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# Optimal estimates for condition numbers and norms of resolvents in terms of the spectrum

Oleg Szehr<sup>1,\*</sup> and Rachid Zarouf<sup>2,†</sup>

<sup>1</sup>*Centre for Quantum Information, University of Cambridge,  
Cambridge CB3 0WA, United Kingdom*

<sup>2</sup>*Aix-Marseille Université, CNRS, Centrale Marseille,  
Institut de Mathématiques de Marseille (I2M), UMR 7353, 13453 Marseille, France.*

In numerical analysis it is often necessary to estimate the condition number  $CN(T) = \|T\| \cdot \|T^{-1}\|$  and the norm of the resolvent  $\|(\zeta - T)^{-1}\|$  of a given  $n \times n$  matrix  $T$ . We derive new spectral estimates for these quantities and compute explicit matrices that achieve our bounds. We recover the well-known fact that the supremum of  $CN(T)$  over all matrices with  $\|T\| \leq 1$  and minimal absolute eigenvalue  $r = \min_{i=1, \dots, n} |\lambda_i| > 0$  is the Kronecker bound  $\frac{1}{r}$ . This result is subsequently generalized by computing the corresponding supremum of  $\|(\zeta - T)^{-1}\|$  for any  $|\zeta| \leq 1$ . We find that the supremum is attained by a triangular Toeplitz matrix. This provides a simple class of structured matrices on which condition numbers and resolvent norm bounds can be studied numerically. The occurring Toeplitz matrices are so-called model matrices, i.e. matrix representations of the compressed backward shift operator on the Hardy space  $H_2$  to a finite-dimensional invariant subspace.

Keywords: Condition number, Resolvent, Toeplitz matrix, Model matrix, Blaschke product  
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\*Electronic address: [oleg.szehr@posteo.de](mailto:oleg.szehr@posteo.de)

†Electronic address: [rachid.zarouf@univ-amu.fr](mailto:rachid.zarouf@univ-amu.fr)

## I. INTRODUCTION

Let  $\mathcal{M}_n$  be the set of complex  $n \times n$  matrices and let  $\|T\|$  denote the spectral norm of  $T \in \mathcal{M}_n$ . We denote by  $\sigma = \sigma(T)$  the spectrum of  $T$  and by  $m_T$  its minimal polynomial. We denote by  $|m_T|$  the degree of  $m_T$ . In this article we are interested in estimates of the type

$$\|R(\zeta, T)\| \leq \Phi(|m_T|, \sigma, \zeta) \quad (1)$$

where  $R(\zeta, T) = (\zeta - T)^{-1}$  denotes the resolvent of  $T$  at point  $\zeta \in \mathbb{C} - \sigma$  and  $\Phi$  is a function of  $|m_T|$ ,  $\sigma$  and  $\zeta$ . We present a general method that yields optimal estimates of the above type and allows us to pinpoint the “worst” matrices for this problem. As it turns out for any  $\zeta \notin \sigma$  among these matrices are so-called analytic Toeplitz matrices. Generally, Toeplitz matrices are characterized by the existence of a sequence of complex numbers  $a = (a_k)_{k=-n+1}^{k=n-1}$  with

$$T = \begin{pmatrix} a_0 & a_{-1} & \cdot & \cdot & a_{-n+1} \\ a_1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & a_{-1} & \cdot \\ a_{n-1} & \cdot & \cdot & a_1 & a_0 \end{pmatrix}.$$

We call  $T_a$  an *analytic* Toeplitz matrix if  $a_k = 0$  for all  $k < 0$  and we will denote by  $\mathcal{T}_n \subset \mathcal{M}_n$  the set of Toeplitz matrices and by  $\mathcal{T}_n^a \subset \mathcal{T}_n$  the analytic Toeplitz matrices.

We will think of an estimate of the above type as an extremal problem. That is, under certain constraints on the set of admissible matrices  $T$  and fixed  $\zeta$ , we are looking to maximize  $\|R(\zeta, T)\|$  over this set. To guarantee a finite bound we at least need a constraint on the *norm* and the *spectrum* of possible  $T$ . In our discussion we will generally impose that  $\|T\| \leq 1$  and call such  $T$  a *contraction*. Note that this condition can always be achieved by normalization  $T/\|T\|$ .  $\mathcal{C}_n \subset \mathcal{M}_n$  denotes the set of contractions. To ensure that the resolvent is finite,  $\zeta$  must be separated from  $\sigma$ . Depending on the situation it will be convenient to measure this separation in *Euclidean* distance

$$d(z, w) := |z - w|, \quad z, w \in \mathbb{C}$$

or *pseudo-hyperbolic* distance

$$p(z, w) := \left| \frac{z - w}{1 - \bar{z}w} \right|, \quad z, w \in \mathbb{C}.$$

The case  $\zeta = 0$  in (1) corresponds to the study of the *condition number*  $CN(T) = \|T\| \cdot \|T^{-1}\|$ . It was shown by Kronecker in the 19th century that

$$\sup \{ \|T^{-1}\| : T \in \mathcal{C}_n, p(0, \sigma) = r \} = \frac{1}{r^n}. \quad (2)$$

The upper bound can be seen using polar decomposition [NN1, p. 137]. To prove the reverse inequality, one can use A. Horn's theorem (see [AH] and also [MO, Chap. 9, Sect. E]) that gives a converse to the famous Weyl inequalities [NN1, p. 137].

The case  $|\zeta| = 1$  was studied by Davies and Simon and applied to characterize the localization of zeros of random orthogonal polynomials on the unit circle [DS]. The corresponding estimate for  $|\zeta| = 1$  is

$$\sup \{d(\zeta, \sigma) \|R(\zeta, T)\| : T \in \mathcal{C}_n\} = \cot\left(\frac{\pi}{4n}\right). \quad (3)$$

Note that  $|\zeta| = 1$  implies that we have  $p(\zeta, \sigma) = 1$  for any  $\sigma$  such that we could add this condition to the optimization problem. In this paper we provide an approach, which

1) allows us to treat the problems (2) and (3) simultaneously and generalize them to any  $|\zeta| \leq 1$ ,

2) strengthens the result (3) for  $|\zeta| = 1$ , by considering the sup over  $T \in \mathcal{C}_n$  with fixed minimal polynomial and

3) provides explicit analytic Toeplitz matrices that achieve the estimates (1), (2) and (3).

Already for  $\zeta = 0$  it is a non-trivial question which matrices achieve the estimate (2). A theoretic classification of such matrices was given in [NN1]. However, it seems rather difficult to compute explicit matrix representations from this classification. It was suspected in [RZ] that the estimate (2) is not reached by any Toeplitz matrix; this claim is refuted here.

