(\psi(d))}{n+1}\right) = \sum_{k=0}^{3}(-1)^k \frac{\psi^{(k)}(d)}{k!}\left(\frac{\theta(\psi(d))}{n+1}\right)^k + O\left(\frac{1}{n^4}\right),$$

we obtain (6). By Lemmas 2.1 and 2.2,

$$\psi(d) = \frac{g''(0)}{2}\, d^2 + O(d^4) = O(d^2),$$
$$\psi'(d) = g''(0)\, d + O(d^3) = O(d),$$
$$\theta(\psi(d)) = -\frac{w_0}{2}\, d + O(d^3) = O(d).$$

Clearly, $\psi^{(k)}(d) = O(1)$ for $k \ge 0$. Hence for $k \ge 2$,

$$\psi^{(k)}(d)\left(\frac{\theta(\psi(d))}{n+1}\right)^k = O\left(\frac{d^k}{n^k}\right) = O\left(\frac{d^2}{n^2}\right) = O\left(\frac{j^2}{n^4}\right) = O\left(\frac{j^4}{n^4}\right).$$

The terms with $k = 0$ and $k = 1$ give

$$\begin{aligned}\psi(d) - \frac{\psi'(d)\theta(\psi(d))}{n+1} &= \frac{g''(0)}{2}d^2 + O(d^4) - \frac{1}{n+1}\left(g''(0)d + O(d^3)\right)\left(-\frac{w_0}{2}d + O(d^3)\right)\\ &= \frac{g''(0)}{2}\left(\frac{\pi j}{n+1}\right)^2 + \frac{g''(0)}{2}\left(\frac{\pi j}{n+1}\right)^2\frac{w_0}{n+1} + O\left(\frac{j^4}{n^4}\right).\end{aligned}$$

This is (7). Formula (8) is an immediate consequence of (7). Thus, the proof of Theorem 1.5 is complete. □

Remark 5.1. As already noted in the paragraph after Theorem 1.5, the preceding proof also works under the sole assumption that $j/n \le C_0$, yielding that the constants in the O terms depend on C_0 and a but on nothing else.

Remark 5.2. Proceeding as in the previous proofs but starting with $\lambda_{j,2}^{(n)}, \lambda_{j,3}^{(n)}, \ldots$ instead of $\lambda_{j,1}^{(n)}$ one can get as many terms of the expansion (4) as desired. For example, Theorem 4.3 gives

$$\lambda_{j,*}^{(n)} = \lambda_{j,2}^{(n)} + O\left(\frac{\psi'(d)\theta(\psi(d))}{n^3}\right) = \lambda_{j,2}^{(n)} + O\left(\frac{1}{n^3}\right)$$

with

$$\begin{aligned}\lambda_{j,2}^{(n)} &= \psi\left(d - \frac{\theta(\lambda_{j,1}^{(n)})}{n+1}\right) \\ &= \psi(d) - \psi'(d)\frac{\theta(\lambda_{j,1}^{(n)})}{n+1} + \frac{\psi''(d)}{2}\left(\frac{\theta(\lambda_{j,1}^{(n)})}{n+1}\right)^2 + O\left(\frac{1}{n^3}\right)\end{aligned}$$

and

$$\begin{aligned}\theta(\lambda_{j,1}^{(n)}) &= \theta\left(\psi\left(d - \frac{\theta(\psi(d))}{n+1}\right)\right) \\ &= \theta\left(\psi(d) - \frac{\psi'(d)\theta(\psi(d))}{n+1} + \frac{\psi''(d)}{2}\left(\frac{\theta(\psi(d))}{n+1}\right)^2 + O\left(\frac{1}{n^3}\right)\right) \\ &= \theta(\psi(d)) - \theta'(\psi(d))\left(\frac{\psi'(d)\theta(\psi(d))}{n+1} - \frac{\psi''(d)}{2}\left(\frac{\theta(\psi(d))}{n+1}\right)^2\right) \\ &\quad + \frac{\theta''(d)}{2}\left(\frac{\psi'(d)\theta(\psi(d))}{n+1}\right)^2 + O\left(\frac{1}{n^3}\right),\end{aligned}$$

which is more complicated but by one order better than (5). □

Finally, here are a few simple consequences of our main results.

