ZEROS AND RATIO ASYMPTOTICS FOR MATRIX ORTHOGONAL POLYNOMIALS

By

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Abstract. Ratio asymptotics for matrix orthogonal polynomials with recurrence coefficients A_n and B_n having limits A and B, respectively, (the matrix Nevai class) were obtained by Durán. In the present paper, we obtain an alternative description of the limiting ratio. We generalize it to recurrence coefficients which are asymptotically periodic with higher periodicity, and/or which are slowly varying as a function of a parameter. Under such assumptions, we also find the limiting zero distribution of the matrix orthogonal polynomials, thus generalizing results by Durán-López-Saff and Dette-Reuther to the non-Hermitian case. Our proofs are based on "normal family" arguments and on the solution of a quadratic eigenvalue problem. As an application of our results, we obtain new explicit formulas for the spectral measures of the matrix Chebyshev polynomials of the first and second kind and derive the asymptotic eigenvalue distribution for a class of random band matrices which generalize the tridiagonal matrices introduced by Dumitriu-Edelman.

1 Introduction

Let $(P_n(x))_{n=0}^{\infty}$ be a sequence of matrix-valued polynomials of size $r \times r$ ($r \geq 1$) generated by the recurrence relation

$$xP_n(x) = A_{n+1}P_{n+1}(x) + B_nP_n(x) + A_n^*P_{n-1}(x), \quad n \geq 0, \tag{1.1}$$

with initial conditions $P_{-1}(x) \equiv 0 \in \mathbb{C}^{r\times r}$ and $P_0(x) \equiv I_r$, with I_r the identity matrix of size $r \times r$. The coefficients A_k and B_k are complex matrices of size $r \times r$. We assume that each matrix A_k is non-singular and B_k is Hermitian. The star superscript denotes the Hermitian conjugation.

The polynomials generated by (1.1) satisfy orthogonality relations with respect to a matrix-valued measure (spectral measure) on the real line (Favard's theorem

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[8]) and are therefore called **matrix orthogonal polynomials**. The study of such polynomials goes back at least to [19]; we refer to the survey paper [8] for a detailed discussion of the available literature and for many more references. Some recent developments and applications of matrix orthogonal polynomials can be found in [4, 6, 9, 17], among many others.

To the recurrence (1.1) we associate the **block Jacobi matrix**

$$J_n = \begin{pmatrix} B_0 & A_1 & & & 0 \\ A_1^* & B_1 & A_2 & & \\ & A_2^* & \ddots & \ddots & \\ & & \ddots & \ddots & A_{n-1} \\ 0 & & & A_{n-1}^* & B_{n-1} \end{pmatrix}_{rn\times rn}, \tag{1.2}$$

which is a Hermitian, block tridiagonal matrix. It is well known that

$$\det P_n(x) = c_n \det(xI_n - J_n),$$

with $c_n = \det(A_n^{-1}\cdots A_2^{-1}A_1^{-1}) \neq 0$; see [8, 14]. By the *zeros* of the matrix polynomial $P_n(x)$ we mean the zeros of the determinant $\det P_n(x)$ or, equivalently, the eigenvalues of the matrix J_n defined in (1.2) (counting multiplicities).

The polynomials $(P_n(x))_{n=0}^{\infty}$ are said to belong to the **matrix Nevai class** if the limits

$$\lim_{n\to\infty} A_n = A, \quad \lim_{n\to\infty} B_n = B, \tag{1.3}$$

exist, where we assume throughout this paper that A is non-singular.

One famous classical result on orthogonal polynomials is Rakhmanov's theorem [25]; see [1, 9, 28] for a survey of the recent advances in this direction. Rakhmanov's theorem for matrix orthogonal polynomials on the real line is discussed in [9, 30]. These results give a sufficient condition on the spectral measure of matrix orthogonal polynomials for them to belong to the matrix Nevai class, with limiting values $A = I_r$ and $B = 0$. For a discussion of the matrix Nevai class in this case, see [18].

Durán [13] showed that in the matrix Nevai class (1.3), the limiting matrix ratio

$$R(x) := \lim_{n\to\infty} P_n(x)P_{n+1}^{-1}(x), \quad x \in \mathbb{C}\setminus[-M, M], \tag{1.4}$$

exists and depends analytically on $x \in \mathbb{C}\setminus[-M, M]$. Here $M > 0$ is a constant such that all the zeros of the matrix polynomials $P_n(x)$ are in $[-M, M]$. Moreover, Durán also proved in [13] that $R(x)A^{-1}$ is the Stieltjes transform of the spectral measure for the matrix Chebyshev polynomials of the second kind generated by the constant recurrence coefficients A and B; see Section 4.

The present paper serves several purposes. First, we give a different formulation of Durán's result on ratio asymptotics [13]. In particular, we give a self-contained proof of the existence of the limiting ratio $R(x)$ and express it in terms of a quadratic eigenvalue problem. Second, our approach can also be used to obtain ratio asymptotics for some extensions to the matrix Nevai class. More precisely, we allow the coefficients A_n and B_n to be slowly varying as a function of a parameter, or to be asymptotically periodic with higher periodicity. In both cases, we prove the existence of the limiting ratio (the limit may be local or periodic) and give an explicit formula for it.

To prove these results we work with *normal families* in the sense of Montel's theorem. Similar arguments can be found at various places in the literature; our approach is based, in particular, on the work by Kuijlaars-Van Assche [22] and its further developments in [3, 7, 11, 20]. We point out that an alternative approach to obtaining ratio asymptotics is to use the *Generalized Poincaré Theorem* (see [24, 27] for this theorem). However, the normal family argument has the advantage that it also works for slowly varying recurrence coefficients; see Section 3.1 for more details.

The third purpose of the paper is to obtain a new description of the limiting zero distribution of the matrix polynomials $(P_n(x))_{n=0}^{\infty}$. Durán-López-Saff [15] showed that in the matrix Nevai class (1.3), and assuming that A is Hermitian, the zero distribution of $P_n(x)$ has a limit as $n \to \infty$ in the sense of the weak convergence of measures. They expressed the limiting zero distribution of $P_n(x)$ in terms of the spectral measure for the matrix Chebyshev polynomials of the first kind; see Section 5 for the details. In contrast to the work of [15], the results derived in the present paper are also applicable in the case when the matrix A is non-singular but not necessarily Hermitian. Perhaps not surprisingly, the limiting eigenvalue distribution of the matrix J_n in (1.2)–(1.3) is the same as the limiting eigenvalue distribution for $n \to \infty$ of the **block Toeplitz matrix**

$$T_n = \begin{pmatrix} B & A & & & 0 \\ A^* & B & A & & \\ & A^* & \ddots & \ddots & \\ & & \ddots & \ddots & A \\ 0 & & & A^* & B \end{pmatrix}_{rn \times rn}. \tag{1.5}$$

The eigenvalue counting measure of the matrix T_n has a weak limit as $n \to \infty$ [29], and a description of the limiting measure can be obtained from [5, 10, 29].

In this paper, we establish the limiting zero distribution of the matrix polynomials $P_n(x)$ as a consequence of our results on ratio asymptotics. We also find the limiting zero distribution for the previously mentioned extensions to the matrix Nevai class. That is, the coefficients A_n and B_n are again allowed to be slowly varying as a function of a parameter or to be asymptotically periodic with higher periodicity.

Incidentally, we mention that it is possible to devise an alternative, linear algebra theoretic, proof of the fact that the matrices J_n and T_n have the same weak limiting eigenvalue distribution, using the fact that the block Jacobi matrix (1.2) is Hermitian [21]; however, our approach has the advantage that it can be also used in the non-Hermitian case, at least in principle. This means that most of the methodology derived in this paper is also applicable in the case when the recurrence matrix (1.2) generating the polynomials $P_n(x)$ is no longer Hermitian or when it has a larger band width in its block lower triangular part, as in [3]. In fact, the key places where we use the Hermiticity are in the proof of Proposition 2.1 and in the proof of Lemma 7.1 (see [11]); but it is reasonable to expect that both facts remain true for some specific non-Hermitian cases as well. This may be an interesting topic for further research.

The remaining part of this paper is organized as follows. In the next section, we state our results for the case of the matrix Nevai class. In Section 3, we generalize these findings to the context of recurrence coefficients with slowly varying or asymptotically periodic behavior. In Section 4, we apply our results to find new formulas for the spectral measures of the matrix Chebyshev polynomials of the first and second kind. In Section 5, we relate our formula for the limiting zero distribution to the one of Durán-López-Saff [15]. In Section 6, we indicate some potential applications in the context of random matrices. In particular, we derive the limiting eigenvalue distribution for a class of random band matrices which generalize the random tridiagonal representations of the β-ensembles which were introduced in [12]. Finally, Section 7 contains proofs of the main results.

2 Statement of results: the matrix Nevai class

2.1 The quadratic eigenvalue problem. Throughout this section, we work in the matrix Nevai class (1.2)–(1.3). Observe that the limiting ratio $R(x)$ in (1.4) satisfies the matrix relation

$$A^*R(x) + B - xI_r + AR^{-1}(x) = 0, \quad x \in \mathbb{C} \setminus [-M, M], \tag{2.1}$$

which is an easy consequence of the three term recurrence (1.1). For a simple motivation for our approach, we assume temporarily that for each $x \in \mathbb{C}\setminus[-M, M]$, $R(x)$ is diagonalizable and has distinct eigenvalues $z_k = z_k(x)$, $k = 1, \ldots, r$. Let $\mathbf{v}_k(x) \in \mathbb{C}^r$ be the corresponding eigenvectors, so that $R(x)\mathbf{v}_k(x) = z_k(x)\mathbf{v}_k(x)$ for $k = 1, \ldots, r$. Multiplying (2.1) on the right by $\mathbf{v}_k(x)$ gives

$$\left(z_k(x)A^* + B - xI_r + z_k^{-1}(x)A\right)\mathbf{v}_k(x) = \mathbf{0}, \tag{2.2}$$

where $\mathbf{0}$ denotes the column vector with all entries equal to zero. This relation implies, in particular, that

$$\det\left(z_k(x)A^* + B - xI_r + z_k^{-1}(x)A\right) = 0. \tag{2.3}$$

We can view (2.3) as a *quadratic eigenvalue problem* in the variable $z = z_k(x)$, and it gives us an algebraic equation for the eigenvalues of the limiting ratio $R(x)$. The corresponding eigenvectors $\mathbf{v}_k(x)$ can then be found from (2.2). Note that the equation (2.3) has $2r$ roots $z = z_k(x)$, $k = 1, \ldots, 2r$. Ordering these roots by increasing modulus

$$0 < |z_1(x)| \leq |z_2(x)| \leq \ldots \leq |z_r(x)| \leq |z_{r+1}(x)| \leq \ldots \leq |z_{2r}(x)|, \tag{2.4}$$

we see below that the eigenvalues of $R(x)$ are precisely the r smallest modulus roots $z_1(x), \ldots, z_r(x)$.

In order to treat the general case of eigenvalues with multiplicity larger than 1, we now proceed more formally. Inspired by the above discussion, we define the algebraic equation

$$0 = f(z, x) := \det(zA^* + B + z^{-1}A - xI_r), \tag{2.5}$$

where z and x denote two complex variables. As mentioned, one may consider (2.5) to be a (usual) eigenvalue problem in the variable x and a quadratic eigenvalue problem in the variable z.

Expanding the determinant in (2.5), we can write it as a Laurent polynomial in z:

$$f(z, x) = \sum_{k=-r}^{r} f_k(x)z^k, \tag{2.6}$$

where the coefficients $f_k(x)$ are polynomials in x of degree at most r, and where the outermost coefficients $f_r(x)$ and $f_{-r}(x)$ are given by

$$f_r(x) \equiv f_r = \det A^*, \quad f_{-r}(x) \equiv f_{-r} = \det A.$$

Solving the algebraic equation $f(z,x) = 0$ for z yields $2r$ roots (counting multiplicities) $z_k = z_k(x)$, which we order by increasing modulus as in (2.4). If $x \in \mathbb{C}$ is such that two or more roots $z_k(x)$ have the same modulus, we may label them arbtirarily such that (2.4) holds.