## II. RESOLVENT BOUNDS

Before we state our main results we need to introduce some further notation. We denote by  $\mathbb{D} = \{z \in \mathbb{C} : |z| < 1\}$  the open unit disc in the complex plane,  $\overline{\mathbb{D}}$  is its closure and  $\partial\mathbb{D}$  its boundary. For any finite set  $\sigma \subset \mathbb{D}$  we define

$$s(\zeta, \sigma) := \max \left\{ \frac{1 - |\lambda|^2}{|1 - \bar{\lambda}\zeta|} : \lambda \in \sigma, p(\zeta, \lambda) = p(\zeta, \sigma) \right\}.$$

The function  $s$  is related to the Stolz angle [JC, p. 23] between  $\zeta \in \overline{\mathbb{D}} - \sigma$  and  $\lambda \in \sigma$ . For  $T \in \mathcal{C}_n$  the function  $\zeta \mapsto s(\zeta, \sigma(T))$  is bounded on  $\overline{\mathbb{D}}$  by  $1 + \rho(T) \leq 2$ , where

$$\rho(T) := \max\{|\lambda| : \lambda \in \sigma(T)\}$$

is the spectral radius of  $T$ . Of particular importance to our discussion will be the analytic Toeplitz matrix  $X_{r,\beta}$  given entry-wise by

$$(X_{r,\beta})_{ij} = \begin{cases} 0 & \text{if } i < j \\ r^{n-1} & \text{if } i = j \\ \beta r^{n-(i-j+1)} & \text{if } i > j \end{cases} \quad (4)$$

with  $r \in [0, 1]$  and  $\beta \in [0, 2]$ . The spectral norm of  $X_{r,\beta}$  is computed below in Proposition II.6.

### A. Optimal upper bounds

**Theorem II.1.** *Let  $T \in \mathcal{C}_n$  with minimal polynomial  $m$  and spectrum  $\sigma$ . For any  $\zeta \in \overline{\mathbb{D}} - \sigma$ , it holds for the resolvent of  $T$  that*

$$\|R(\zeta, T)\| \leq \frac{1}{d(1, \bar{\sigma}\zeta)} \frac{1}{r^{|m|}} \|X_{r, \beta}\|, \quad (5)$$

where  $X_{r, \beta}$  is the  $|m| \times |m|$  analytic Toeplitz matrix defined in (4),  $r = p(\zeta, \sigma)$  and  $\beta = s(\zeta, \sigma)$ . Moreover, for any  $\zeta \in [-1, 1]$  and  $\lambda \in (-1, 1)$ ,  $\lambda \neq \zeta$  the analytic  $n \times n$  Toeplitz matrix

$$T^* = \begin{pmatrix} \lambda & 0 & \dots & \dots & 0 \\ 1 - \lambda^2 & \lambda & \ddots & \cdot & \vdots \\ -\lambda(1 - \lambda^2) & 1 - \lambda^2 & \lambda & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ (-\lambda)^{n-2}(1 - \lambda^2) & \dots & -\lambda(1 - \lambda^2) & 1 - \lambda^2 & \lambda \end{pmatrix},$$

is a contraction of minimal polynomial  $m = (z - \lambda)^n$  that achieves (5).

#### Remarks:

1. Setting  $\zeta = 0$  in Theorem II.1 we recover Kronecker's result for condition numbers. Moreover, an analytic Toeplitz matrix is extremal for the Kronecker maximization problem (2). This answers the questions raised in [RZ].
2. Considering Theorem II.1 for  $\zeta \in \partial\mathbb{D}$ , and bounding

$$\|X_{1, s(\zeta, \sigma(T))}\| \leq \|X_{1, 1+\rho(T)}\| \leq \|X_{1, 2}\|,$$

we recover the resolvent estimate of [DS] as  $\|X_{1, 2}\| = \cot(\frac{\pi}{4n})$  (cf. Proposition II.6 below). However, if e.g.  $\rho(T)$  is known we can improve on [DS].

3. Equality is achieved by a so-called *model matrix* corresponding to a fully degenerate spectrum. This matrix arises as a representation of the compressed backward shift operator of  $H_2$  with respect to the *Malmquist-Walsh basis*, see Section III below for details. The model matrix is a natural generalization of a simple Jordan block of size  $n$  to the situation when the spectrum is  $\sigma = \{a\} \subset \overline{\mathbb{D}}$ .

The next proposition treats the case  $\sigma(T) \subset \partial\mathbb{D}$ .

**Proposition II.2.** *Let  $T \in \mathcal{C}_n$  with spectrum  $\sigma \subset \partial\mathbb{D}$ . Then for any  $\zeta \in \mathbb{C} - \sigma$*

$$\|R(\zeta, T)\| \leq \frac{1}{d(\zeta, \sigma)}. \quad (6)$$

It follows that if  $T$  is a contraction such that  $\sigma(T) \subset \partial\mathbb{D}$  then it satisfies a *Linear Resolvent Growth* with constant 1, see [BN]. Clearly, any diagonal matrix in  $\mathcal{C}_n$  achieves the inequality (6).

Theorem II.1 has the disadvantage that the upper bound depends on the slightly unyielding quantity  $\|X_{r,\beta}\|$ . Taking together Theorem II.4 with Proposition II.6 (both below) leads directly to the following.

**Theorem II.3.** *Let  $T \in \mathcal{C}_n$  with minimal polynomial  $m$  and spectrum  $\sigma$ . For any  $\zeta \in \mathbb{D} - \sigma$  let  $p(\zeta, \sigma) = r$  denote the pseudo-hyperbolic distance of  $\zeta$  to  $\sigma$ . Then it holds for the resolvent of  $T$  that*

$$\|R(\zeta, T)\| \leq \frac{1}{d(1, \bar{\sigma}\zeta)} \frac{1}{r^{|m|}(1-r|\zeta|)}.$$

The estimate is sharp in the limit of large  $|m|$ .

### B. Constrained maximization of the resolvent

For any given  $\zeta \in \overline{\mathbb{D}}$  and  $r \in [0, 1]$  we study the quantity

$$\mathcal{R}(\zeta, r) := \sup \{d(1, \bar{\sigma}\zeta) \|R(\zeta, T)\| : T \in \mathcal{C}_n, p(\zeta, \sigma) = r\}, \quad (7)$$

where  $\bar{\sigma} = \{\bar{\lambda} : \lambda \in \sigma\}$ .  $\mathcal{R}$  also depends on  $n$  but we keep the notation simple and do not write this explicitly.

**Theorem II.4.** *For any  $\zeta \in \mathbb{D}$  and  $r \in (0, 1)$  we have that*

$$\mathcal{R}(\zeta, r) = \frac{1}{r^n} \|X_{r, \beta_{\max}}\|,$$

where  $\beta_{\max} = \frac{1-r^2}{1-r|\zeta|}$ . The estimate is achieved by an analytic Toeplitz matrix and in the limit of large matrices we find

$$\mathcal{R}(\zeta, r) \sim \frac{1}{r^n} \frac{1}{1-r|\zeta|} \quad \text{as } n \rightarrow \infty.$$

Recall that Kronecker's result (2) is

$$\mathcal{R}(0, r) = \frac{1}{r^n}.$$

Davies and Simon (3) have shown that

$$\mathcal{R}(\zeta, 1) = \cot\left(\frac{\pi}{4n}\right), \quad \zeta \in \partial\mathbb{D} - \{1\},$$

which can be seen in the above theorem by continuously moving  $\zeta$  to  $\partial\mathbb{D}$ . Note, however, the fundamental difference in the large  $n$  behavior of the resolvent for  $\zeta \in \mathbb{D}$  and  $\zeta \in \partial\mathbb{D}$ . This is a consequence of the fact that for  $\zeta$  inside the unit disk  $\|X_{r,\beta}\|$  is bounded from above, see Proposition II.6.

Finally for  $\zeta \in \partial\mathbb{D}$  and a polynomial  $P_\sigma$  with zero set  $\sigma$  so that  $p(\zeta, \sigma) = 1$  we can compute the constant

$$\mathcal{K}(\zeta, P_\sigma) = \sup \{d(\zeta, \sigma) \|R(\zeta, T)\| : T \in \mathcal{C}_n, m_T = P_\sigma\}, \quad (8)$$

which is bounded by  $\mathcal{R}(\zeta, r)$ .