Corollary 5.3. *Let $n \to \infty$. Then $\lambda_{j+1}^{(n)} - \lambda_j^{(n)}$ equals*

$$\frac{\pi^2\psi''(0)}{2}\,\frac{2j+1}{(n+1)^2} + O\left(\frac{j^3}{(n+1)^3}\right) \quad \text{as } j/n \to 0,$$

$$\frac{\pi}{\varphi'(\lambda_x)}\,\frac{1}{n+1} + O\left(\left(\frac{j}{n+1} - x\right)^2 + \frac{1}{n^2}\right) \quad \text{as } j/n \to x \in (0,1),$$

$$\frac{\pi^2|\psi''(\pi)|}{2}\,\frac{2n+1-2j}{(n+1)^2} + O\left(\left(1 - \frac{j}{n+1}\right)^2\right) \quad \text{as } j/n \to 1.$$

Proof. This is immediate from Theorem 1.4 and (8). □

Corollary 5.4. *Given $\varepsilon > 0$, there is an $n_0 = n_0(a, \varepsilon)$ such that if $n \ge n_0$ and $0 \le \alpha < \beta \le M$, then*

$$\left| |\{j : \lambda_j^{(n)} \in (\alpha,\beta)\}| - (n+1)\frac{\varphi(\beta) - \varphi(\alpha)}{\pi} - \frac{\theta(\beta) - \theta(\alpha)}{\pi} \right| < 1 + \varepsilon.$$

Proof. From Theorem 1.2 we know that if n is sufficiently large, then $\alpha < \lambda_j^{(n)} < \beta$ if and only if

$$A < (n+1)\varphi(\lambda_j^{(n)}) + \theta(\lambda_j^{(n)}) < B$$

where $A = (n+1)\varphi(\alpha) + \theta(\alpha)$ and $B = (n+1)\varphi(\beta) + \theta(\beta)$. By the same theorem,

$$(n+1)\varphi(\lambda_j^{(n)}) + \theta(\lambda_j^{(n)}) = \pi j + \varrho_j^{(n)}$$

where $|\varrho_j^{(n)}| \le C\mathrm{e}^{-\delta n}$ with some constant $C < \infty$ independent of j. Thus,

$$|\{j : \lambda_j^{(n)} \in (\alpha,\beta)\}| = \left|\left\{j : \frac{A}{\pi} < j + \frac{\varrho_j^{(n)}}{\pi} < \frac{B}{\pi}\right\}\right|.$$

We may assume that $C\mathrm{e}^{-\delta n} < \pi\varepsilon/2$. Then

$$\begin{aligned}\left|\left\{j : \frac{A}{\pi} < j + \frac{\varrho_j^{(n)}}{\pi} < \frac{B}{\pi}\right\}\right| &< \left|\left\{j : \frac{A}{\pi} - \frac{\varepsilon}{2} < j < \frac{B}{\pi} + \frac{\varepsilon}{2}\right\}\right| \\ &< \left(\frac{B}{\pi} + \frac{\varepsilon}{2}\right) - \left(\frac{A}{\pi} - \frac{\varepsilon}{2}\right) + 1 = \frac{B-A}{\pi} + 1 + \varepsilon\end{aligned}$$

and

$$\left|\left\{j : \frac{A}{\pi} < j + \frac{\varrho_j^{(n)}}{\pi} < \frac{B}{\pi}\right\}\right| > \left|\left\{j : \frac{A}{\pi} + \frac{\varepsilon}{2} < j < \frac{B}{\pi} - \frac{\varepsilon}{2}\right\}\right|$$
$$> \left(\frac{B}{\pi} - \frac{\varepsilon}{2}\right) - \left(\frac{A}{\pi} + \frac{\varepsilon}{2}\right) - 1 = \frac{B - A}{\pi} - 1 - \varepsilon. \quad \square$$

In [15] it is shown that

$$\left| |\{j : \lambda_j^{(n)} \in (\alpha, \beta)\}| - (n+1)\frac{\varphi(\beta) - \varphi(\alpha)}{\pi} \right| \le 6r$$

where r is the degree of the trigonometric polynomial $g(x) = a(e^{ix})$. As the increment of the argument of function (16) is at most 2π, the maximal value of θ on $(0, M)$ cannot exceed $2\pi(r-1)$. Thus, $\theta(\beta) - \theta(\alpha) \le 4\pi(r-1)$ and Corollary 5.4 therefore implies that

$$\left| |\{j : \lambda_j^{(n)} \in (\alpha, \beta)\}| - (n+1)\frac{\varphi(\beta) - \varphi(\alpha)}{\pi} \right| \le 4(r-1) + 1 + \varepsilon$$

for all sufficiently large n. Note that, however, our assumptions on a are stronger than those required in [15].

6. Examples

This section provides some numerical examples which reveal that our asymptotic formulas deliver not only extremely good approximations for large matrix dimensions but even good approximations for matrices of moderate size.