Define

$$\Gamma_0 := \{x \in \mathbb{C} \mid |z_r(x)| = |z_{r+1}(x)|\}. \tag{2.7}$$

It turns out that the set Γ_0 attracts the eigenvalues of the block Toeplitz matrix T_n in (1.5) for $n \to \infty$; see [5, 10, 29]. This set also attracts the eigenvalues of the matrix J_n in (1.2). The structure of Γ_0 is given in the following result, which is proved in Section 7.1.

Proposition 2.1. Γ_0 *is a subset of the real line. It is compact and can be written as the disjoint union of at most r intervals.*

2.2 Ratio asymptotics. For any $x \in \mathbb{C}$ and root $z = z_k(x)$ of the quadratic eigenvalue problem (2.5), we can choose a column vector $\mathbf{v}_k(x) \in \mathbb{C}^r$ in the right null space of the matrix $z_k(x)A^* + B - xI_r + z_k^{-1}(x)A$; see (2.2). If the null space is one-dimensional, we can fix $\mathbf{v}_k(x)$ by requiring it to be the unique vector having unit norm and first non-zero component positive.

If the null space is two or more dimensional, the vector $\mathbf{v}_k(x)$ is not uniquely determined from (2.2). We need some terminology. (The following paragraphs are a bit more technical and the reader may wish to move directly to Theorem 2.3.) For $x, z \in \mathbb{C}$, define $d(z,x)$ as the geometric dimension of the null space in (2.2), i.e.,

$$d(z,x) := \dim\{\mathbf{v} \in \mathbb{C}^r \mid (A^*z + B + Az^{-1} - xI_r)\mathbf{v} = \mathbf{0}\}. \tag{2.8}$$

Also define the algebraic multiplicities

$$m_1(z,x) := \max\{k \in \mathbb{Z}_{\geq 0} \mid (Z-z)^k \text{ divides } Z^r f(Z,x)\}, \tag{2.9}$$

$$m_2(z,x) := \max\{k \in \mathbb{Z}_{\geq 0} \mid (X-x)^k \text{ divides } f(z,X)\}, \tag{2.10}$$

where Z and X are auxiliary variables and division is understood to be in the ring of polynomials in Z and X respectively.

In the spirit of linear algebra, we can think of $d(z,x)$ as the *geometric multiplicity* of $(z,x) \in \mathbb{C}^2$, while $m_1(z,x)$ and $m_2(z,x)$ are the *algebraic multiplicities* of (z,x) with respect to the variables z and x, respectively.

The next lemma is a generalization of a result of Durán [13, Lemma 2.2].

Lemma 2.2 (Algebraic and geometric multiplicities)**.** *Let $A, B \in \mathbb{C}^{r\times r}$ be matrices, A non-singular and B Hermitian. Define $f(z,x)$ by* (2.5)*. The algebraic and geometric multiplicities in* (2.8)–(2.10) *are the same for all but finitely many $z, x \in \mathbb{C}$, i.e., $d(z,x) = m_1(z,x) = m_2(z,x)$ for all but finitely many $z, x \in \mathbb{C}$.*

Lemma 2.2 is proved in Section 7.2. We note that the particular Hermitian structure of the problem is needed in the proof.

Now let $x \in \mathbb{C}$ and consider the roots $z_1(x), \dots, z_{2r}(x)$ in (2.4) with algebraic multiplicities taken into account. Lemma 2.2 ensures that for all but finitely many $x \in \mathbb{C}$, we can find corresponding vectors $\mathbf{v}_1(x), \dots, \mathbf{v}_{2r}(x)$ having unit norm, satisfying (2.2), and such that

$$\dim\{\mathbf{v}_l(x) \mid l \in \{1,\dots,2r\},\ z_l(x) = z_k(x)\} = d(z_k(x), x) = m_1(z_k(x), x), \tag{2.11}$$

for each fixed k. In what follows, we always assume that the vectors $\mathbf{v}_k(x)$ are chosen in this way. We let $S \subset \mathbb{C}$ denote the set of those $x \in \mathbb{C}$ for which (2.11) *cannot* be achieved. Thus S has finite cardinality.

Now we are ready to describe the ratio asymptotics for the matrix Nevai class. The next result should be compared to that of Durán [13].

Theorem 2.3 (Ratio asymptotics)**.** *Let $A, B \in \mathbb{C}^{r\times r}$ be matrices, with A non-singular and B Hermitian. Let $P_n(x)$ satisfy* (1.1) *and* (1.3)*. Let $M > 0$ be such that all the zeros of the polynomials $\det P_n(x)$ lie in $[-M, M]$, and let $S \subset \mathbb{C}$ be the set of finite cardinality defined in the previous paragraphs. Then for all $x \in \mathbb{C} \setminus ([-M,M] \cup S)$, the limiting $r \times r$ matrix $\lim_{n\to\infty} P_n(x)P_{n+1}^{-1}(x)$ exists entrywise and is diagonalizable. Moreover,*

$$\left(\lim_{n\to\infty} P_n(x)P_{n+1}^{-1}(x)\right)\mathbf{v}_k(x) = z_k(x)\mathbf{v}_k(x), \quad k = 1,\dots,r,$$

uniformly for $k \in \{1,\dots,r\}$ and for x on compact subsets of $\mathbb{C} \setminus ([-M,M] \cup S)$. (Here, we take into account multiplicities as explained in the paragraphs before the statement of the theorem.)

Theorem 2.3 is proved in Section 7.3. See also Section 3 for the generalization of Theorem 2.3 beyond the matrix Nevai class.

Since the determinant of a matrix is the product of its eigenvalues, Theorem 2.3 implies the following result.

Corollary 2.4. *Under the assumptions of Theorem 2.3,*

$$\lim_{n\to\infty} \frac{\det P_n(x)}{\det P_{n+1}(x)} = z_1(x)\dots z_r(x)$$

uniformly on compact subsets of $\mathbb{C} \setminus [-M, M]$.

Note that the convergence in Corollary 2.4 holds in $\mathbb{C} \setminus [-M, M]$ rather than in $\mathbb{C} \setminus ([-M, M] \cup S)$. This is due to Lemma 7.1. See Section 4 below for some further corollaries of Theorem 2.3 in terms of the matrix Chebychev polynomials.

2.3 Limiting zero distribution. With the above results on ratio asymptotics in place, it is rather routine to obtain the limiting zero distribution for the polynomials $(P_n(x))_{n=0}^{\infty}$ in the matrix Nevai class. Recall that the zeros of the matrix polynomial $P_n(x)$ are defined as the zeros of $\det P_n(x)$, or equivalently, the eigenvalues of the Hermitian matrix J_n in (1.2). We denote these zeros by $x_1 \leq x_2 \leq \ldots \leq x_{rn}$ (taking into account multiplicities) and then define the **normalized zero counting measure** by

$$\nu_n = \frac{1}{rn} \sum_{k=1}^{rn} \delta_{x_k}, \tag{2.12}$$

where δ_x is the Dirac measure at the point x.

Theorem 2.5. *Under the assumptions of Theorem 2.3, the normalized zero counting measure ν_n defined in* (2.12) *has a weak limit μ_0 as $n \to \infty$. The (probability) measure μ_0 is supported on the set Γ_0 defined in* (2.7) *and has logarithmic potential*

$$\int \log |x - t|^{-1} \, \mathrm{d}\mu_0(t) = \frac{1}{r} \log |z_1(x) \ldots z_r(x)| + C, \quad x \in \mathbb{C} \setminus \Gamma_0, \tag{2.13}$$

where $C = -\log |\det A|/r$.

Recall that a measure on the real line is completely determined from its logarithmic potential [26].

Theorem 2.5 is proved in Section 7.4 with the help of Corollary 2.4. In the proof, we obtain a stronger version of (2.13), with the absolute value signs in the logarithms removed. Moreover, in Section 3, we extend Theorem 2.5 beyond the matrix Nevai class.

It can be shown that the measure μ_0 in Theorem 2.5 is absolutely continuous on $\Gamma_0 \subset \mathbb{R}$ with density (see also [3, 10])

$$\mathrm{d}\mu_0(x) = \frac{1}{r} \frac{1}{2\pi i} \sum_{j=1}^{r} \left(\frac{z'_{j+}(x)}{z_{j+}(x)} - \frac{z'_{j-}(x)}{z_{j-}(x)} \right) \mathrm{d}x, \quad x \in \Gamma_0. \tag{2.14}$$

Here, the prime denote derivation with respect to x, and $z_{j+}(x)$ and $z_{j-}(x)$ are the boundary values of $z_j(x)$ obtained from the upper and lower part of the complex plane respectively. These boundary values exist for all but a finite number of points $x \in \Gamma_0$; see Section 5 for a comparison to the formulas of [15].

2.4 Alternative description of the limiting zero distribution. First, let us give an alternative description of the set Γ_0 in (2.7). For the proof, see Section 7.5.

Proposition 2.6.

$$\Gamma_0 = \{x \in \mathbb{C} \mid \textit{there exists } z \in \mathbb{C} \textit{ with } f(z,x) = 0 \textit{ and } |z| = 1\} \subset \mathbb{R}. \tag{2.15}$$

Here, $f(z,x)$ is as defined in (2.5).

Now let $\mathcal{I} := (x_1, x_2) \subset \Gamma_0$ be an open interval disjoint from the set of branch points of the algebraic equation $f(z,x) = 0$. We can choose a labeling of the roots so that each $z_k(x)$, $x \in \mathcal{I}$, is the restriction to $\mathcal{I}$ of an analytic function defined in an open complex neighborhood $\Omega \supset \mathcal{I}$. Note that we are not using the ordering (2.4) anymore. If k is such that $|z_k(x)| = 1$ throughout the interval $\mathcal{I}$, we write $z_k(x) = e^{i\theta_k(x)}$, $x \in \mathcal{I}$, with θ_k a real-valued, differentiable argument function on $\mathcal{I}$. Observe that

$$\frac{z_k'(x)}{z_k(x)} = i\theta_k'(x), \quad x \in \mathcal{I}.$$

Moreover $\theta_k'(x)$ describes how fast $z_k(x)$ runs on the unit circle as a function of $x \in \mathcal{I}$.

We can now give an alternative description of the measure μ_0 in (2.14)..

Proposition 2.7. *With the above notation,*

$$\begin{aligned} \frac{\mathrm{d}\mu_0(x)}{\mathrm{d}x} &= \frac{1}{2\pi r} \sum_{k:|z_k(x)|=1} \left| \frac{z_k'(x)}{z_k(x)} \right| \\ &= \frac{1}{2\pi r} \sum_{k:|z_k(x)|=1} \left|\theta_k'(x)\right|, \quad x \in \mathcal{I}. \end{aligned} \tag{2.16}$$

Moreover, $\theta_k'(x) \neq 0$ *for any* $x \in \mathcal{I}$ *and for any* k *with* $|z_k(x)| = 1$.

Proposition 2.7 is proved in Section 7.6.

3 Generalizations of the matrix Nevai class

3.1 Slowly varying recurrence coefficients. In this section, we consider a first type of generalization of the matrix Nevai class. We assume, as in Dette-Reuther [11], that the recurrence coefficients A_n and B_n depend on an additional variable $N > 0$, and we write $A_{n,N}$ and $B_{n,N}$. For each fixed $N > 0$, we define the matrix-valued polynomials $P_{n,N}(x)$ generated by the recurrence (compare with (1.1))

$$xP_{n,N}(x) = A_{n+1,N}P_{n+1,N}(x) + B_{n,N}P_{n,N}(x) + A_{n,N}^*P_{n-1,N}(x), \quad n \geq 0, \tag{3.1}$$

again with the initial conditions $P_{0,N} = I_r$ and $P_{-1,N} = 0$.