**Proposition II.5.** *Let  $P_\sigma$  be a polynomial with zero set  $\sigma = \sigma_1 \cup \sigma_2$ ,  $\sigma_1 \subset \mathbb{D}$  and  $\sigma_2 \subset \partial\mathbb{D}$  so that  $P_\sigma = P_{\sigma_1} P_{\sigma_2}$ . For any  $\zeta \in \partial\mathbb{D} - \sigma$ , we have*

$$\mathcal{K}(\zeta, P_\sigma) \leq \max(1, \|X_{1,s(\zeta,\sigma_1)}\|) \leq \|X_{1,2}\| = \cot\left(\frac{\pi}{4|P_{\sigma_1}|}\right), \quad (9)$$

where  $X_{1,s(\zeta,\sigma)}$ ,  $X_{1,2} \in \mathcal{M}_{|P_{\sigma_1}|}(\mathbb{C})$ . Moreover, fixing  $\zeta \in \partial\mathbb{D} - \sigma$ ,  $n_1, n_2 \geq 1$  and  $0 \leq \rho_1 < 1$  and taking the supremum of  $\mathcal{K}(\zeta, P_\sigma)$  over all sets  $\sigma = \sigma_1 \cup \sigma_2$  with  $n_1 = |P_{\sigma_1}|$  and  $n_2 = |P_{\sigma_2}|$  such that  $\max_{\lambda \in \sigma_1} |\lambda| \leq \rho_1$  we get:

$$\sup \mathcal{K}(\zeta, P_\sigma) = \|X_{1,1+\rho_1}\| \quad (10)$$

where  $X_{1,1+\rho_1} \in \mathcal{M}_{n_1}(\mathbb{C})$ . In particular, the supremum of the above quantity taken over  $0 \leq \rho_1 < 1$  is equal to

$$\cot\left(\frac{\pi}{4n_1}\right).$$

### C. Computing $\|X_{r,\beta}\|$

In this subsection we study the quantity  $\|X_{r,\beta}\|$  for  $r \in (0, 1]$  and  $\beta \in [0, 2]$ . We provide an implicit formula for  $\|X_{r,\beta}\|$ .

**Proposition II.6.** *Let  $X_{r,\beta}$  with  $r \in (0, 1]$  and  $\beta \in [0, 2]$  be the  $n \times n$  matrix introduced in (4). The following assertions hold.*

- i) *If  $\beta = 1 - r^2$  then  $\|X_{r,\beta}\| = 1$ .*
- ii) *At fixed  $n$ ,  $\|X_{r,\beta}\|$  grows monotonically with  $r$  and  $\beta$ .*
- iii) *At fixed  $r$  and  $1 - r^2 \leq \beta$ ,  $\|X_{r,\beta}\|$  grows monotonically with  $n$ .*
- iv) *Let  $U_n$  denote the  $n$ -th degree Chebychev polynomial of second kind, i.e.  $U_n(\cos(\theta)) = \frac{\sin((n+1)\theta)}{\sin(\theta)}$ . If  $\beta \neq 1 - r^2$  then  $\|X_{r,\beta}\| = |\lambda^*|$ , where  $\lambda^*$  is the largest in magnitude solution of the polynomial equation*

$$\mu^{n+1} r U_n\left(\frac{\gamma}{2\mu}\right) + \mu^n (\lambda^2 - r^{2n-2}(\beta - 1)^2) U_{n-1}\left(\frac{\gamma}{2\mu}\right) = 0 \quad (11)$$

with  $\mu = \lambda^2 + r^{2n-2}(\beta - 1)$  and  $\gamma = -\lambda^2(r + 1/r) + r^{2n-2}(r + \frac{1}{r}(\beta - 1)^2)$ .

v) If  $r \in (0, 1)$  and  $1 - r^2 \leq \beta$  we have the limit

$$\|X_{r, \beta}\| \rightarrow \frac{\beta}{1 - r^2}, \quad n \rightarrow \infty.$$

vi) For any  $n$ ,  $r \in (0, 1)$ ,  $\beta_{\max} \in (0, 2]$  and  $1 - r^2 \leq \beta \leq \beta_{\max}$  we have

$$\|X_{r, \beta}\| \leq \frac{\beta_{\max}}{1 - r^2}.$$

The equations in iv) (see (11)) are discussed in Lemma II.7 below. For instance we can recover known values of  $\|X_{1, \beta}\|$  from Proposition II.6, iv). In this case

$$\|X_{1, \beta}\| = \frac{1}{2} \sqrt{(\beta - 2)^2 + \frac{\beta^2}{\cot(\theta^*/2)}},$$

where  $\theta^*$  is the unique solution of (11) in  $[\frac{2n-1}{2n}\pi, \pi)$  and it follows, see [OS], that

$$\|X_{1, 0}\| = 1, \quad \|X_{1, 1}\| = \frac{1}{2 \sin(\frac{\pi}{4n+2})}, \quad \|X_{1, 2}\| = \cot(\frac{\pi}{4n}).$$

**Lemma II.7.** *Let  $r \in (0, 1]$  and  $\beta \in (0, 2]$  such that  $\beta - 1 + r^2 \neq 0$ . We consider the equation*

$$\cot(n\theta) + \frac{(2 - \beta)r}{r^2 + (\beta - 1)} \frac{1}{\sin(\theta)} + \frac{r^2 - (\beta - 1)}{r^2 + (\beta - 1)} \cot(\theta) = 0. \quad (12)$$

1. If  $r = 1$ , then (12) has exactly  $2n$  distinct solutions in  $[-\pi, \pi)$ .
2. If  $r = |\beta - 1| \notin \{0, 2\}$ , we distinguish two subcases:
  - (a) if  $\beta < 1$ , then (12) has exactly  $2n - 2$  distinct solutions in  $[-\pi, \pi)$  for any  $n \geq 1$ ,
  - (b) if  $\beta > 1$ , then (12) has exactly  $2n - 2$  distinct solutions in  $[-\pi, \pi)$  if and only if  $n > \frac{\beta}{2(2-\beta)}$ . If  $n \leq \frac{\beta}{2(2-\beta)}$ , then (12) has exactly  $2n$  distinct solutions in  $[-\pi, \pi)$ .
3. If  $\beta > 1$ , and  $r \notin \{1, \beta - 1\}$ , we distinguish two subcases:
  - (a) if  $1 < \beta < 1 + r$ , then (12) has exactly  $2n - 2$  distinct solutions in  $[-\pi, \pi)$  if and only if  $n > \frac{\beta - 1 + r^2}{(1-r)(r + \beta - 1)}$ . If  $n \leq \frac{\beta - 1 + r^2}{(1-r)(r + \beta - 1)}$ , then (12) has exactly  $2n$  distinct solutions in  $[-\pi, \pi)$ .
  - (b) If  $\beta > 1 + r$ , and  $n \geq 2$ , then (12) has exactly  $2n - 4$  distinct solutions in  $[-\pi, \pi)$  if and only if  $n > \frac{\beta - 1 + r^2}{(1-r)(r + \beta - 1)}$ . If  $\frac{\beta - 1 + r^2}{(1+r)(\beta - 1 - r)} < n \leq \frac{\beta - 1 + r^2}{(1-r)(r + \beta - 1)}$ , then (12) has exactly  $2n - 2$  distinct solutions in  $[-\pi, \pi)$ . Finally, if  $n \leq \frac{\beta - 1 + r^2}{(1+r)(\beta - 1 - r)}$ , then (12) has exactly  $2n$  distinct solutions in  $[-\pi, \pi)$ .