We consider $T_n(a)$, denote by $\lambda_j^{(n)}$ the jth eigenvalue, by $\lambda_{j,*}^{(n)}$ the approximation to $\lambda_j^{(n)}$ given by Theorem 1.2, and by $\lambda_{j,k}^{(n)}$ the kth approximation to $\lambda_j^{(n)}$ delivered by the iteration introduced in Section 4. We put

$$\Delta_*^{(n)} = \max_{1\le j\le n} |\lambda_j^{(n)} - \lambda_{j,*}^{(n)}|, \qquad \Delta_k^{(n)} = \max_{1\le j\le n} |\lambda_j^{(n)} - \lambda_{j,k}^{(n)}|.$$

We let w_0 be the constant (9), denote by

$$\lambda_{j,W}^{(n)} = \frac{g''(0)}{2}\left(\frac{\pi j}{n+1}\right)^2\left(1 + \frac{w_0}{n+1}\right)$$

Widom's approximation for the jth extreme eigenvalue given by (7), and put

$$\Delta_{j,W}^{(n)} = \frac{(n+1)^4}{\pi^4 j^4} |\lambda_j^{(n)} - \lambda_{j,W}^{(n)}|.$$

The computations in the following examples were performed using the computer algebra system PARI/GP [16], which is distributed under the terms of the GNU General Public License. To calculate the exponentially small errors $\Delta_*^{(n)}$, we used multi-precision arithmetic with 130 decimal digits and truncated power series with 70 terms. The quick calculation of the functions φ, θ, and ψ was based on polynomial interpolation of degree 61 with 1000 node points. At the extreme points 0 and M we made the exchanges $\mu = \sqrt{\lambda}$ and $\mu = \sqrt{M - \lambda}$. For example, we interpolated the function $\mu \mapsto \varphi(\mu^2)$ near $\mu = 0$ rather than $\lambda \mapsto \varphi(\lambda)$ near $\lambda = 0$. On a computer with a 2.8 GHz processor, the calculation of the interpolation polynomials took about 2 min in Example 6.4. The time to calculate $\lambda_{j,*}^{(n)}$ for a single value of j does not grow with n, and we calculated all eigenvalues for $n = 10000$ in 10 s.

In the following examples, the function g can always be checked to be strictly increasing on $(0, \varphi_0)$ and to be strictly decreasing on $(\pi_0, 2\pi)$. The values of φ_0 and of $g''(\varphi_0)$ will be explicitly given.

Example 6.1 (*A Symmetric Pentadiagonal Matrix*). Let $a(t) = 8 - 5t - 5t^{-1} + t^2 + t^{-2}$. In that case

$$g(x) = 8 - 10\cos x + 2\cos 2x = 4\sin^2\frac{x}{2} + 16\sin^4\frac{x}{2},$$

$\varphi_0 = \pi$, $g''(\varphi_0) = -18$, $a(\mathbf{T}) = [0, 20]$, and for $\lambda \in [0, 20]$, the roots of $a(z) - \lambda$ are $e^{-i\varphi(\lambda)}$, $e^{i\varphi(\lambda)}$, $u(\lambda)$, $1/u(\lambda)$ with

$$\varphi(\lambda) = \arccos\frac{5 - \sqrt{1+4\lambda}}{4} = 2\arcsin\frac{\sqrt{\sqrt{1+4\lambda} - 1}}{2\sqrt{2}},$$
$$u(\lambda) = \frac{5 + \sqrt{1+4\lambda}}{4} + \frac{\sqrt{5 + 2\lambda + 5\sqrt{1+4\lambda}}}{2\sqrt{2}}$$

and we have

$$g''(0) = 2, \qquad w_0 = \frac{4}{u(0) - 1} = 2\sqrt{5} - 2.$$

The errors $\Delta_*^{(n)}$ are

	$n = 10$	$n = 20$	$n = 50$	$n = 100$	$n = 150$
$\Delta_*^{(n)}$	$5.4 \cdot 10^{-7}$	$1.1 \cdot 10^{-11}$	$5.2 \cdot 10^{-25}$	$1.7 \cdot 10^{-46}$	$9.6 \cdot 10^{-68}$

and for $\Delta_k^{(n)}$ and $\Delta_{j,W}^{(n)}$ we have

	$n = 10$	$n = 100$	$n = 1000$	$n = 10\,000$
$\Delta_1^{(n)}$	$9.0 \cdot 10^{-2}$	$1.1 \cdot 10^{-4}$	$1.1 \cdot 10^{-6}$	$1.1 \cdot 10^{-8}$
$\Delta_2^{(n)}$	$2.2 \cdot 10^{-4}$	$2.8 \cdot 10^{-7}$	$2.9 \cdot 10^{-10}$	$2.9 \cdot 10^{-13}$
$\Delta_3^{(n)}$	$1.1 \cdot 10^{-5}$	$1.5 \cdot 10^{-9}$	$1.5 \cdot 10^{-13}$	$1.5 \cdot 10^{-17}$