Assume that the limits

$$\lim_{n/N\to s} A_{n,N} =: A_s, \qquad \lim_{n/N\to s} B_{n,N} =: B_s, \tag{3.2}$$

exist for each $s > 0$, where $\lim_{n/N\to s}$ means that n and N tend to infinity in such a way that the ratio n/N converges to $s > 0$. We assume that each A_s is non-singular. We trust that the notation A_s, B_s $(s > 0)$ does not lead to confusion with our previous usage of A_n, B_n $(n \in \mathbb{Z}_{\geq 0})$.

For each $s > 0$, define the algebraic equation

$$0 = f_s(z, x) := \det(A_s^* z + B_s + A_s z^{-1} - xI_r). \tag{3.3}$$

We again define the roots $z_k(x, s)$, $k = 1, \dots, 2r$ of this equation, ordered as in (2.4), and find the corresponding null space vectors $\mathbf{v}_k(x, s)$ as in (2.2). We also define the finite cardinality set $S_s \subset \mathbb{C}$ as before and $\Gamma_0(s)$ as in (2.7).

We now formulate the extensions of Theorems 2.3 and 2.5 to the present setting.

Theorem 3.1. *Fix $s > 0$ and assume that the limits A_s, B_s in* (3.1) *and* (3.2) *depend continuously on $s \geq 0$. For all $x \in \mathbb{C} \setminus ([-M, M] \cup S_s)$, the limiting $r \times r$ matrix* $\lim_{n/N\to s} P_{n,N}(x)P_{n+1,N}^{-1}(x)$ *exists entrywise and is diagonalizable, with*

$$\left(\lim_{n/N\to s} P_{n,N}(x)P_{n+1,N}^{-1}(x)\right) \mathbf{v}_k(x, s) = z_k(x, s)\mathbf{v}_k(x, s), \quad k = 1, \dots, r,$$

uniformly for x on compact subsets of $\mathbb{C} \setminus ([-M, M] \cup S_s)$. *Also,*

$$\lim_{n/N\to s} \frac{\det P_{n,N}(x)}{\det P_{n+1,N}(x)} = z_1(x, s) \dots z_r(x, s)$$

uniformly on compact subsets of $\mathbb{C} \setminus [-M, M]$.

Theorem 3.2. *Under the assumptions of Theorem 3.1, the normalized zero counting measure of* $\det P_{n,N}(x)$ *for $n/N \to s$ has a weak limit $\mu_{0,s}$, with logarithmic potential given by*

$$\int \log |x - t|^{-1}\, \mathrm{d}\mu_{0,s}(t) = \frac{1}{rs} \int_0^s \log |z_1(x, u) \dots z_r(x, u)|\, \mathrm{d}u + C_s, \tag{3.4}$$
$$x \in \mathbb{C} \setminus \bigcup_{0\leq u\leq s} \Gamma_0(u)$$

for some constant C_s which can be given explicitly.

In other words, $\mu_{0,s}$ is precisely the average (or integral) of the individual limiting measures for fixed u, integrated over $u \in [0, s]$.

Theorems 3.1 and 3.2 are proved in Section 7.7, and an application of these results in the context of random band matrices is given in Section 6.

3.2 Asymptotically periodic recurrence coefficients. In this section, we consider a second type of generalization of the Nevai class. We assume that the matrices A_n and B_n have *periodic* limits with period $p \in \mathbb{Z}_{>0}$ in the sense that

$$\lim_{n\to\infty} A_{pn+j} =: A^{(j)}, \quad \lim_{n\to\infty} B_{pn+j} =: B^{(j)}, \tag{3.5}$$

for any fixed $j = 0, 1, \dots, p-1$.

The role that was previously played by $zA^* + B + z^{-1}A - xI_r$ is now played by the matrix

$$F(z,x) := \begin{pmatrix} B^{(0)} - xI_r & A^{(1)} & 0 & 0 & zA^{(0)*} \\ A^{(1)*} & B^{(1)} - xI_r & A^{(2)} & 0 & 0 \\ 0 & A^{(2)*} & \ddots & \ddots & 0 \\ 0 & 0 & \ddots & \ddots & A^{(p-1)} \\ z^{-1}A^{(0)} & 0 & 0 & A^{(p-1)*} & B^{(p-1)} - xI_r \end{pmatrix}_{pr\times pr}, \tag{3.6}$$

where we abbreviate $A^{(j)*} := (A^{(j)})^*$. We define

$$f(z,x) := \det F(z,x). \tag{3.7}$$

This can be expanded as a Laurent polynomial in z

$$f(z,x) = \sum_{k=-r}^{r} f_k(x) z^k, \tag{3.8}$$

where now the outermost coefficients $f_r(x)$, $f_{-r}(x)$ are given by

$$f_r(x) \equiv f_r = (-1)^{(p-1)r^2} \det(A^{(0)*} \dots A^{(p-1)*}),$$
$$f_{-r}(x) \equiv f_{-r} = (-1)^{(p-1)r^2} \det(A^{(0)} \dots A^{(p-1)}).$$

We again order the roots $z_k(x)$, $k = 1, \dots, 2r$ of (3.8) as in (2.4). We define Γ_0 as in (2.7). Proposition 2.1 now takes the following form.

Proposition 3.3. *Γ_0 is a subset of the real line. It is compact and can be written as the disjoint union of at most pr intervals.*

As before, we denote by $\mathbf{v}_k(x)$, $k = 1, \dots, 2r$, the normalized null space vectors of the matrix $F(z_k(x), x)$. We partition these vectors into blocks as

$$\mathbf{v}_k(x) = \begin{pmatrix} \mathbf{v}_{k,0}(x) \\ \vdots \\ \mathbf{v}_{k,p-1}(x) \end{pmatrix}, \tag{3.9}$$

where each $\mathbf{v}_{k,j}(x)$, $j = 0, 1, \ldots, p-1$, is a column vector of length r. Lemma 2.2 also holds in the present setting.

Now we can state the analogues of Theorems 2.3 and 2.5.

Theorem 3.4. *For all $x \in \mathbb{C} \setminus ([-M, M] \cup S)$ and $j \in \{0, 1, \ldots, p-1\}$, the limiting $r \times r$ matrix $\lim_{n\to\infty} P_{pn+j}(x)P^{-1}_{pn+j+p}(x)$ exists entrywise and is diagonalizable, with*

$$\left(\lim_{n\to\infty} P_{pn+j}(x)P^{-1}_{pn+j+p}(x)\right) \mathbf{v}_{k,j}(x) = z_k(x)\mathbf{v}_{k,j}(x), \tag{3.10}$$

uniformly for $k \in \{1, \ldots, r\}$ and for x in compact subsets of $\mathbb{C} \setminus ([-M, M] \cup S)$. Moreover,

$$\lim_{n\to\infty} \frac{\det P_n(x)}{\det P_{n+p}(x)} = z_1(x) \ldots z_r(x) \tag{3.11}$$

uniformly for x in compact subsets of $\mathbb{C} \setminus [-M, M]$.

Theorem 3.4 is proved in Section 7.8, where we establish in fact a stronger variant (7.18) of (3.10). The proof uses some ideas from [3]. Note that the eigenvectors in (3.10) depend on the residue class modulo p, $j \in \{0, 1, \ldots, p-1\}$, while the eigenvalues are independent of j.

Theorem 3.5. *Under the assumptions of Theorem 3.4, the normalized zero counting measure of $\det P_n(x)$ for $n \to \infty$ has a weak limit μ_0, supported on Γ_0, with logarithmic potential given by*

$$\int \log |x-t|^{-1} \, \mathrm{d}\mu_0(t) = \frac{1}{pr} \log |z_1(x) \ldots z_r(x)| + C, \quad x \in \mathbb{C} \setminus \Gamma_0, \tag{3.12}$$

where $C = -\log |\det(A^{(0)} \ldots A^{(p-1)})|/pr$.

Finally, we point out that the results in the present section can be combined with those in Section 3.1. That is, one could allow for slowly varying recurrence coefficients $A_{n,N}$, $B_{n,N}$ with periodic local limits of period p. The corresponding modifications are straightforward and are left to the interested reader.

4 Formulas for matrix Chebychev polynomials

Throughout this section, we let A be a fixed non-singular matrix and B be a fixed Hermitian $r \times r$ matrix. The matrix Chebyshev polynomials of the second kind are defined from the recursion (1.1), with the standard initial conditions $P_0(x) \equiv I_r$, $P_{-1}(x) \equiv 0$, and with constant recurrence coefficients $A_n \equiv A$ and $B_n \equiv B$ for all n. The matrix Chebyshev polynomials of the first kind are defined in the same way, but now with $A_1 = \sqrt{2}A$ and $A_n = A$ for all $n \geq 2$.

Let X and W be the spectral measures for the matrix Chebychev polynomials of the first and second kind, respectively, normalized by $\int_{\mathbb{R}} \mathrm{d}X = \int_{\mathbb{R}} \mathrm{d}W = I_r$, as in [13, 15]. Here the integrals are taken entrywise. Denote the corresponding Stieltjes transforms (or Cauchy transforms) by

$$F_X(x) = \int \frac{\mathrm{d}X(t)}{x-t}, \quad F_W(x) = \int \frac{\mathrm{d}W(t)}{x-t}.$$

Theorem 2.3 can be reformulated as

$$\lim_{n\to\infty} P_n(x)P_{n+1}^{-1}(x) = V(x)D(x)V^{-1}(x), \quad x \in \mathbb{C} \setminus ([-M, M] \cup S), \tag{4.1}$$

where $D(x)$ is the diagonal matrix with entries $z_k(x)$, $k = 1, \dots, r$, and $V(x)$ is the matrix whose columns are the corresponding vectors $\mathbf{v}_k(x)$ in (2.2).

In turns out that the Stieltjes transforms F_W and F_X can be expressed in terms of the matrices $D = D(x)$ and $V = V(x)$ as well.

Proposition 4.1.

$$F_W(x) = V(x)D(x)V^{-1}(x)A^{-1} \tag{4.2}$$

$$F_X(x) = \left[xI_r - B - 2A^*F_W(x)A\right]^{-1} \tag{4.3}$$

$$= V\left[AVD^{-1} - A^*VD\right]^{-1} \tag{4.4}$$

for all but finitely many $x \in \mathbb{C} \setminus \Gamma_0$. Hence the matrix-valued measures W and X are both supported on Γ_0 together with a finite, possibly empty, set of mass points on $\mathbb{R}$.

Proof. By comparing (4.1) with Durán's result [13, Thm. 1.1], we get the claimed expression (4.2). The formula (4.3) follows from the theory of the matrix continued fraction expansion; see [2] and [31]. Formula (4.4) is then a consequence of (4.2)–(4.3) and the matrix relation

$$-(xI_r - B)V + A^*VD + AVD^{-1} = 0, \tag{4.5}$$

which is obvious from the definitions of $D = D(x)$ and $V = V(x)$.

To prove the remaining claims, we note that the right hand side of (4.2) is analytic for $x \in \mathbb{C} \setminus (\Gamma_0 \cup S \cup \tilde{S})$ with $\tilde{S}$ the set of branch points of (2.5); so $F_W(x)$ is also analytic there, and therefore the measure W has its support in a subset of $(\Gamma_0 \cup S \cup \tilde{S}) \cap \mathbb{R}$. Finally, the determinant of the matrix in square brackets in (4.3) is analytic and not identically zero for $x \in \mathbb{C} \setminus (\Gamma_0 \cup S \cup \tilde{S})$, so it has only finitely many zeros there. This yields the claim about the support of the measure X. □

The above descriptions considerably simplify if A is Hermitian. In that case, the algebraic equation (2.5) becomes

$$0 = f(z,x) = \det(Aw + B - xI_r), \tag{4.6}$$

where

$$w := z + z^{-1}. \tag{4.7}$$

As in Section 2.4, for any open interval $\mathcal{I} := (x_1, x_2) \subset \Gamma_0$ disjoint from the set of branch points of the algebraic equation (2.5), we can choose an ordering of the roots $z_k(x)$, $x \in \mathcal{I}$, so that each $z_k(x)$ is the restriction to $\mathcal{I}$ of an analytic function defined on an open complex neighborhood $\Omega \supset \mathcal{I}$. Thereby we drop the ordering constraint (2.4). By (4.6)–(4.7) we may assume that

$$z_{2r-k}(x) = z_k(x)^{-1}, \quad k = 1, \ldots, r, \tag{4.8}$$

for all $x \in \Omega \supset \mathcal{I}$ and write

$$w_k(x) = z_k(x) + z_k(x)^{-1}, \quad k = 1, \ldots, r. \tag{4.9}$$

If $w_k(x) \in (-2,2)$ for all $x \in \mathcal{I}$, we write

$$w_k(x) = 2\cos\theta_k(x), \quad 0 < \theta_k(x) < \pi, \tag{4.10}$$

with θ_k a real-valued, differentiable argument function on $\mathcal{I}$. Denote by $V(x)$ the matrix formed by the normalized null space vectors $\mathbf{v}_k(x)$ for the roots $w_k(x)$, $x \in \mathcal{I}$.