4. If  $\beta < 1$ , and  $r \notin \{1, 1 - \beta\}$ , we distinguish two subcases:

(a) if  $1 - r^2 < \beta < 1$ , then (12) has exactly  $2n - 2$  distinct solutions in  $[-\pi, \pi)$  if and only if  $n > \frac{\beta - 1 + r^2}{(1-r)(r+\beta-1)}$ ,

(b) if  $0 < \beta < 1 - r^2$ , we distinguish two subcases:

i. if  $0 < \beta < 1 - r$ , then (12) has exactly  $2n - 4$  distinct solutions in  $[-\pi, \pi)$  if and only if  $n > \frac{\beta - 1 + r^2}{(1-r)(r+\beta-1)}$ . If  $n \leq \frac{\beta - 1 + r^2}{(1-r)(r+\beta-1)}$ , then (12) has exactly  $2n$  distinct solutions in  $[-\pi, \pi)$ .

ii. If  $1 - r < \beta < 1 - r^2$ , then (12) has exactly  $2n - 2$  distinct solutions on  $[-\pi, \pi)$  for any  $n \geq 2$ .

5. If  $\beta = 1$  then (12) has exactly  $2n - 2$  distinct solutions in  $[-\pi, \pi)$  if and only if  $n > \frac{r}{1-r}$ . If  $n \leq \frac{r}{1-r}$ , then (12) has exactly  $2n$  distinct solutions in  $[-\pi, \pi)$ .

### III. MODEL SPACES AND MODEL OPERATORS

This section lays down the theoretical framework on which our results are footed. We refer to [NN3] for an in-depth study of the topic. To the minimal polynomial  $m = m_T$  of  $T \in \mathcal{M}_n$  we associate a Blaschke product

$$B(z) := \prod_i \frac{z - \lambda_i}{1 - \bar{\lambda}_i z}.$$

The product is taken over all  $i$  such that the corresponding linear factor  $z - \lambda_i$  occurs in the minimal polynomial  $m$ . Thus, the numerator of  $B$  as defined here is exactly the associated minimal polynomial. The space of holomorphic functions on  $\mathbb{D}$  is denoted by  $Hol(\mathbb{D})$ . The Hardy spaces considered here are

$$H_2 := \left\{ f \in Hol(\mathbb{D}) : \|f\|_{H_2}^2 := \sup_{0 \leq r < 1} \frac{1}{2\pi} \int_0^{2\pi} |f(re^{i\phi})|^2 d\phi < \infty \right\},$$

and

$$H_\infty := \left\{ f \in Hol(\mathbb{D}) : \|f\|_{H_\infty} := \sup_{z \in \mathbb{D}} |f(z)| < \infty \right\}.$$

Let  $B$  be the Blaschke product associated to the minimal polynomial of  $T \in \mathcal{M}_n$ . We define the  $|m|$ -dimensional model space

$$K_B := H_2 \ominus BH_2 := H_2 \cap (BH_2)^\perp,$$

where we employ the usual scalar product from  $L^2(\partial\mathbb{D})$ . The model operator  $M_B$  acts on  $K_B$  as

$$\begin{aligned} M_B : K_B &\rightarrow K_B \\ f &\mapsto M_B(f) := P_B(zf), \end{aligned}$$

where  $P_B$  denotes the orthogonal projection on  $K_B$ . In other words,  $M_B$  is the compression of the multiplication operation by  $z$  to the model space  $K_B$ . Multiplication by  $z$  has operator norm 1 so that  $\|M_B\| \leq 1$ . Moreover, it is not hard to show that the eigenvalues of  $M_B$  are exactly the zeros of the corresponding Blaschke product, see [NN2].

For our subsequent discussion we will assume that  $T$  can be diagonalized. This does not result in any difficulties since the upper bounds obtained in the special case extend by continuity to bounds for non-diagonalizable  $T$ , see [OS]. One natural orthonormal basis for  $K_B$  (for diagonalizable  $T$ ) is the Malmquist-Walsh basis  $\{e_k\}_{k=1,\dots,|m|}$  with ([NN3, p. 137])

$$e_k(z) := \frac{(1 - |\lambda_k|^2)^{1/2}}{1 - \bar{\lambda}_k z} \prod_{i=1}^{k-1} \frac{z - \lambda_i}{1 - \bar{\lambda}_i z}$$

with

$$e_1(z) = \frac{(1 - |\lambda_1|^2)^{1/2}}{1 - \bar{\lambda}_1 z}.$$

## IV. PROOFS

### A. Proofs of Theorem II.1 and Proposition II.2

We recall [OS, Theorem III.2] that given a finite Blaschke product  $B = \prod_{i=1}^N \frac{z - \nu_i}{1 - \bar{\nu}_i z}$ , of degree  $N \geq 1$ , with zeros  $\nu_i \in \mathbb{D}$ , the components of the resolvent of the model operator  $M_B$  at any point  $\zeta \in \mathbb{C} - \{\nu_1, \dots, \nu_N\}$  with respect to the Malmquist-Walsh basis are given by

$$\left( (\zeta - M_B)^{-1} \right)_{1 \leq i, j \leq N} = \frac{1}{B(\zeta)} \begin{cases} 0 & \text{if } i < j \\ \frac{1}{1 - \bar{\nu}_i \zeta} \prod_{s \neq i} \frac{\zeta - \nu_s}{1 - \bar{\nu}_s \zeta} & \text{if } i = j \\ \frac{(1 - |\nu_i|^2)^{1/2}}{1 - \bar{\nu}_i \zeta} \frac{(1 - |\nu_j|^2)^{1/2}}{1 - \bar{\nu}_j \zeta} \prod_{s \notin \{j, \dots, i\}} \frac{\zeta - \nu_s}{1 - \bar{\nu}_s \zeta} & \text{if } i > j \end{cases} \quad (13)$$

We begin by proving Proposition II.2.

*Proof of Proposition II.2.* We consider  $T \in \mathcal{C}_n$  and assume for a moment that  $\sigma(T) \subset \mathbb{D}$ . It follows from [OS, Theorem III.2] that for any  $\zeta \in \mathbb{C} - \sigma(T)$  the resolvent of  $T$  is bounded by

$$\|R(\zeta, T)\| \leq \|R(\zeta, M_B)\|,$$

where  $B$  is the Blaschke product associated with  $m_T$ . We conclude from (13) that

$$\left( (\zeta - M_B)^{-1} \right)_{1 \leq i, j \leq |m|} = \begin{cases} 0 & \text{if } i < j \\ \frac{1}{\zeta - \lambda_i} & \text{if } i = j \\ \frac{(1 - |\lambda_i|^2)^{1/2}}{1 - \bar{\lambda}_i \zeta} \frac{(1 - |\lambda_j|^2)^{1/2}}{1 - \bar{\lambda}_j \zeta} \prod_{k=j}^i \frac{1 - \bar{\lambda}_k \zeta}{\zeta - \lambda_k} & \text{if } i > j \end{cases}$$