	$n = 10$	$n = 100$	$n = 1000$	$n = 10\,000$	$n = 100\,000$
$\Delta_{1,W}^{(n)}$	1.462	1.400	1.383	1.381	1.381
$\Delta_{2,W}^{(n)}$	0.997	1.046	1.034	1.033	1.033
$\Delta_{3,W}^{(n)}$	0.840	0.979	0.970	0.968	0.968

Example 6.2 (*A Symmetric Heptadiagonal Matrix*). Consider

$$a(t) = 34 - 21t - 21t^{-1} + 8t^2 + 8t^{-2} - 4t^3 - 4t^{-3},$$
$$g(x) = 100 \sin^2 \frac{x}{2} - 256 \sin^4 \frac{x}{2} + 256 \sin^6 \frac{x}{2}.$$

Now $\varphi_0 = \pi$ and $g''(\varphi_0) = -178$. We have $g''(0) = 50$ and the two roots of the polynomial $z^3 a(z)$ that lie outside the unit disk are $u_1(0) = 2\mathrm{i}$ and $u_2(0) = -2\mathrm{i}$, which gives $w_0 = -8/5$. The tables show $\Delta_k^{(n)}$, $\Delta_k^{(n)}$, $\Delta_{j,W}^{(n)}$.

	$n = 10$	$n = 20$	$n = 50$	$n = 100$	$n = 150$
$\Delta_*^{(n)}$	$7.6 \cdot 10^{-3}$	$2.7 \cdot 10^{-5}$	$4.6 \cdot 10^{-12}$	$8.0 \cdot 10^{-23}$	$1.7 \cdot 10^{-33}$

	$n = 10$	$n = 100$	$n = 1000$	$n = 10\,000$
$\Delta_1^{(n)}$	$4.4 \cdot 10^{-1}$	$5.2 \cdot 10^{-3}$	$5.3 \cdot 10^{-5}$	$5.3 \cdot 10^{-7}$
$\Delta_2^{(n)}$	$3.9 \cdot 10^{-2}$	$7.5 \cdot 10^{-5}$	$7.6 \cdot 10^{-8}$	$7.6 \cdot 10^{-11}$
$\Delta_3^{(n)}$	$8.2 \cdot 10^{-3}$	$2.7 \cdot 10^{-6}$	$2.8 \cdot 10^{-10}$	$2.8 \cdot 10^{-14}$

	$n = 10$	$n = 100$	$n = 1000$	$n = 10\,000$	$n = 100\,000$
$\Delta_{1,W}^{(n)}$	8.51	12.65	13.16	13.21	13.22
$\Delta_{2,W}^{(n)}$	10.83	16.24	16.81	16.86	16.87
$\Delta_{3,W}^{(n)}$	9.92	16.88	17.48	17.54	17.54

Example 6.3 (*A Hermitian Pentadiagonal Matrix*). Let

$$a(t) = 8 + (-4 - 2\mathrm{i})t + (-4 - 2\mathrm{i})t^{-1} + it^2 - it^{-2},$$
$$g(x) = 8 - 8\cos x + 4\sin x - 2\sin 2x = 16 \sin^2 \frac{x}{2} + 16 \sin^3 \frac{x}{2} \cos \frac{x}{2}.$$

Here $\varphi_0 \approx 2.527$, $g''(\varphi_0) \approx -16.38$, $M \approx 18.73$, $g''(0) = 8$. The polynomial $z^2 a(z)$ has the roots 1, 1, $u(0)$, $1/\overline{u}(0)$ with $u(0) = -(\sqrt{3} + 2)i$. It follows that

$$w_0 = 4 \,\mathrm{Re}\, \frac{1}{u(0) - 1} = \sqrt{3} - 2. \tag{32}$$

Numerical results are in the tables.