Proposition 4.2. *Assume that A is Hermitian. Then with the above notation, the density of the absolutely continuous part of the measures X and W is given by*

$$\frac{\mathrm{d}X(x)}{\mathrm{d}x} = V(x)\Lambda_X(x)V^{-1}(x)A^{-1}, \quad x \in \Gamma_0,$$
$$\frac{\mathrm{d}W(x)}{\mathrm{d}x} = V(x)\Lambda_W(x)V^{-1}(x)A^{-1}, \quad x \in \Gamma_0,$$

where

$$\Lambda_X(x) = \frac{1}{\pi}\operatorname{diag}\left(\frac{\mathbf{1}_{w_k(x)\in(-2,2)}}{\sqrt{4 - w_k(x)^2}}\, \mathit{sign}\, w_k'(x)\right)_{k=1}^{r},$$
$$\Lambda_W(x) = \frac{1}{2\pi}\operatorname{diag}\left(\mathbf{1}_{w_k(x)\in(-2,2)}\sqrt{4 - w_k(x)^2}\, \mathit{sign}\, w_k'(x)\right)_{k=1}^{r},$$

and the characteristic function $\mathbf{1}_{w_k \in (-2,2)}$ takes the value 1 if $w_k \in (-2,2)$ and zero otherwise.

Proposition 4.2 is proved in Section 7.9. If A is positive definite, the factors $\operatorname{sign} w_k'(x)$ in the above formulas can be removed. This follows from (5.2) below. Then one can show that the above formulas correspond to those in [13, 15].

5 The results of Durán-López-Saff revisited

In this section, we show how Theorem 2.5 on the limiting zero distribution of $P_n(x)$ in the matrix Nevai class relates to the formulas of Durán-López-Saff [15] for the case where the matrix A is positive definite or Hermitian.

Throughout this section, we write the algebraic equation $f(z,x) = 0$ as in (4.6)–(4.7). First, we assume that A is positive definite. Thus $A^{1/2}$ exists, and we can replace the algebraic equation (4.6) with $0 = \det(wI_r + A^{-1/2}BA^{-1/2} - xA^{-1})$. Hence the roots w are the eigenvalues of the matrix $xA^{-1} - A^{-1/2}BA^{-1/2}$. If $x \in \mathbb{R}$, this matrix is Hermitian; we denote its spectral decomposition by

$$xA^{-1} - A^{-1/2}BA^{-1/2} = U(x)D_w(x)U^{-1}(x), \tag{5.1}$$

where $D_w(x) = \operatorname{diag}(w_1(x), \ldots, w_r(x))$ is the diagonal matrix containing the eigenvalues and $U(x)$ is the corresponding eigenvector matrix. We can assume that $U(x)$ is unitary, i.e., $U^{-1}(x) = U^*(x)$.

As in the previous section, we fix an open interval $\mathcal{I} := (x_1, x_2) \subset \Gamma_0$, disjoint from the set of branch points of the algebraic equation (2.5), and choose an ordering of the roots $z_k(x)$, $x \in \mathcal{I}$, so that each $z_k(x)$ is the restriction to $\mathcal{I}$ of an analytic function defined on an open complex neighborhood $\Omega \supset \mathcal{I}$. The same then holds for $w_k(x)$ in (4.9).

Lemma 5.1. *If A is positive definite, then with the above notation,*

$$w_k'(x) = (U^{-1}(x)A^{-1}U(x))_{k,k} > 0, \quad k = 1, \ldots, p, \tag{5.2}$$

where $M_{k,k}$ denotes the (k,k) entry of a matrix M.

Proof. Take the derivative of (5.1) with respect to x. This yields (we suppress the dependence on x for simplicity)

$$\begin{aligned} A^{-1} &= U'D_wU^{-1} + UD_w'U^{-1} + UD_w(U^{-1})', \quad \text{or} \\ U^{-1}A^{-1}U &= U^{-1}U'D_w + D_w' + D_w(U^{-1})'U. \end{aligned}$$

Invoking the fact that $(U^{-1})' = -U^{-1}U'U^{-1}$, we see that this becomes

$$U^{-1}A^{-1}U = D_w' + [U^{-1}U', D_w],$$

where the square brackets denote the commutator. The equality in (5.2) then follows by taking the (k,k) diagonal entry of this matrix relation and noting that the diagonal entries of the commutator $[U^{-1}U', D_w]$ are all zero, since D_w is diagonal. Finally, the inequality in (5.2) follows because A is positive definite and U is unitary, $U^{-1} = U^*$. □

From (4.9), we have

$$\frac{z_k'(x)}{z_k(x)} = \pm i \frac{w_k'(x)}{\sqrt{4 - w_k(x)^2}}. \tag{5.3}$$

Thus the density of the limiting zero distribution μ_0 in (2.16) becomes

$$\frac{\mathrm{d}\mu_0(x)}{\mathrm{d}x} = \frac{1}{\pi r} \sum_{k=1}^{r} \frac{w_k'(x)}{\sqrt{4 - w_k(x)^2}} \mathbf{1}_{w_k \in (-2,2)}, \tag{5.4}$$

where we have used the fact that $w_k'(x) > 0$, and where again the characteristic function $\mathbf{1}_{w_k \in (-2,2)}$ takes the value 1 if $w_k \in (-2, 2)$ and zero otherwise. Note that the factor 2 in the denominator of (2.16) is canceled since for any $w_k \in (-2, 2)$, there are *two* solutions z_k of (4.9), one leading to the plus sign and the other to the minus sign in (5.3).

Inserting (5.2) in (5.4), we obtain

$$\begin{aligned} \frac{\mathrm{d}\mu_0(x)}{\mathrm{d}x} &= \frac{1}{\pi r} \sum_{k=1}^{r} \frac{(U^{-1}(x)A^{-1}U(x))_{k,k}}{\sqrt{4 - w_k(x)^2}} \mathbf{1}_{w_k \in (-2,2)} \\ &= \frac{1}{r} \mathrm{Tr} \left(U^{-1}(x) A^{-1} U(x) \Lambda_X(x) \right), \end{aligned}$$

where $\mathrm{Tr}(C)$ denotes the trace of the matrix C and

$$\Lambda_X(x) = \frac{1}{\pi} \operatorname{diag} \left(\frac{\mathbf{1}_{w_k \in (-2,2)}}{\sqrt{4 - w_k(x)^2}} \right)_{k=1}^{r}.$$

Since the trace of a matrix product is invariant under cyclic permutations, we obtain

$$\frac{\mathrm{d}\mu_0(x)}{\mathrm{d}x} = \frac{1}{r} \mathrm{Tr} \left(A^{-1/2} U(x) \Lambda_X(x) U^{-1}(x) A^{-1/2} \right).$$

This is the result of Durán-López-Saff for the case where A is positive definite [15].

Next suppose that A is Hermitian but not necessarily positive definite. Then we can basically repeat the above procedure. Rather than taking the square root $A^{1/2}$, we now write (4.6) in the form $0 = \det(wI_r + A^{-1}B - xA^{-1})$. Hence the roots w are the eigenvalues of the matrix $xA^{-1} - A^{-1}B$. Supposing that this matrix is diagonalizable, we write

$$xA^{-1} - A^{-1}B = V(x) D_w(x) V^{-1}(x), \tag{5.5}$$

with $D_w = \operatorname{diag}(w_1, \ldots, w_r)$ but with V not necessarily unitary. The notation V is compatible with that in the previous section, by virtue of (4.5). We then again have the equality in (5.2) (with U replaced with V), although the positivity $w_k'(x) > 0$ may be violated. Similarly to the above paragraphs, we have

$$\frac{\mathrm{d}\mu_0(x)}{\mathrm{d}x} = \frac{1}{r}\mathrm{Tr}\left(V(x)\Lambda_X(x)V^{-1}(x)A^{-1}\right),$$

with Λ_X defined in Proposition 4.2, which then implies

$$\frac{\mathrm{d}\mu_0(x)}{\mathrm{d}x} = \frac{1}{r}\mathrm{Tr}\left(\frac{\mathrm{d}X(x)}{\mathrm{d}x}\right).$$

This is the result of Durán-López-Saff for the case where A is Hermitian [15].

6 An application to random matrices

In a fundamental paper, Dumitriu-Edelman [12] introduced a tridiagonal random matrix

$$G_n^{(1)} = \begin{pmatrix} N_1 & \frac{1}{\sqrt{2}}\mathcal{X}_{(n-1)\beta} & & & & \\ \frac{1}{\sqrt{2}}\mathcal{X}_{(n-1)\beta} & N_2 & \frac{1}{\sqrt{2}}\mathcal{X}_{(n-2)\beta} & & & \\ & \frac{1}{\sqrt{2}}\mathcal{X}_{(n-2)\beta} & N_3 & & & \\ & & & \ddots & & \\ & & & & N_{n-1} & \frac{1}{\sqrt{2}}\mathcal{X}_{\beta} \\ & & & & \frac{1}{\sqrt{2}}\mathcal{X}_{\beta} & N_n \end{pmatrix},$$

where $N_1, \ldots, N_n$ are independent identically distributed standard normal random variables and $\mathcal{X}_{1\beta}^2, \ldots, \mathcal{X}_{(n-1)\beta}^2$ are independent random variables also independent of $N_1, \ldots, N_n$ such that $\mathcal{X}_{j\beta}^2$ is a chi-square distribution with $j\beta$ degrees of freedom. They showed that the density of the eigenvalues $\lambda_1 \le \cdots \le \lambda_n$ of G_n is given by the so called beta ensemble

$$c_\beta \prod_{i<j} |\lambda_i - \lambda_j|^\beta \cdot \exp\Big(-\sum_{j=1}^n \frac{\lambda_j^2}{2}\Big),$$

where $c_\beta > 0$ is an appropriate normalizing constant (see [16] or [23], among many others). It is well known that the empirical eigenvalue distribution of $G_n/\sqrt{n}$ converges weakly (almost surely) to Wigner's semi-circle law. In the following discussion, we use the results of Section 3.1 to derive a corresponding result for a $(2r+1)$-band matrix of a similar structure. To be precise, let $G_n^{(r)} = 1/\sqrt{2}$ times the matrix

$$\begin{pmatrix}
\sqrt{2}\,N_1 & \mathcal{X}_{(n-1)\gamma_1} & \cdots & \mathcal{X}_{(n-r)\gamma_r} & & & & & \\
\mathcal{X}_{(n-1)\gamma_1} & \sqrt{2}\,N_2 & \cdots & \mathcal{X}_{(n-r)\gamma_{r-1}} & \mathcal{X}_{(n-r-1)\gamma_r} & & & & \\
\mathcal{X}_{(n-2)\gamma_2} & \mathcal{X}_{(n-2)\gamma_1} & \ddots & \ddots & \ddots & \ddots & \ddots & & \\
 & \mathcal{X}_{(n-3)\gamma_2} & & \ddots & \ddots & \ddots & \ddots & \ddots & \\
\vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \\
\mathcal{X}_{(n-r)\gamma_r} & \mathcal{X}_{(n-r)\gamma_{r-1}} & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \\
 & \mathcal{X}_{(n-r-1)\gamma_r} & & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\
 & & & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\
 & & & \ddots & \ddots & \ddots & \ddots & \ddots & \\
 & & & & & & & \mathcal{X}_{2\gamma_1} & \mathcal{X}_{\gamma_2} \\
 & & & & & & \mathcal{X}_{2\gamma_1} & \sqrt{2}\,N_{n-1} & \mathcal{X}_{\gamma_1} \\
 & & & & & & \mathcal{X}_{\gamma_2} & \mathcal{X}_{\gamma_1} & \sqrt{2}\,N_n
\end{pmatrix},$$