Taking the limit  $|\lambda_i| \rightarrow 1$  we have that for  $\zeta \in \mathbb{C} - \sigma(T)$  the norm of the resolvent is bounded by the norm of the diagonal matrix

$$\begin{pmatrix} \frac{1}{\zeta - \lambda_1} & & \\ & \ddots & \\ & & \frac{1}{\zeta - \lambda_n} \end{pmatrix},$$

which is  $\frac{1}{d(\zeta, \sigma)}$ .  $\square$

*Proof of Theorem II.1.* We begin by showing that (5) holds. As before we suppose  $\sigma(T) \subset \mathbb{D}$ . The more general case  $\sigma(T) \subset \bar{\mathbb{D}}$  follows immediately by continuously moving the eigenvalue towards  $\partial\mathbb{D}$ . As before we have that  $\|R(\zeta, T)\| \leq \|R(\zeta, M_B)\|$  and that

$$\left( (\zeta - M_B)^{-1} \right)_{1 \leq i, j \leq |m|} = \begin{cases} 0 & \text{if } i < j \\ \frac{1}{1 - \bar{\lambda}_i \zeta} \frac{1}{b_{\lambda_i}} & \text{if } i = j \\ \frac{(1 - |\lambda_i|^2)^{1/2}}{1 - \bar{\lambda}_i \zeta} \frac{(1 - |\lambda_j|^2)^{1/2}}{1 - \bar{\lambda}_j \zeta} \frac{1}{\prod_{k=j}^i b_{\lambda_k}} & \text{if } i > j \end{cases},$$

where we abbreviated  $b_{\lambda_i} = \frac{\zeta - \lambda_i}{1 - \bar{\lambda}_i \zeta}$ . Recall that for any  $n \times n$  matrices  $A = (a_{ij})$  and  $A' = (a'_{ij})$ , the condition  $|a_{ij}| \leq a'_{ij}$  implies that  $\|A\| \leq \|A'\|$ . Hence, we estimate

$$\left| (\zeta - M_B)^{-1}_{i,j} \right| \leq \begin{cases} 0 & \text{if } i < j \\ \frac{1}{|1 - \bar{\lambda}_i \zeta|} \frac{1}{|b_{\lambda_i}|} & \text{if } i = j \\ \frac{(1 - |b_{\lambda_i}|^2)^{\frac{1}{2}} (1 - |b_{\lambda_j}|^2)^{\frac{1}{2}}}{1 - |\zeta|^2} \frac{1}{\prod_{k=j}^i |b_{\lambda_k}|} & \text{if } i > j \end{cases},$$

where we made use of the well-known [JG] fact that

$$\frac{1 - |\lambda|^2}{|1 - \bar{\lambda} \zeta|^2} = \frac{1 - |b_{\lambda}(\zeta)|^2}{1 - |\zeta|^2}, \quad \lambda \neq \zeta.$$

By assumption  $\min_i |b_{\lambda_i}| = p(\zeta, \sigma) = r$  and for any  $l$  with  $|b_{\lambda_l}| = r$  we have

$$\left| (\zeta - M_B)^{-1}_{i,j} \right| \leq \begin{cases} 0 & \text{if } i < j \\ \frac{1}{|1 - \bar{\lambda}_i \zeta|} \frac{1}{r} & \text{if } i = j \\ \frac{1 - |b_{\lambda_l}(\zeta)|^2}{1 - |\zeta|^2} \frac{1}{r^{i-j+1}} & \text{if } i > j \end{cases},$$

and since

$$\frac{1 - |b_{\lambda_l}(\zeta)|^2}{1 - |\zeta|^2} = \frac{1 - |\lambda_l|^2}{|1 - \bar{\lambda}_l \zeta|^2} \leq \frac{1}{d(1, \bar{\sigma} \zeta)} \frac{1 - |\lambda_l|^2}{|1 - \bar{\lambda}_l \zeta|} \leq \frac{\beta}{d(1, \bar{\sigma} \zeta)},$$

with  $\beta = s(\zeta, \sigma)$  we conclude that

$$\left| (\zeta - M_B)_{i,j}^{-1} \right| \leq \frac{1}{d(1, \bar{\sigma}\zeta)} \frac{1}{r^{|m|}} \begin{cases} 0 & \text{if } i < j \\ r^{|m|-1} & \text{if } i = j \\ \beta r^{|m|-(i-j+1)} & \text{if } i > j \end{cases}$$

Next we discuss the sharpness of (5). We consider  $\zeta \in [-1, 1]$  and the model operator  $M_B$  with  $B = b_\lambda^n$  and  $\lambda \in (-1, 1)$ . In this case  $d(1, \bar{\sigma}\zeta) = |1 - \bar{\lambda}\zeta|$  and  $p(\zeta, \sigma) = |b_\lambda(\zeta)|$  and  $s(\zeta, \sigma) = \frac{1-|\lambda|^2}{|1-\lambda\zeta|}$ . We find that

$$(\zeta - M_B)_{i,j}^{-1} = \frac{1}{d(1, \bar{\sigma}\zeta)} \frac{1}{B(\zeta)} \begin{cases} 0 & \text{if } i < j \\ (b_\lambda(\zeta))^{n-1} & \text{if } i = j \\ \frac{1-|\lambda|^2}{|1-\lambda\zeta|} (b_\lambda(\zeta))^{n-(i-j+1)} & \text{if } i > j \end{cases}.$$

If  $b_\lambda(\zeta) > 0$  then the equality

$$\|R(\zeta, M_B)\| = \frac{1}{d(1, \bar{\sigma}\zeta)} \frac{1}{r^n} \|X_{r,\beta}\|$$

is clear. If  $b_\lambda(\zeta) < 0$  equality still holds because the Toeplitz matrices  $a = (a_k)_{k \geq 0}$  and  $b = ((-1)^k a_k)_{k \geq 0}$  have the same norm. To see this write  $D = \text{diag}(-1, \dots, -1)$  and note that  $DT_a D^\dagger = T_b$ . As  $D$  is unitary  $\|T_a\| = \|T_b\|$ .  $\square$

## B. Proofs of Theorem II.4 and Propositions II.5, II.6

**Lemma IV.1.** *For any  $\zeta \in \mathbb{D}$  and  $r \in (0, 1)$*

$$\mathcal{R}_n(\zeta, r) = \mathcal{R}_n(|\zeta|, r).$$

*Proof.* Indeed, writing  $\zeta = |\zeta| \exp(i\theta)$  we have  $|1 - \bar{\lambda}\zeta| = |1 - \exp(i\theta)\bar{\lambda}|\zeta||$  and  $\|R(\zeta, T)\| = \|(|\zeta| - \exp(-i\theta)T)^{-1}\|$ , which entails that

$$d(1, \overline{\sigma(T)}\zeta) \|R(\zeta, T)\| = d(1, \overline{\sigma(T')}|\zeta|) \|R(|\zeta|, T')\|$$

with  $T' = \exp(-i\theta)T$ . Clearly  $T \in \mathcal{C}_n \Leftrightarrow T' \in \mathcal{C}_n$  and  $p(\zeta, \sigma(T)) = p(|\zeta|, \sigma(T'))$ . The same argument implies  $T \in \mathcal{T}_n^a \Leftrightarrow T' \in \mathcal{T}_n^a$ .  $\square$

The lemma says that for our optimization task it is sufficient to consider real  $\zeta$ .

*Proof of Theorem II.4.* We consider a matrix  $T \in \mathcal{C}_n$  with  $p(\zeta, \sigma(T)) = r$  and the function  $s$  in (5). The function  $\lambda \mapsto \frac{1-|\lambda|^2}{|1-\lambda\zeta|}$  is maximized on the pseudo-hyperbolic circle of center  $|\zeta|$  and radius  $r$  at  $\lambda_{\max} = \frac{|\zeta|-r}{1-r|\zeta|}$  and takes the value  $\beta_{\max} = \frac{1-|\lambda_{\max}|^2}{1-\lambda_{\max}|\zeta|} = \frac{1-r^2}{1-r|\zeta|}$ . Thus using Lemma IV.1 and Theorem II.1 we find that  $\mathcal{R}_n(\zeta, r) = \mathcal{R}_n(|\zeta|, r) \leq \frac{1}{r^n} \|X_{r,\beta_{\max}}\|$ .