	$n = 10$	$n = 20$	$n = 50$	$n = 100$	$n = 150$
$\Delta_*^{(n)}$	$3.8 \cdot 10^{-8}$	$2.8 \cdot 10^{-13}$	$2.9 \cdot 10^{-30}$	$5.9 \cdot 10^{-58}$	$1.5 \cdot 10^{-85}$

	$n = 10$	$n = 100$	$n = 1000$	$n = 10\,000$
$\Delta_1^{(n)}$	$7.2 \cdot 10^{-3}$	$8.2 \cdot 10^{-5}$	$8.4 \cdot 10^{-7}$	$8.4 \cdot 10^{-9}$
$\Delta_2^{(n)}$	$3.5 \cdot 10^{-4}$	$4.8 \cdot 10^{-7}$	$5.0 \cdot 10^{-10}$	$5.0 \cdot 10^{-13}$
$\Delta_3^{(n)}$	$1.7 \cdot 10^{-5}$	$3.1 \cdot 10^{-9}$	$3.2 \cdot 10^{-13}$	$3.2 \cdot 10^{-17}$

	$n = 10$	$n = 100$	$n = 1000$	$n = 10\,000$	$n = 100\,000$
$\Delta_{1,W}^{(n)}$	1.287	1.533	1.559	1.561	1.561
$\Delta_{2,W}^{(n)}$	1.216	1.548	1.575	1.578	1.578
$\Delta_{3,W}^{(n)}$	1.055	1.549	1.578	1.581	1.581

Let us also use this example to demonstrate that w_0 may not only be computed via (32) but also with the help of the integral formula (9). In the case at hand, $g''(0) = 8$, $g'''(0) = 12$, and the function under the integral equals

$$\begin{aligned}\left(\frac{g'(x)}{g(x)} - \cot\frac{x}{2} - \frac{1}{2}\right)\cot\frac{x}{2} &= \left(\frac{16\sin\frac{x}{2}\cos\frac{x}{2} + 24\sin^2\frac{x}{2}\cos^2\frac{x}{2} - 8\sin^4\frac{x}{2}}{16\sin^2\frac{x}{2} + 16\sin^3\frac{x}{2}\cos\frac{x}{2}} - \cot\frac{x}{2} - \frac{1}{2}\right)\cot\frac{x}{2}\,\mathrm{d}x \\ &= \left(\frac{2t(1+t^2) + 3t^2 - t^4}{2t^2(1+t^2) + 2t^3} - \frac{1}{t} - \frac{1}{2}\right)\frac{1}{t} \\ &= -\frac{1+2t}{1+t+t^2}\end{aligned}$$

where $t = \tan\frac{x}{2}$. Making the change $t = \tan\frac{x}{2}$ in the integral we come to

$$w_0 = \frac{1}{\pi}\int_{-\infty}^{+\infty} \frac{-(1+2t)\,\mathrm{d}t}{(1+t^2)(1+t+t^2)} = \sqrt{3} - 2.$$

Example 6.4 (*A Hermitian Heptadiagonal Matrix*). Let finally

$$a(t) = 24 + (-12 - 3\mathrm{i})t + (-12 + 3\mathrm{i})t^{-1} + \mathrm{i}t^3 - \mathrm{i}t^{-3},$$
$$g(x) = 48\sin^2\frac{x}{2} + 8\sin^3 x.$$

This time $\varphi_0 = \pi$ and $g''(\varphi_0) = -24$. To obtain w_0, we applied a numerical rootfinder to the polynomial $z^3 a(z)$ on the one hand and numerically computed the integral (9) with $g''(0) = 24$ and $g'''(0) = 48$ on the other. Both methods give the same value $w_0 \approx -0.2919$. The tables contain more numerical results.

	$n = 10$	$n = 20$	$n = 50$	$n = 100$	$n = 150$
$\Delta_*^{(n)}$	$6.6 \cdot 10^{-6}$	$1.2 \cdot 10^{-10}$	$7.6 \cdot 10^{-24}$	$1.4 \cdot 10^{-45}$	$3.3 \cdot 10^{-67}$

	$n = 10$	$n = 100$	$n = 1000$	$n = 10\,000$
$\Delta_1^{(n)}$	$1.0 \cdot 10^{-2}$	$1.4 \cdot 10^{-4}$	$1.5 \cdot 10^{-6}$	$1.5 \cdot 10^{-8}$
$\Delta_2^{(n)}$	$3.2 \cdot 10^{-4}$	$5.8 \cdot 10^{-7}$	$5.9 \cdot 10^{-10}$	$5.9 \cdot 10^{-13}$
$\Delta_3^{(n)}$	$1.4 \cdot 10^{-5}$	$2.4 \cdot 10^{-9}$	$2.5 \cdot 10^{-13}$	$2.6 \cdot 10^{-17}$

	$n = 10$	$n = 100$	$n = 1000$	$n = 10\,000$	$n = 100\,000$
$\Delta_{1,W}^{(n)}$	5.149	7.344	7.565	7.587	7.589
$\Delta_{2,W}^{(n)}$	4.106	7.386	7.623	7.645	7.647
$\Delta_{3,W}^{(n)}$	2.606	7.370	7.633	7.656	7.658

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