where $n = mr$, all random variables in the matrix $G_n^{(r)}$ are independent and N_j is standard normal distributed ($j = 1, \dots, n$), while for $j = 1, \dots, n-1$, $k = 1, \dots, r$ $\mathcal{X}^2_{j\gamma_k}$ has a chi-square distribution with $j\gamma_k$ degrees of freedom ($\gamma_1, \dots, \gamma_r \geq 0$). It now follows by arguments similar to those in [11] that the empirical distribution of the eigenvalues $\lambda_1^{(n,r)} \leq \cdots \leq \lambda_n^{(n,r)}$ of $G_n^{(r)}/\sqrt{n}$ has the same asymptotic properties as the limiting distribution of the roots of the orthogonal matrix polynomials $R_{m,n}(x)$ defined by ($R_{-1,n}(x) = 0, R_{0,n}(x) = I_r$)

$$xR_{k,n}(x) = A_{k+1,n}R_{k+1,n}(x) + B_{k,n}R_{k,n}(x) + A^*_{k,n}R_{k-1,n}(x), \quad k \geq 0,$$

where the $r \times r$ matrices $\sqrt{2n}A_{i,n}$ and $\sqrt{2n}B_{i,n}$ are given by

$$\begin{pmatrix}
\sqrt{((i-1)r+1)\gamma_r} & 0 & 0 & \cdots & 0 \\
\sqrt{((i-1)r+2)\gamma_{r-1}} & \sqrt{((i-1)r+2)\gamma_r} & 0 & \cdots & 0 \\
\vdots & \ddots & \ddots & \ddots & \vdots \\
\sqrt{(ir-1)\gamma_2} & \cdots & \sqrt{(ir-1)\gamma_{r-1}} & \sqrt{(ir-1)\gamma_r} & 0 \\
\sqrt{ir\gamma_1} & \cdots & \sqrt{ir\gamma_{r-2}} & \sqrt{ir\gamma_{r-1}} & \sqrt{ir\gamma_r}
\end{pmatrix},$$

and

$$\begin{pmatrix}
0 & \sqrt{(ir+1)\gamma_1} & \sqrt{(ir+1)\gamma_2} & \cdots & \sqrt{(ir+1)\gamma_{r-1}} \\
\sqrt{(ir+1)\gamma_1} & 0 & \sqrt{(ir+2)\gamma_1} & \cdots & \sqrt{(ir+2)\gamma_{r-2}} \\
\vdots & \ddots & \ddots & \ddots & \vdots \\
\sqrt{(ir+1)\gamma_{r-2}} & \cdots & \sqrt{((i+1)r-2)\gamma_1} & 0 & \sqrt{((i+1)r-2)\gamma_1} \\
\sqrt{(ir+1)\gamma_{r-1}} & \cdots & \sqrt{((i+1)r-2)\gamma_2} & \sqrt{((i+1)r-1)\gamma_1} & 0
\end{pmatrix},$$

respectively. Now it is easy to see that for any $u \in (0, 1)$

$$\lim_{\frac{i}{n}\to u} B_{i,n} = B(u), \lim_{\frac{i}{n}\to u} A_{i,n} = A(u),$$

where

$$A(u) := \sqrt{\frac{ur}{2}} \begin{pmatrix} \sqrt{\gamma_r} & 0 & 0 & \cdots & 0 \\ \sqrt{\gamma_{r-1}} & \sqrt{\gamma_r} & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \sqrt{\gamma_2} & \cdots & \sqrt{\gamma_{r-1}} & \sqrt{\gamma_r} & 0 \\ \sqrt{\gamma_1} & \cdots & \sqrt{\gamma_{r-2}} & \sqrt{\gamma_{r-1}} & \sqrt{\gamma_r} \end{pmatrix} \in \mathbb{R}^{r\times r}, \tag{6.1}$$

$$B(u) := \sqrt{\frac{ur}{2}} \begin{pmatrix} 0 & \sqrt{\gamma_1} & \sqrt{\gamma_2} & \cdots & \sqrt{\gamma_{r-1}} \\ \sqrt{\gamma_1} & 0 & \sqrt{\gamma_1} & \cdots & \sqrt{\gamma_{r-2}} \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \sqrt{\gamma_{r-2}} & \cdots & \sqrt{\gamma_1} & 0 & \sqrt{\gamma_1} \\ \sqrt{\gamma_{r-1}} & \cdots & \sqrt{\gamma_2} & \sqrt{\gamma_1} & 0 \end{pmatrix} \in \mathbb{R}^{r\times r}. \tag{6.2}$$

Theorem 3.2 shows that the normalized counting measure of the roots of the matrix orthogonal polynomial $R_{m,n}(x)$ has a weak limit $\mu_{0,1/r}$, defined by its logarithmic potential

$$\int \log|x-t|^{-1} d\mu_{0,1/r}(t) = \int_0^{1/r} \log|z_1(x,u), \ldots, z_r(x,u)| du + c(r),$$

where $z_1(x, u), \ldots, z_r(x, u)$ are the roots of the equation

$$\det(A^*(u)z + B(u) + A(u)z^{-1} - xI_r) = 0 \tag{6.3}$$

corresponding to the smallest moduli. Observing the structure of the matrices in (6.1) and (6.2), we see that $z_j(x, u) = z_j\left(x/\sqrt{u}\right)$, where $z_1(x), \ldots, z_r(x)$ are the roots of (6.3) for $u = 1$ (with smallest modulus). Arguments similar to those used in the proof of Proposition 2.7 now show that the measure $\mu_{0,1/r}$ is absolutely continuous with density defined by

$$\frac{d\mu_{0,1/r}(x)}{dx} = \int_0^{1/r} \frac{1}{2\pi} \sum_{k:|z_k(x,u)|=1} \left| \frac{\frac{\partial}{\partial x} z_k(x,u)}{z_k(x,u)} \right| du \tag{6.4}$$

$$= \frac{1}{2\pi} \int_0^{1/r} \frac{1}{\sqrt{u}} \sum_{k:|z_k(x/\sqrt{u})|=1} \left| \frac{z_k'(x/\sqrt{u})}{z_k(x/\sqrt{u})} \right| du. \tag{6.5}$$

By the same reasoning as in [11], we therefore obtain the following result (δ_x denotes the Dirac measure).

Theorem 6.1. *Let $\lambda_1^{(n,r)} \leq \cdots \leq \lambda_n^{(n,r)}$ be the eigenvalues of the random matrix $G_n^{(r)}/\sqrt{n}$ with $\gamma_1, \ldots, \gamma_r > 0$. Then the empirical eigenvalue distribution $\sum_{j=1}^n \delta_{\lambda_j^{(n,r)}}/n$ converges weakly (almost surely) to the measure $\mu_{0,1/r}$ defined in* (6.4).

We conclude this section with a brief example illustrating Theorem 6.1 in the case $r = 2$. In the left part of Figure 1, we show the simulated eigenvalue distribution of the matrix $G_n^{(r)}/\sqrt{n}$ in the case $n = 5000$, $\gamma_1 = \gamma_2 = 1$, while the corresponding limiting density is shown in the right part of the figure. Similar results in the case $r = 2$, $\gamma_1 = 1$, and $\gamma_2 = 5$ are depicted in Figure 2. Note that the derivatives $z_k'(x)$ can be evaluated numerically using the formula (Implicit Function Theorem)

$$z_k'(x) = -\frac{\frac{\partial f}{\partial x}(z_k(x), x)}{\frac{\partial f}{\partial z}(z_k(x), x)}.$$

7 Proofs

7.1 Proof of Proposition 2.1. First, we consider the behavior of the roots $z_k(x)$ for $x \to \infty$. It is easy to check that in this limit,

$$\begin{aligned} z_k(x) &\to 0, \quad k = 1, \ldots, r, \\ |z_k(x)| &\to \infty, \quad k = r+1, \ldots, 2r; \end{aligned} \tag{7.1}$$

see, e.g., [10]. In particular, $|z_r(x)| < |z_{r+1}(x)|$ if $|x|$ is large enough, showing the compactness of Γ_0.

Next, we ask the following question. For which $x \in \mathbb{C}$ can we have a root $z_k = z_k(x)$ such that $|z_k| = 1$? In this case, (2.5) becomes

$$0 = f(z_k, x) = \det(z_k A^* + B + \overline{z_k} A - x I_r),$$

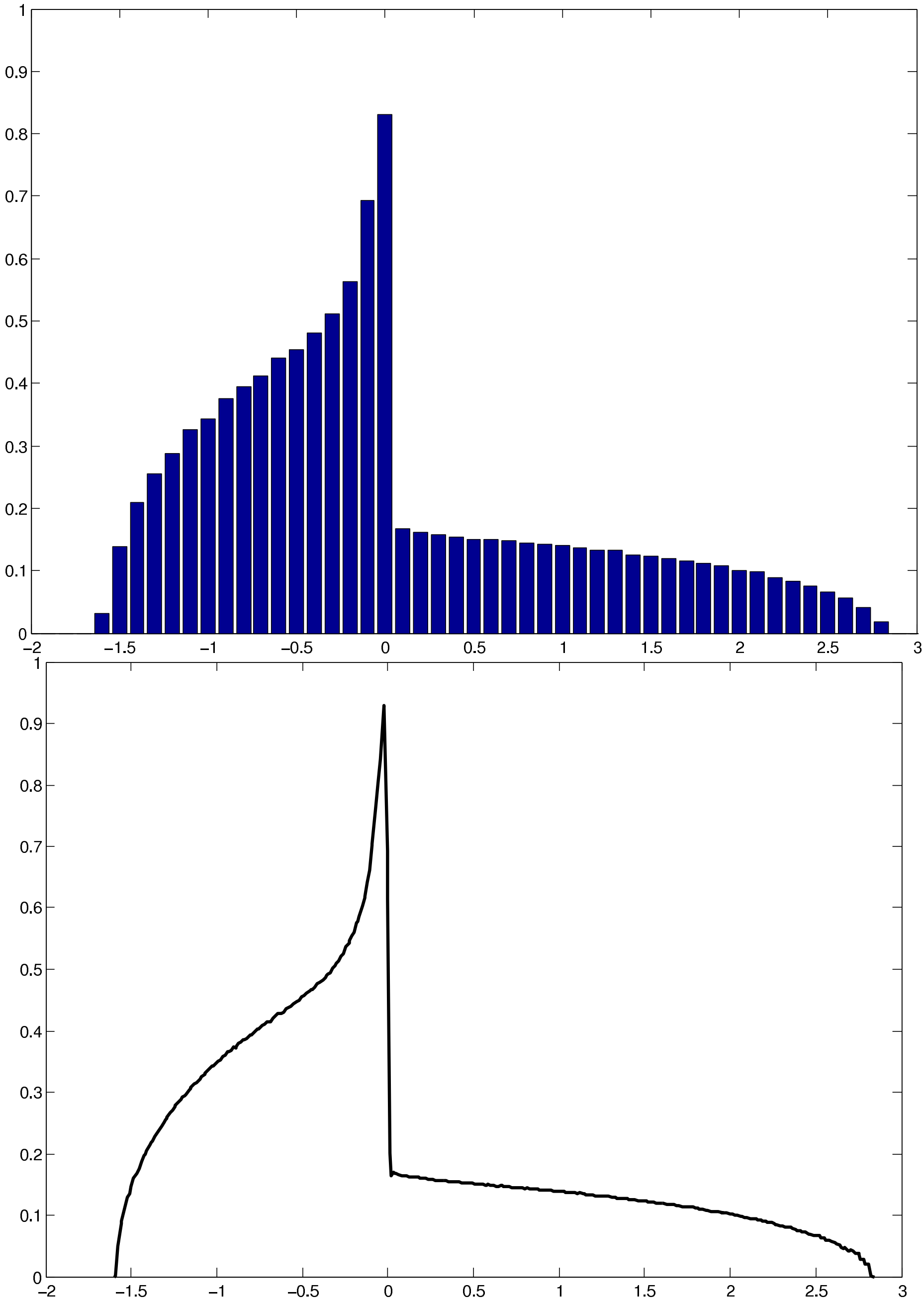

Figure 1. Simulated and limiting spectral density of the random block matrix $G_n^{(r)}/\sqrt{n}$ in the case $r = 2$, $\gamma_1 = 1$, $\gamma_2 = 1$. In the simulation, the eigenvalue distribution of a 5000×5000 matrix was calculated (i.e. $m = n/r = 2500$).