According to the proof of Theorem II.1 the model operator corresponding to Blaschke product  $B = b_\lambda^n$  with  $\lambda \in (-1, 1)$ ,  $\lambda \neq |\zeta|$  satisfies

$$\|R(|\zeta|, M_B)\| = \frac{1}{d(1, \bar{\sigma}|\zeta|)} \frac{1}{r^n} \|X_{r,\beta}\|.$$

We choose  $\lambda_{\max} = \frac{|\zeta| - r}{1 - r|\zeta|}$  and have  $p(|\zeta|, \sigma) = r$  and  $s(|\zeta|, \sigma) = \beta_{\max} = \frac{1 - r^2}{1 - r|\zeta|}$ . It follows that  $\mathcal{R}_n(\zeta, r) \geq \frac{1}{r^n} \|X_{r, \beta}\|$  and the “worst” matrix for the extremal problem in (7) is the analytic Toeplitz matrix  $M_B$  with  $B = b_{\lambda_{\max}}^n$ .

The monotonicity properties and the asymptotic behaviour of  $\mathcal{R}_n(\zeta, r)$  are consequences of our study of  $\|X_{r, \beta_{\max}}\|$ , which is summarized in Proposition II.6.  $\square$

*Proof of Proposition II.5.* We first prove (9). We consider  $T \in \mathcal{C}_n$  with spectrum  $\sigma$  and assume for a moment that  $\sigma_2 \subset \mathbb{D}$ . It follows from [OS, Theorem III.2] that for any  $\zeta \in \mathbb{C} - \sigma$  the resolvent of  $T$  is bounded by

$$\|R(\zeta, T)\| \leq \|R(\zeta, M_B)\|,$$

where  $B$  is the Blaschke product associated with  $P_\sigma$ . We conclude from (13) that the matrix of the resolvent of the model operator  $M_B$  at any point  $\zeta \in \mathbb{C} - \sigma$  (with respect to the Malmquist-Walsh basis) is given by a block-diagonal matrix

$$\begin{pmatrix} A_1 & 0 \\ 0 & A_2 \end{pmatrix},$$

where  $A_1 \in \mathcal{M}_{|P_{\sigma_1}|}(\mathbb{C})$  and  $A_2 \in \mathcal{M}_{|P_{\sigma_2}|}(\mathbb{C})$  are respectively defined by (taking now the limit as  $|\mu| \rightarrow 1$  for  $\mu \in \sigma_2$ ):

$$(A_1)_{1 \leq i, j \leq |P_{\sigma_1}|} = \begin{cases} 0 & \text{if } i < j \\ \frac{1}{\zeta - \lambda_i} & \text{if } i = j \\ \frac{(1 - |\lambda_i|^2)^{1/2}}{1 - \lambda_i \zeta} \frac{(1 - |\lambda_j|^2)^{1/2}}{1 - \lambda_j \zeta} \prod_{k=j}^i \frac{1 - \bar{\lambda}_k \zeta}{\zeta - \lambda_k} & \text{if } i > j \end{cases},$$

and

$$A_2 = \begin{pmatrix} \frac{1}{\zeta - \mu_1} & & \\ & \ddots & \\ & & \frac{1}{\zeta - \mu_{n_2}} \end{pmatrix},$$

where  $\mu_i$  are the unimodular eigenvalues of  $M_B$ . To conclude, it remains to remark that the spectral norm of  $R(\zeta, T)$  is nothing but

$$\max(\|A_1\|, \|A_2\|),$$

that  $\|A_2\| = \frac{1}{d(\zeta, \sigma_2)}$ , while the inequality

$$\|A_1\| \leq \frac{1}{d(\zeta, \sigma_1)} \|X_{1, s(\zeta, \sigma_1)}\|,$$

follows directly from Theorem II.1. This proves the first inequality in (9). The second one is due to the fact that  $s(\zeta, \sigma_1)$  is bounded from above by 2 and the equality refers to the resolvent estimate in [DS] or more generally to our Proposition II.6.

Now, let us prove (10). We consider  $T \in \mathcal{C}_n$  with spectrum  $\sigma = \sigma_1 \cup \sigma_2$ ,  $n_1 = |P_{\sigma_1}|$  and  $n_2 = |P_{\sigma_2}|$  such that  $\max_{\lambda \in \sigma_1} |\lambda| \leq \rho_1$ . We fix  $\zeta \in \partial\mathbb{D} - \sigma$ . The last inequality, combined with the trivial observation that  $s(\zeta, \sigma_1) \leq \rho_1$ , proves that

$$\|A_1\| \leq \|X_{1, \rho_1}\|.$$

To complete the proof of (10), we first remark that by rotation invariance (as in the proof of Lemma IV.1) the sup defined in the statement of (10) does not depend on  $\zeta$  and coincides with its value at point  $\zeta = 1$ . We consider the spectrum  $\sigma = \sigma_1 \cup \sigma_2$  defined by setting  $P_{\sigma_1} = (z - \rho_1)^{n_1}$  and  $P_{\sigma_2} = (z + 1)^{n_2}$ . Let  $B$  be the Blaschke product associated with  $P_\sigma$ . We repeat the proof of (9) to the model operator  $M_B$ . The matrix of its resolvent at point 1 (with respect to the Malmquist-Walsh basis) is given by the block-diagonal matrix

$$\begin{pmatrix} A_1 & 0 \\ 0 & A_2 \end{pmatrix},$$

where

$$\begin{aligned} (A_1)_{1 \leq i, j \leq n_1} &= \frac{1}{d(1, \sigma_1)} \frac{1}{B(1)} \begin{cases} 0 & \text{if } i < j \\ (b_{\rho_1}(1))^{n-1} & \text{if } i = j \\ \frac{1-|\rho_1|^2}{|1-\rho_1|} (b_{\rho_1}(1))^{n-(i-j+1)} & \text{if } i > j \end{cases} \\ &= \frac{X_{1, 1+\rho_1}}{|1-\rho_1|}. \end{aligned}$$

and  $A_2 = \frac{1}{2}I_{n_2}$ , where  $I_{n_2}$  is the identity matrix of  $\mathcal{M}_{n_2}(\mathbb{C})$ . Thus,

$$\|R(1, M_B)\| = \max\left(\frac{1}{|1-\rho_1|} \|X_{1, 1+\rho_1}\|, \frac{1}{2}\right),$$

but  $d(1, \sigma) = d(1, \sigma_1) = |1 - \rho_1|$ , and as a consequence:

$$d(1, \sigma) \|R(1, M_B)\| = \max(\|X_{1, 1+\rho_1}\|, \frac{|1-\rho_1|}{2}).$$

The above maximum is equal to  $\|X_{1, 1+\rho_1}\|$ : indeed, according to Proposition II.6,

$$\|X_{1, 1+\rho_1}\| \geq \|X_{1, 1}\| = \frac{1}{2 \sin(\frac{\pi}{4n_1+2})},$$

and the latter quantity  $\frac{1}{2 \sin(\frac{\pi}{4n_1+2})}$  is always greater than  $\frac{1}{2}$  (increasing with  $n_1$ ) since  $n_1 \geq 1$ . The last part of the statement relies again on Proposition II.6 and the fact that  $\rho \mapsto \|X_{1, 1+\rho}\|$  is increasing on  $[0, 1]$ .  $\square$

*Proof of Proposition II.6.* Our approach is guided by the methods developed in [EE, DS, OS]. Often it will be convenient to transform the Toeplitz matrix  $X_{r, \beta}$  to an associated Hankel matrix  $\tilde{X}_{r, \beta}$ , see [DS, OS]. We set  $\tilde{X}_{r, \beta} = X_{r, \beta} J$ , where

$$J = \begin{pmatrix} & & & 1 \\ & & & \\ & & \ddots & \\ & & & \\ 1 & & & \end{pmatrix}.$$

$\tilde{X}$  is a Hermitian Hankel matrix that satisfies  $\|\tilde{X}\| = \|X_{r,\beta}\|$ . Hence, in our discussion we can focus on the largest in magnitude eigenvalue of  $\tilde{X}$ . (We omit indices in  $\tilde{X}$  for simpler notation.)