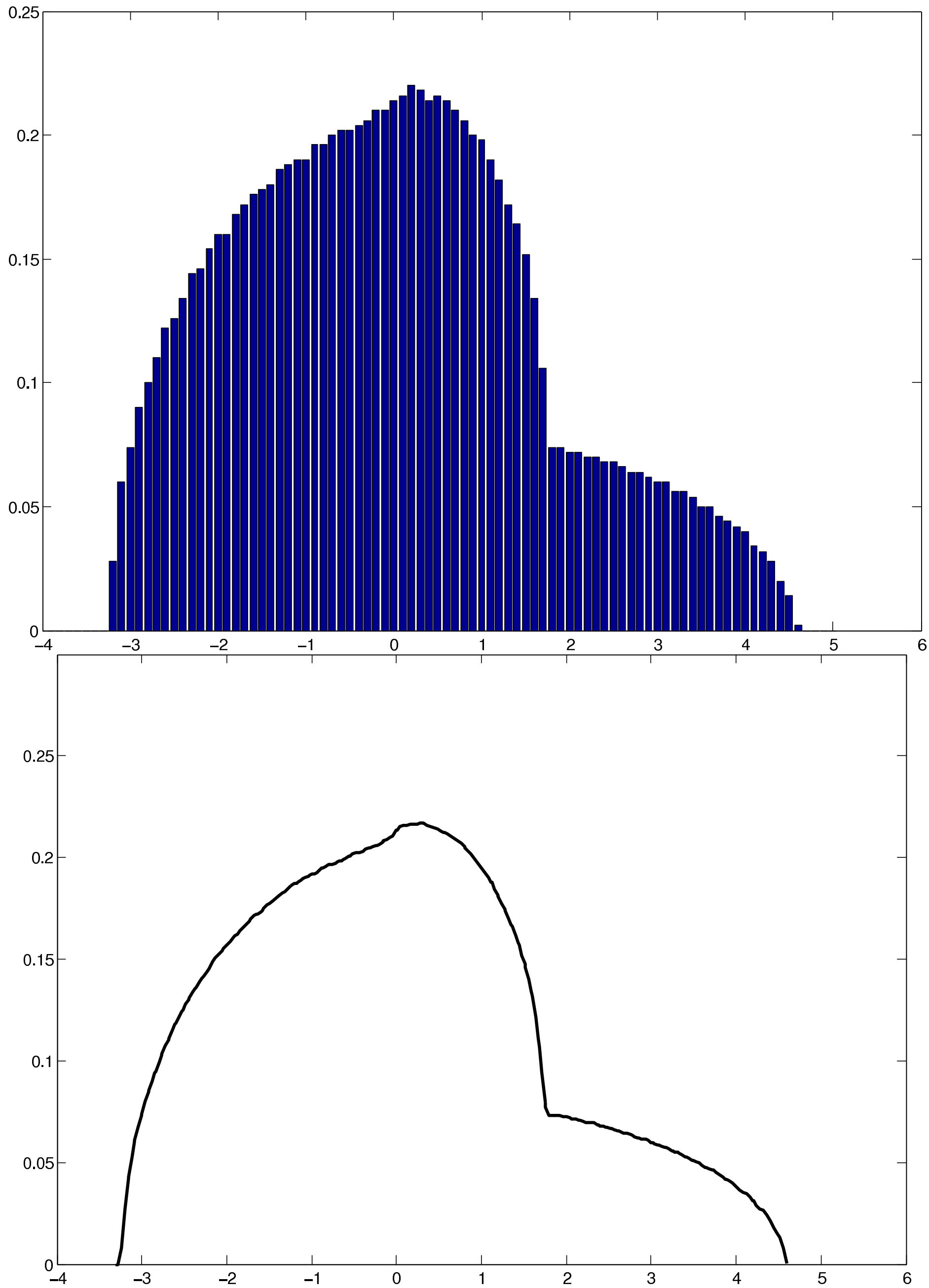

Figure 2. Simulated and limiting spectral density of the random block matrix $G_n^{(r)}/\sqrt{n}$ in the case $r = 2$, $\gamma_1 = 1$, $\gamma_2 = 5$. In the simulation, the eigenvalue distribution of a 5000×5000 matrix was calculated (i.e. $m = n/r = 2500$).

so x is an eigenvalue of the Hermitian matrix $z_k A^* + B + \overline{z_k} A$. In particular, it follows that

$$|z_k(x)| = 1 \;\Rightarrow\; x \in \mathbb{R}. \tag{7.2}$$

Now for $x \to \infty$, (7.1) implies that precisely r roots $z_k(x)$ satisfy $|z_k(x)| < 1$. By (7.2) and continuity, this must then hold for all $x \in \mathbb{C} \setminus \mathbb{R}$, i.e.,

$$x \in \mathbb{C} \setminus \mathbb{R} \;\Rightarrow\; \begin{cases} |z_k(x)| < 1, & k = 1, \dots, r, \\ |z_k(x)| > 1, & k = r+1, \dots, 2r. \end{cases}$$

In particular, we see that $|z_r(x)| < 1 < |z_{r+1}(x)|$ for $x \in \mathbb{C} \setminus \mathbb{R}$, implying that $\Gamma_0 \subset \mathbb{R}$.

Finally, the claim that $\Gamma_0 \subset \mathbb{R}$ is the disjoint union of at most r intervals follows from [10, 29]. □

7.2 Proof of Lemma 2.2 The proof uses ideas from Durán [13, Proof of Lemma 2.2]. We invoke a general result known as the *square-free factorization for multivariate polynomials*. In our context, it implies that there exists a factorization of the bivariate polynomial $z^r f(z, x)$ of the form

$$z^r f(z, x) = \prod_{k=1}^{K} g_k(z, x)^{m_k} \tag{7.3}$$

for certain $K \in \mathbb{Z}_{>0}$, multiplicities $m_1, \dots, m_K \in \mathbb{Z}_{>0}$, and non-constant bivariate polynomials $g_1(z, x), \dots, g_K(z, x)$, in such a way that

$$g(z, x) := \prod_{k=1}^{K} g_k(z, x) \tag{7.4}$$

is square-free; i.e., for all but finitely many $x \in \mathbb{C}$, the roots z of $g(z, x) = 0$ are all distinct, and vice versa with the roles of x and z reversed.

The existence of the square-free factorization of the previous paragraph can be obtained from a repeated use of Euclid's algorithm. For example, if $z^r f(z, x) = 0$ has a multiple root $z = z(x)$ for all $x \in \mathbb{C}$, then we apply Euclid's algorithm with input polynomials $z^r f(z, x)$ and $\frac{\partial}{\partial z}(z^r f(z, x))$, viewed as polynomials in z with coefficients in $\mathbb{C}[x]$. This gives us the greatest common divisor of these two polynomials and yields a factorization $z^r f(z, x) = g_1(z, x) g_2(z, x)$ for two bivariate polynomials g_1, g_2 which both depend non-trivially on z. Note that the factorization can be taken fraction free, i.e., with g_1, g_2 being polynomials in x rather than rational functions. If one of the factors g_1 or g_2 has a multiple root $z = z(x)$ for all $x \in \mathbb{C}$, then we repeat the above procedure. If g_1 and g_2 have a common root $z = z(x)$ for all $x \in \mathbb{C}$, then we apply Euclid's algorithm with input polynomials g_1 and g_2 viewed again as polynomials in z with coefficients in $\mathbb{C}[x]$. Repeating this procedure sufficiently many times yields the square-free factorization in the required form. Note that the factors $g_k(z, x)$ in (7.3) all depend non-trivially on both z and x. For if $g_k(z, x)$ were a polynomial in z alone (say), then there would exist $z \in \mathbb{C}$ such that $f(z, x) = 0$ for all $x \in \mathbb{C}$, which is easily seen to contradict (2.5).

From the above paragraphs, we easily get the symmetry relation $m_1(z, x) = m_2(z, x)$, for all but finitely many $z, x \in \mathbb{C}$. This proves one part of Lemma 2.2.

It remains to show that $m_2(z, x) = d(z, x)$ for all but finitely many $z, x \in \mathbb{C}$. From the definitions, this is equivalent to showing that the matrix $zA^* + B + z^{-1}A$ is diagonalizable for all but finitely many $z \in \mathbb{C}$. This is certainly true if $|z| = 1$, since then $zA^* + B + z^{-1}A$ is Hermitian; so, in particular, it is diagonalizable. The claim then follows in exactly the same way as in [13, Proof of Lemma 2.2]. □

7.3 Proof of Theorem 2.3. Before going to the proof of Theorem 2.3, let us recall the following result of Dette-Reuther [11]. As previously mentioned, this result uses the Hermitian structure of (1.2) in an essential way.

Lemma 7.1 (See [11])**.** *If all roots of the matrix orthogonal polynomials $P_n(x)$ are located in the interval $[-M, M]$, then*

$$|\mathbf{v}^* P_n(z) P_{n+1}^{-1}(z) A_{n+1}^{-1} \mathbf{v}| \leq \frac{1}{\operatorname{dist}(z, [-M, M])}$$

for all complex numbers z and all column vectors $\mathbf{v}$ with euclidean norm $||\mathbf{v}|| = 1$.

We need the following variant of Lemma 7.1.

Corollary 7.2. *In the matrix Nevai class* (1.3)*, there exists $M > 0$ as in Lemma 7.1 such that*

$$|\mathbf{w}^* P_n(z) P_{n+1}^{-1}(z) \mathbf{v}| \leq \frac{8||A||}{\operatorname{dist}(z, [-M, M])} \tag{7.5}$$

for all n sufficiently large, all column vectors $\mathbf{v}, \mathbf{w}$ with $||\mathbf{v}|| = ||\mathbf{w}|| = 1$, and all complex numbers z. Here, $||A||$ denotes the operator norm (also known as 2-norm, or maximal singular value) of the matrix A.

Proof. For fixed n and fixed $z \in \mathbb{C}$, define the sesquilinear form

$$\langle \mathbf{v}, \mathbf{w} \rangle_A := \mathbf{w}^* P_n(z) P_{n+1}^{-1}(z) A_{n+1}^{-1} \mathbf{v}.$$

This form is linear in its first argument and anti-linear in its second argument. Also define $||\mathbf{v}||_A^2 := \langle \mathbf{v}, \mathbf{v} \rangle_A$. (This "norm" is not necessarily positive!) The polar identity asserts that

$$\langle \mathbf{v}, \mathbf{w} \rangle_A = \frac{1}{4} \left(||\mathbf{v} + \mathbf{w}||_A^2 - ||\mathbf{v} - \mathbf{w}||_A^2 + i||\mathbf{v} + i\mathbf{w}||_A^2 - i||\mathbf{v} - i\mathbf{w}||_A^2 \right).$$

Combining this with Lemma 7.1, we obtain

$$|\mathbf{w}^* P_n(z) P_{n+1}^{-1}(z) A_{n+1}^{-1} \mathbf{v}| =: |\langle \mathbf{v}, \mathbf{w} \rangle_A| \leq \frac{4}{\operatorname{dist}(z, [-M, M])}$$

for all pairs of vectors $\mathbf{v}, \mathbf{w}$ with $||\mathbf{v}|| = ||\mathbf{w}|| = 1$ and all complex numbers z. Taking n so large that $||A_{n+1}|| < 2||A||$ (recall (1.3)), we get the desired inequality (7.5). □

Proof of Theorem 2.3. The proof is based on a normal family argument. Fix $k \in \{1, \ldots, r\}$ and $z_0 \in \mathbb{C} \setminus [-M, M]$. By (7.5), $P_n(z) P_{n+1}^{-1}(z) \mathbf{v}_k(z)$ is uniformly bounded entrywise in a neighborhood of $z = \infty$. By Montel's theorem, we can take a subsequence of indices $(n_i)_{i=0}^{\infty}$ such that $\lim_{i \to \infty} P_{n_i}(z) P_{n_i+1}^{-1}(z) \mathbf{v}_k(z)$ exists uniformly in this neighborhood. We prove by induction on $l = 0, 1, 2, \ldots$ that

$$\lim_{i \to \infty} P_{n_i}(x) P_{n_i+1}^{-1}(x) \mathbf{v}_k(x) = z_k(x) \mathbf{v}_k(x) + O(x^{-l}), \quad x \to \infty. \tag{7.6}$$

For $l = 0$ (or $l = 1$), this follows from (7.5) and the fact that $z_k(x) = O(x^{-1})$ as $x \to \infty$.

Now assume that (7.6) is satisfied for a certain value of l and for *every* sequence $(n_i)_i$ for which the limit exists. Fixing such a sequence $(n_i)_i$, we prove that (7.6) holds with l replaced with $l + 2$. By moving to a subsequence of $(n_i)_i$ if necessary, we may assume, without loss of generality, that the limiting matrices $\lim_{i \to \infty} P_{n_i}(x) P_{n_i+1}^{-1}(x)$ and $\lim_{i \to \infty} P_{n_i-1}(x) P_{n_i}^{-1}(x)$ both exist. The induction hypothesis asserts that (7.6) holds for *every* sequence (n_i) for which the limit exists, so in particular,

$$\lim_{i \to \infty} P_{n_i-1}(x) P_{n_i}^{-1}(x) \mathbf{v}_k(x) = z_k(x) \mathbf{v}_k(x) + O(x^{-l}), \quad x \to \infty. \tag{7.7}$$

Now write the three-term recurrence (1.1) in the form

$$A_{n_i}^* P_{n_i-1}(x) P_{n_i}^{-1}(x) + (B_{n_i} - x I_r) + A_{n_i+1} P_{n_i+1}(x) P_{n_i}^{-1}(x) = 0.$$

Multiplying on the right by $\mathbf{v}_k(x)$, taking the limit as $i \to \infty$, and using the facts that $\lim_n A_n = A$ and $\lim_n B_n = B$, we get

$$A^* \lim_{i\to\infty} \left(P_{n_i-1}(x)P_{n_i}^{-1}(x)\right) \mathbf{v}_k(x)+(B-xI_r)\mathbf{v}_k(x)+A\lim_{i\to\infty}\left(P_{n_i+1}(x)P_{n_i}^{-1}(x)\right)\mathbf{v}_k(x) = 0.$$

With the help of (7.7) and (2.2), this implies

$$A\lim_{i\to\infty}\left(P_{n_i+1}(x)P_{n_i}^{-1}(x)\right)\mathbf{v}_k(x) = Az_k^{-1}(x)\mathbf{v}_k(x) + O(x^{-l}), \quad x \to \infty.$$

Multiplying this relation on the left by $z_k(x)\lim_{n\to\infty}\left(P_{n_i}(x)P_{n_i+1}^{-1}(x)\right)A^{-1}$, and using (7.5) and the fact that $z_k(x) = O(x^{-1})$ for $x \to \infty$, we obtain

$$\lim_{i\to\infty} P_{n_i}(x)P_{n_i+1}^{-1}(x)\mathbf{v}_k(x) = z_k(x)\mathbf{v}_k(x) + O(x^{-l-2}), \quad x \to \infty,$$

showing that the induction hypothesis (7.6) holds with l replaced with $l+2$. □

7.4 Proof of Theorem 2.5. Write the telescoping product

$$\det P_n(x) = \left(\det P_n(x)P_{n-1}^{-1}(x)\right)\ldots\left(\det P_2(x)P_1^{-1}(x)\right)\left(\det P_1(x)P_0^{-1}(x)\right)\det P_0(x).$$

Taking logarithms and dividing by rn, we get

$$\frac{1}{rn}\log\det P_n(x) = \frac{1}{rn}\left(\left(\sum_{k=1}^{n}\log\det P_k(x)P_{k-1}^{-1}(x)\right) + \log\det P_0(x)\right).$$

(Here, we use the logarithm as a complex multi-valued function.) Taking the limit $n \to \infty$ and using the ratio asymptotics in Corollary 2.4, we obtain

$$-\lim_{n\to\infty}\frac{1}{rn}\log(\det P_n(x)) = \frac{1}{r}\log(z_1(x)\ldots z_r(x)), \quad x \in \mathbb{C}\setminus[-M,M].$$

Now take the real part of both sides of this equation. The left hand side becomes precisely the logarithmic potential of μ_0, up to an additive constant C. So we obtain (2.13); the constant C can be determined by calculating the asymptotics for $x \to \infty$. □

7.5 Proof of Proposition 2.6. From Proposition 2.1 and its proof, we know that both the left and right hand sides of the equation in (2.15) are subsets of the real axis. Now for $x \in \mathbb{R}$, we have the symmetry relation

$$\begin{aligned}\overline{f(z,x)} &:= \overline{\det(A^*z + B + Az^{-1} - xI_r)} = \det(A\bar{z} + B + A^*\bar{z}^{-1} - xI_r)\\ &= f(\bar{z}^{-1}, x),\end{aligned} \tag{7.8}$$

where the bar denotes complex conjugation. We have used the fact that $\overline{\det M} = \det(M^*)$ for any square matrix M. This implies that for each solution $z = z_k(x)$ of the equation $f(z, x) = 0$, the complex conjugated inverse $z = \bar{z}_k^{-1}(x)$ is a solution as well, with the same multiplicity. So with the ordering (2.4), $|z_k(x)| \cdot |z_{2r-k}(x)| = 1$ for any $k = 1, \ldots, r$. In particular, $|z_r(x)| = |z_{r+1}(x)|$ if and only if $|z_r(x)| = 1$. □

7.6 Proof of Proposition 2.7. We use the notation in Section 2.4. Fix $x \in \mathcal{I} \subset \Gamma_0$ and define the sets

(7.9) $$S_+(x) = \{z_k(x) \mid |z_k(y)| < 1 \text{ for all } y \in \Omega \cap \mathbb{C}_+\},$$

(7.10) $$S_-(x) = \{z_k(x) \mid |z_k(y)| < 1 \text{ for all } y \in \Omega \cap \mathbb{C}_-\}.$$

So $S_+(x)$ (or $S_-(x)$) contains all the roots $z_k(x)$ for which $|z_k(y)| < 1$ for y in the upper half plane (or lower half plane, respectively) close to x.

Let $z_k(x)$ be a root of modulus strictly less than 1. By continuity, this root belongs to both sets $S_+(x)$ and $S_-(x)$, with the same multiplicity, and hence the contributions from the +- and −-terms in (2.14) corresponding to this root $z_k(x)$ cancel out.

Next, let $z_k(x)$ be a root of modulus 1. Assume again that $z_k(y) = e^{i\theta_k(y)}$ with $\theta_k(y)$ real and differentiable for $y \in \mathcal{I} \subset \mathbb{R}$. Suppose that $\theta_k'(x) > 0$. Then the Cauchy-Riemann equations applied to $\log z_k(y)$ imply that $|z_k(y)| < 1$ for y in the upper half plane close to x, and $|z_k(y)| > 1$ for y in the lower half plane close to x. So $z_k(x)$ lies in the set $S_+(x)$ in (7.9) but not in $S_-(x)$. Similarly, if $\theta_k'(x) < 0$ then $z_k(x)$ lies in the set $S_-(x)$ but not in $S_+(x)$. In both cases, the contribution from $z_k(x)$ in the right hand side of (2.14) has a positive sign, and so we obtain the desired equality (2.16).

Finally, the claim that $\theta'(x) \neq 0$ for any $x \in \mathcal{I} \subset \Gamma_0$ follows since if this fails, then general considerations (e.g., in [27, Proof of Theorem 11.1.1(v)]) would imply that $\Gamma_0 \not\subset \mathbb{R}$, which is a contradiction. □

7.7 Proof of Theorem 3.1. The proof of Theorem 2.3 and 2.5 can be easily extended to prove Theorem 3.1. The difference is that the limits $\lim_{n_i \to \infty}$ should be replaced by local limits of the form $\lim_{n_i/N \to s}$. The details are straightforward and left to the reader. (For similar reasoning, see also [3, 7, 11, 20, 22], among others.)

7.8 Proof of Theorem 3.4. The proof of Theorem 3.4 follows the same scheme as the proof of Theorem 2.3, but it is more complicated because of the higher periodicity. To deal with the periodicity, we use some ideas from [3]. It is convenient to make the substitution $z = y^p$ and work with the transformed matrix

$$G(y,x) := \operatorname{diag}(1, y, \ldots, y^{p-1})F(y^p, x) \cdot \operatorname{diag}(1, y^{-1}, \ldots, y^{-(p-1)}) \tag{7.11}$$

$$= \begin{pmatrix} B^{(0)} - xI_r & y^{-1}A^{(1)} & 0 & 0 & yA^{(0)*} \\ yA^{(1)*} & B^{(1)} - xI_r & y^{-1}A^{(2)} & 0 & 0 \\ 0 & yA^{(2)*} & \ddots & \ddots & 0 \\ 0 & 0 & \ddots & \ddots & y^{-1}A^{(p-1)} \\ y^{-1}A^{(0)} & 0 & 0 & yA^{(p-1)*} & B^{(p-1)} - xI_r \end{pmatrix}_{pr \times pr}. \tag{7.12}$$

Consistent with the substitution $z = y^p$, we set $y_k(x) = z_k^{1/p}(x)$, $k = 1, \ldots, 2r$, for an arbitrary but fixed choice of the pth root. The ordering (2.4) implies that

$$0 < |y_1(x)| \leq |y_2(x)| \leq \ldots \leq |y_r(x)| \leq |y_{r+1}(x)| \leq \ldots \leq |y_{2r}(x)|. \tag{7.13}$$

Note that each $y = y_k(x)$ is a root of the algebraic equation

$$\det G(y,x) \equiv \det F(y^p, x) = 0.$$

From (7.12), it is then easy to check that (see, e.g., [10])

$$y_k(x) \propto \begin{cases} x^{-1}, & k = 1, \ldots, r, \quad x \to \infty, \\ x, & k = r+1, \ldots, 2r, \quad x \to \infty, \end{cases} \tag{7.14}$$

where the symbol $\propto$ means that the ratio of the left and right hand sides is bounded both from below and above in absolute value as $x \to \infty$.

Denote by $\mathbf{w}_k(x)$ a normalized null space vector such that

$$G(y_k(x), x)\mathbf{w}_k(x) = \mathbf{0}. \tag{7.15}$$

If there are roots $y_k(x)$ with higher multiplicities, we pick the vectors $\mathbf{w}_k(x)$ as explained in Section 2.2. We again partition $\mathbf{w}_k(x)$ into blocks as

$$\mathbf{w}_k(x) = \begin{pmatrix} \mathbf{w}_{k,0}(x) \\ \vdots \\ \mathbf{w}_{k,p-1}(x) \end{pmatrix}, \tag{7.16}$$

where each $\mathbf{w}_{k,j}(x)$, $j = 0, 1, \ldots, p-1$, is a column vector of length r. Assuming the normalization $||\mathbf{w}_k(x)|| = 1$, we then have

$$\lim_{x\to\infty} ||\mathbf{w}_{k,j}(x)|| = C_{k,j} > 0, \quad j = 0, 1, \ldots, p-1. \tag{7.17}$$

This follows from (7.15)–(7.16), (7.14), and inspection of the dominant terms for $x \to \infty$ in the matrix (7.12).