*i)* In the case  $\beta = 1 - r^2$  we have

$$\frac{1}{r^n} X_{r,\beta} = \frac{1}{r^n} \begin{cases} 0 & \text{if } i < j \\ r^{n-1} & \text{if } i = j \\ (1 - r^2)r^{n-(i-j+1)} & \text{if } i > j \end{cases} = (M_{b_{-r}^{-1}})_{1 \leq i, j \leq n},$$

where the second equality is (13). It is well known [NN1, Theorem 3.12, p.147], [OS, Lemma III.5] that (see the cited articles for a discussion)

$$\|M_B^{-1}\| = \|1/z\|_{H_\infty/BH_\infty} = \frac{1}{|B(0)|} = \prod_{\lambda \in \sigma} \frac{1}{|\lambda|}.$$

In particular, we find  $\|M_{b_{-r}^{-1}}^{-1}\| = \frac{1}{r^n}$  and  $\|X_{r,\beta}\| = 1$ .

*ii)*  $\tilde{X}$  is an entry-wise non-negative matrix. A standard result in Perron-Froebienius theory [HM, Theorem 4.2] asserts that the spectral radius of such matrices is a non-negative eigenvalue and the corresponding eigenvector is entry-wise non-negative<sup>1</sup>. Furthermore the spectral radius is monotonically increasing in the matrix-entries [HM, Corollary 2.1], i.e.  $\tilde{X} \leq B$  entry-wise implies  $\rho(\tilde{X}) \leq \rho(B)$ .

*iii)* Here, we show a simple proof for  $\beta > 1$ . The more general discussion under the condition  $1 - r^2 \leq \beta$  can be found below. Let  $\tilde{X}_n \in \mathcal{M}_n$  and  $\tilde{X}_{n+1} \in \mathcal{M}_{n+1}$ . We show  $\|\tilde{X}_n\| \leq \|\tilde{X}_{n+1}\|$ . Let  $x^*$  with  $\|x^*\| = 1$  and  $\tilde{X}_n x^* = \|\tilde{X}_n\| x^*$ . Computing entries of vectors and using  $\beta \geq 1$  we see that

$$\|\tilde{X}_n x^*\| \leq \left\| \tilde{X}_{n+1} \begin{pmatrix} x^* \\ 0 \end{pmatrix} \right\|.$$

*iv)* We turn to the case  $r^2 + \beta - 1 \neq 0$ . The discussion is guided by [EE]. The eigenvalues of  $\tilde{X}^2$  are the eigenvalues of  $\tilde{X}$  squared. Hence, we are looking for the largest  $\lambda^2$  such that

$$0 = \det(\tilde{X}^2 - \lambda^2) = \det(\tilde{X} - \lambda) \det(\tilde{X} + \lambda).$$

The matrix  $\tilde{X}^2 - \lambda^2$  can be computed explicitly. We display this matrix for  $n = 5$  for simplicity, see Appendix V for the general matrix. If  $n = 5$  we have

$$\tilde{X}^2 - \lambda^2 = \begin{pmatrix} -\lambda^2 + \beta^2 \frac{1-r^{2 \cdot 4}}{1-r^2} + r^8 & \beta^2 r \frac{1-r^{2 \cdot 3}}{1-r^2} + \beta r^7 & \beta^2 r^2 \frac{1-r^{2 \cdot 2}}{1-r^2} + \beta r^6 & \beta^2 r^3 \frac{1-r^{2 \cdot 1}}{1-r^2} + \beta r^5 & \beta r^4 \\ \beta^2 r \frac{1-r^{2 \cdot 3}}{1-r^2} + \beta r^7 & -\lambda^2 + \beta^2 r^2 \frac{1-r^{2 \cdot 3}}{1-r^2} + r^8 & \beta^2 r^3 \frac{1-r^{2 \cdot 2}}{1-r^2} + \beta r^7 & \beta^2 r^4 \frac{1-r^{2 \cdot 1}}{1-r^2} + \beta r^6 & \beta r^5 \\ \beta^2 r^2 \frac{1-r^{2 \cdot 2}}{1-r^2} + \beta r^6 & \beta^2 r^3 \frac{1-r^{2 \cdot 2}}{1-r^2} + \beta r^7 & -\lambda^2 + \beta^2 r^4 \frac{1-r^{2 \cdot 2}}{1-r^2} + r^8 & \beta^2 r^5 \frac{1-r^{2 \cdot 1}}{1-r^2} + \beta r^7 & \beta r^6 \\ \beta^2 r^3 \frac{1-r^{2 \cdot 1}}{1-r^2} + \beta r^5 & \beta^2 r^4 \frac{1-r^{2 \cdot 1}}{1-r^2} + \beta r^6 & \beta^2 r^5 \frac{1-r^{2 \cdot 1}}{1-r^2} + \beta r^7 & -\lambda^2 + \beta^2 r^6 \frac{1-r^{2 \cdot 1}}{1-r^2} + r^8 & \beta r^7 \\ \beta r^4 & \beta r^5 & \beta r^6 & \beta r^7 & -\lambda^2 + r^8 \end{pmatrix}.$$

The determinant of the above matrix is transformed by the following steps.

<sup>1</sup> In fact, as can be seen easily by computing powers,  $\tilde{X}$  is primitive.

1. We divide the  $k^{\text{th}}$  column and the  $k^{\text{th}}$  row of  $(\tilde{X}^2 - \lambda^2)$  by  $r^{k-1}$ .
2. In the determinant resulting from (1), we subtract the  $k^{\text{th}}$  column from the  $(k-1)^{\text{th}}$  and leave the  $n^{\text{th}}$  unchanged.
3. In the determinant resulting from (2), we subtract the  $(k-1)^{\text{th}}$  row from the  $k^{\text{th}}$  and leave the  $n^{\text{th}}$  unchanged. We obtain the determinant of a tri-diagonal  $n \times n$  matrix.
4. In the determinant resulting from (3), we multiply the  $k^{\text{th}}$  row by  $r^{2k-1}$ .