Theorem 3.4 is a consequence of the following stronger statement.

$$\left(\lim_{n\to\infty} P_{pn+j}(x)P^{-1}_{pn+j+1}(x)\right) \mathbf{w}_{k,j+1}(x) = y_k(x)\mathbf{w}_{k,j}(x), \quad x \to \infty, \tag{7.18}$$

uniformly for x in compact subsets of $\mathbb{C} \setminus ([-M, M] \cup S)$, for all $k \in \{1, \ldots, r\}$ and for all residue classes $j \in \{0, 1, \ldots, p-1\}$ modulo p. (We identify $\mathbf{w}_{k,p}(x) \equiv \mathbf{w}_{k,0}(x)$.) Indeed, Theorem 3.4 follows immediately by iterating (7.18) p times and using that $y_k^p(x) = z_k(x)$.

The rest of the proof is devoted to establishing (7.18). We show by induction on $l \geq 0$ that

$$\left(\lim_{i\to\infty} P_{pn_i+j}(x)P^{-1}_{pn_i+j+1}(x)\right) \mathbf{w}_{k,j+1}(x) = y_k(x)\mathbf{w}_{k,j}(x)(1 + O(x^{-l})), \quad x \to \infty, \tag{7.19}$$

for any $k \in \{1, \ldots, r\}$ and $j \in \{0, 1, \ldots, p-1\}$, and for any increasing sequence $(n_i)_{i=0}^{\infty}$ for which the limit in the left hand side exists.

Assume that the induction hypothesis (7.19) holds for a certain value of $l \geq 0$. We show that it also holds for $l + 2$. Let $(n_i)_{i=0}^{\infty}$ be an increasing sequence for which the limit in the left hand side of (7.19) exists. We can assume, without loss of generality, that $j = p - 1$; a similar argument works for the other values of $j \in \{0, 1, \ldots, p-1\}$. Now, from the three-term recursion, we obtain

$$\begin{pmatrix} A^*_{pn_i} & B_{pn_i} - xI_r & A_{pn_i+1} & & & \\ & A^*_{pn_i+1} & \ddots & \ddots & & \\ & & \ddots & \ddots & A_{pn_i+p-1} & \\ & & & A^*_{pn_i+p-1} & B_{pn_i+p-1} - xI_r & A_{pn_i+p} \end{pmatrix} \begin{pmatrix} P_{pn_i-1}(x) \\ P_{pn_i}(x) \\ \vdots \\ P_{pn_i+p-1}(x) \\ P_{pn_i+p}(x) \end{pmatrix} = 0. \tag{7.20}$$

Applying a diagonal multiplication with appropriate powers of $y := y_k(x)$, we get

$$\begin{pmatrix} yA^*_{pn_i} & B_{pn_i} - xI_r & y^{-1}A_{pn_i+1} & & & \\ & yA^*_{pn_i+1} & \ddots & \ddots & & \\ & & \ddots & \ddots & y^{-1}A_{pn_i+p-1} & \\ & & & yA^*_{pn_i+p-1} & B_{pn_i+p-1} - xI_r & y^{-1}A_{pn_i+p} \end{pmatrix} \times \begin{pmatrix} y^{-p}P_{pn_i-1}(x) \\ y^{-(p-1)}P_{pn_i}(x) \\ \vdots \\ y^{-1}P_{pn_i+p-2}(x) \\ P_{pn_i+p-1}(x) \\ yP_{pn_i+p}(x) \end{pmatrix} = 0. \tag{7.21}$$

Let us focus on the rightmost matrix in the left hand side of (7.21). Multiplying on the right by $P^{-1}_{pn_i+p-1}(x)\mathbf{w}_{k,p-1}(x)$, we see that it becomes

$$\begin{pmatrix} y^{-p}P_{pn_i-1}P^{-1}_{pn_i+p-1}\mathbf{w}_{k,p-1} \\ \vdots \\ y^{-1}P_{pn_i+p-2}P^{-1}_{pn_i+p-1}\mathbf{w}_{k,p-1} \\ \mathbf{w}_{k,p-1} \\ yP_{pn_i+p}P^{-1}_{pn_i+p-1}\mathbf{w}_{k,p-1} \end{pmatrix}. \tag{7.22}$$

(Here, for notational simplicity, we skip the x-dependence.) By considering a subsequence of $(n_i)_{i=0}^{\infty}$, if necessary, and using compactness, we may assume that each block of (7.22) has a limit as $i \to \infty$. Repeated application of the induction hypothesis (7.19) then implies that the limit of (7.22) as $i \to \infty$ behaves as

$$\begin{pmatrix} \mathbf{w}_{k,p-1}(1 + O(x^{-l})) \\ \mathbf{w}_{k,0}(1 + O(x^{-l})) \\ \vdots \\ \mathbf{w}_{k,p-2}(1 + O(x^{-l})) \\ \mathbf{w}_{k,p-1} \\ \varphi(x) \end{pmatrix}$$

for $x \to \infty$, where

$$\varphi(x) := \left(\lim_{i\to\infty} P_{pn_i+p}(x)P^{-1}_{pn_i+p-1}(x)\right) y_k(x)\mathbf{w}_{k,p-1}(x). \tag{7.23}$$

Multiplying (7.21) on the right by $P^{-1}_{pn_i+p-1}(x)\mathbf{w}_{k,p-1}(x)$ and taking the limit as

$i \to \infty$, we get from the above observations that

$$\begin{pmatrix} yA^{(0)*} & B^{(0)} - xI_r & y^{-1}A^{(1)} & & & \\ & yA^{(1)*} & \ddots & \ddots & & \\ & & \ddots & \ddots & y^{-1}A^{(p-1)} & \\ & & & yA^{(p-1)*} & B^{(p-1)} - xI_r & y^{-1}A^{(0)} \end{pmatrix} \times \begin{pmatrix} \mathbf{w}_{k,p-1} \\ \mathbf{w}_{k,0} \\ \vdots \\ \mathbf{w}_{k,p-2} \\ \mathbf{w}_{k,p-1} \\ \varphi(x) \end{pmatrix} = \begin{pmatrix} O(x^{-l+1}) \\ \vdots \\ O(x^{-l+1}) \\ O(x^{-l-1}) \end{pmatrix} \tag{7.24}$$

as $x \to \infty$. Here, we have used the fact that $y \equiv y_k(x) \propto x^{-1}$ as $x \to \infty$. Taking the last block row of this equation yields

$$y_k(x)A^{(p-1)*}\mathbf{w}_{k,p-2} + (B^{(p-1)} - xI_r)\mathbf{w}_{k,p-1} + y_k^{-1}(x)A^{(0)}\varphi(x) = O(x^{-l-1}), \tag{7.25}$$

while by (7.15), (7.16) and (7.12) (evaluated for the last block row), we have that

$$y_k^{-1}(x)A^{(0)}\mathbf{w}_{k,0} + y_k(x)A^{(p-1)*}\mathbf{w}_{k,p-2} + (B^{(p-1)} - xI_r)\mathbf{w}_{k,p-1} = 0.$$

Subtracting this from (7.25) yields

$$A^{(0)}\left(\lim_{i\to\infty} P_{pn_i+p}(x)P^{-1}_{pn_i+p-1}(x)\right)\mathbf{w}_{k,p-1}(x) - y_k^{-1}(x)A^{(0)}\mathbf{w}_{k,0}(x) = O(x^{-l-1})$$

on account of (7.23). The factor $A^{(0)}$ can be ignored. Multiplying on the left by $y_k(x) \times \left(\lim_{i\to\infty} P_{pn_i+p-1}(x)P^{-1}_{pn_i+p}(x)\right)$, we get

$$\left(\lim_{i\to\infty} P_{pn_i+p-1}(x)P^{-1}_{pn_i+p}(x)\right)\mathbf{w}_{k,0}(x) - y_k(x)\mathbf{w}_{k,p-1}(x) = O(x^{-l-3})$$

or, equivalently,

$$\left(\lim_{i\to\infty} P_{pn_i+p-1}(x)P^{-1}_{pn_i+p}(x)\right)\mathbf{w}_{k,0}(x) = y_k(x)\mathbf{w}_{k,p-1}(x)(1 + O(x^{-l-2})).$$

We conclude that (7.19) holds with l replaced with $l + 2$. $\square$

7.9 Proof of Proposition 4.2. Throughout the proof, we use the notation of Section 4. Recall that the Hermitian symmetry $A = A^*$ implies that the roots $z_k(x)$ appear in pairs $\{z_k(x), z_k(x)^{-1}\}$. Both $z_k(x)$ and $z_k(x)^{-1}$ correspond to the same value of $w_k(x) = z_k(x) + z_k(x)^{-1}$ in (4.9), and therefore to the same null space vector $\mathbf{v}_k(x)$.

Now let $x \in \mathbb{R}$. For any $w_k(x) = 2\cos\theta_k(x) \in (-2, 2)$ with $\theta \in (0, \pi)$, $k = 1, \ldots, r$, we have a pair of roots $z_{k_1}(x) = e^{i\theta_k(x)}$ and $z_{k_2}(x) = e^{-i\theta_k(x)}$ with $\{k_1, k_2\} = \{k, 2r - k\}$. Suppose that $w_k'(x) > 0$. Then the Cauchy-Riemann equations show that $z_{k_1}(x)$ lies in the set $S_-(x)$ in (7.10) but not in $S_+(x)$, and vice versa for the root $z_{k_2}(x)$. The reverse situation occurs if $w_k'(x) < 0$.

Fix $x \in \mathbb{R}$ and assume the labeling of roots is such that

$$\max\{|z_1(x)|, \ldots, |z_K(x)|\} < 1, \quad |z_{K+1}(x)| = \ldots = |z_r(x)| = 1$$

with $K \in \{0, \ldots, r\}$. Taking into account the above observations, we find from (4.2) that

$$\begin{aligned}
&\lim_{\epsilon\to 0+} F_W(x + \epsilon i)\\
&\quad = V(x)\left(\lim_{\epsilon\to 0+} D(x+\epsilon i)\right) V^{-1}(x)A^{-1}\\
&\quad = V(x)\,\mathrm{diag}(z_1(x), \ldots, z_K(x), e^{-i\theta_{K+1}(x)\mathrm{sign}\, w'_{K+1}(x)}, \ldots, e^{-i\theta_r(x)\mathrm{sign}\, w'_r(x)})V^{-1}(x)A^{-1}.
\end{aligned}$$

Similarly,

$$\begin{aligned}
&\lim_{\epsilon\to 0+} F_W(x - \epsilon i)\\
&\quad = V(x)\left(\lim_{\epsilon\to 0+} D(x-\epsilon i)\right) V^{-1}(x)A^{-1}\\
&\quad = V(x)\,\mathrm{diag}(z_1(x), \ldots, z_K(x), e^{i\theta_{K+1}(x)\mathrm{sign}\, w'_{K+1}(x)}, \ldots, e^{i\theta_r(x)\mathrm{sign}\, w'_r(x)})V^{-1}(x)A^{-1}.
\end{aligned}$$

Using the Stieltjes inversion principle

$$\frac{\mathrm{d}W(x)}{\mathrm{d}x} = \frac{1}{2\pi i}\lim_{\epsilon\to 0+}\left(F_W(x-\epsilon i) - F_W(x+\epsilon i)\right),$$

we see that the desired formula for $\mathrm{d}W/\mathrm{d}x$ now follows from a straightforward calculation. We also obtain the formula for $\mathrm{d}X/\mathrm{d}x$ similarly from (4.4), taking into account the simplifications due to $A = A^*$. □

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