We obtain that  $\det(\tilde{X}^2 - \lambda^2) = 0$  iff

$$0 = \det \begin{pmatrix} \gamma & \alpha' & 0 & \cdots & 0 \\ \alpha & \gamma & \alpha' & \ddots & \vdots \\ 0 & \alpha & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \gamma & \alpha' \\ 0 & \cdots & 0 & \alpha & y \end{pmatrix} = \det \begin{pmatrix} \gamma & \mu & 0 & \cdots & 0 \\ \mu & \gamma & \mu & \ddots & \vdots \\ 0 & \mu & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \gamma & \mu \\ 0 & \cdots & 0 & \mu & y \end{pmatrix},$$

where  $\alpha = \lambda^2 r + r^{2n-1}(\beta - 1)$ ,  $\alpha' = \frac{\alpha}{r^2}$ ,  $y = -r\lambda^2 + r^{2n-1}$  and  $\gamma = -\lambda^2(r + 1/r) + r^{2n-2}(r + \frac{1}{r}(\beta - 1)^2)$  and we set  $\mu = \alpha/r$  in the last step. We have that

$$\begin{aligned} & \det \begin{pmatrix} \gamma & \mu & 0 & \cdots & 0 \\ \mu & \gamma & \mu & \ddots & \vdots \\ 0 & \mu & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \gamma & \mu \\ 0 & \cdots & 0 & \mu & y \end{pmatrix} \\ &= \det \begin{pmatrix} \gamma & \mu & 0 & \cdots & 0 \\ \mu & \gamma & \mu & \ddots & \vdots \\ 0 & \mu & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \gamma & \mu \\ 0 & \cdots & 0 & \mu & \gamma \end{pmatrix} + \det \begin{pmatrix} \gamma & \mu & 0 & \cdots & 0 \\ \mu & \gamma & \mu & \ddots & \vdots \\ 0 & \mu & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \gamma & 0 \\ 0 & \cdots & 0 & \mu & y - \gamma \end{pmatrix} \\ &= \det \begin{pmatrix} \gamma & \mu & 0 & \cdots & 0 \\ \mu & \gamma & \mu & \ddots & \vdots \\ 0 & \mu & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \gamma & \mu \\ 0 & \cdots & 0 & \mu & \gamma \end{pmatrix} + (y - \gamma) \det \begin{pmatrix} \gamma & \mu & 0 & \cdots & 0 \\ \mu & \gamma & \mu & \ddots & \vdots \\ 0 & \mu & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \gamma & \mu \\ 0 & \cdots & 0 & \mu & \gamma \end{pmatrix}, \end{aligned}$$

where in the last sum the first determinant is of order  $n$ , while the second is of order  $n-1$ . The assumption  $\mu = 0$  is equivalent to  $\lambda^2 = r^{2n-2}(1 - \beta)$  and the determinant equation

turns into  $\gamma y = 0$ . In this case we obtain a solution if  $\beta = 0$  or  $r^2 + \beta - 1 = 0$  but these choices of  $\beta$  are treated differently. (Note that  $\lambda = 1$  implies  $\mu \neq 0$ .) For the determinant of a tri-diagonal Toeplitz matrix we have the well known formula [MV, EP, EE, OS]

$$\det \begin{pmatrix} a & 1 & 0 & \cdots & 0 \\ 1 & a & 1 & \ddots & \vdots \\ 0 & 1 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & a & 1 \\ 0 & \cdots & 0 & 1 & a \end{pmatrix} = U_n(a/2),$$

where  $U_n$  denotes the  $n$ -th degree Chebychev polynomial of the second kind. Hence the eigenvalues of  $\tilde{X}$  correspond to the roots of the polynomial equation

$$\mu^{n+1} U_n \left( \frac{\gamma}{2\mu} \right) + \mu^n (y - \gamma) U_{n-1} \left( \frac{\gamma}{2\mu} \right) = 0.$$

*v)* We make use of properties of  $U_n$  to reveal properties of the roots of equation (11). Let us consider  $\lambda^2$  so that there is *real*  $\theta$  with  $\gamma/2\mu = \cos(\theta)$ , i.e.

$$\lambda^2 = r^{2(n-1)} \frac{(\beta - 1)^2 + r^2 - 2r(\beta - 1) \cos(\theta)}{1 + r^2 + 2r \cos(\theta)}. \quad (14)$$

Using  $U_n(\cos(\theta)) = \frac{\sin((n+1)\theta)}{\sin(\theta)}$  Equation (11) turns into

$$\frac{\sin((n+1)\theta)}{\sin(\theta)} + \frac{1}{r} \frac{\lambda^2 - r^{2n-2}(\beta - 1)^2}{\lambda^2 + r^{2n-2}(\beta - 1)} \frac{\sin(n\theta)}{\sin(\theta)} = 0,$$

which plugging back  $\lambda^2$  is

$$\cot(n\theta) + \frac{1}{\tan(\theta)} \frac{r^2 - (\beta - 1)}{r^2 + \beta - 1} + \frac{(2 - \beta)r}{r^2 + \beta - 1} \frac{1}{\sin(\theta)} = 0. \quad (15)$$

Similarly, if  $\gamma/2\mu \in [1, \infty)$  we set  $\gamma/2\mu = \cosh(\theta)$  with  $\theta \in [0, \infty)$ , which leads to [MH, Section 1.4]

$$\lambda^2 = r^{2(n-1)} \frac{(\beta - 1)^2 + r^2 - 2r(\beta - 1) \cosh(\theta)}{1 + r^2 + 2r \cosh(\theta)} \quad (16)$$

with

$$\frac{\sinh((n+1)\theta)}{\sinh(n\theta)} = - \frac{(2 - \beta)r + 2(1 - \beta) \cosh(\theta)}{r^2 + \beta - 1}. \quad (17)$$

Finally, in case that  $\gamma/2\mu \in [-1, -\infty)$  we set  $\gamma/2\mu = -\cosh(\theta)$  with  $\theta \in [0, \infty)$  and recall that  $U_n(-x) = (-1)^n U_n(x)$  [MH, Section 1.4] to find

$$\lambda^2 = r^{2(n-1)} \frac{(\beta - 1)^2 + r^2 + 2r(\beta - 1) \cosh(\theta)}{1 + r^2 - 2r \cosh(\theta)} \quad (18)$$

with

$$\frac{\sinh((n+1)\theta)}{\sinh(n\theta)} = \frac{(2-\beta)r - 2(1-\beta)\cosh(\theta)}{r^2 + \beta - 1}. \quad (19)$$

We consider the first case. Any solution  $\theta_k$  of (15) leads to a solution  $\lambda_k^2$  of  $\det(\tilde{X}^2 - \lambda^2) = 0$  via (14). An important point about Equation (14) is that all such solutions  $|\lambda_k|^2$  can be bounded by a function that decays exponentially with  $n$ . This allows us to study properties of  $\|\tilde{X}\|$  by counting solutions of equation (15). We observe that

$$\begin{aligned} \frac{1}{\sin(\theta)} &\rightarrow +\infty \quad \text{as } \theta \rightarrow 0^+ & \text{and} & \quad \frac{1}{\tan(\theta)} \rightarrow +\infty \quad \text{as } \theta \rightarrow 0^+ \\ \frac{1}{\sin(\theta)} &\rightarrow +\infty \quad \text{as } \theta \rightarrow \pi^- & \text{and} & \quad \frac{1}{\tan(\theta)} \rightarrow -\infty \quad \text{as } \theta \rightarrow \pi^-. \end{aligned}$$

It follows that if  $1 - r^2 < \beta < 1 + r$  then (see Lemma II.7 for details)

$$\begin{aligned} \frac{1}{\tan(\theta)} \frac{r^2 - (\beta - 1)}{r^2 + \beta - 1} + \frac{(2 - \beta)r}{r^2 + \beta - 1} \frac{1}{\sin(\theta)} &\rightarrow +\infty \quad \text{as } \theta \rightarrow 0^+ \\ \frac{1}{\tan(\theta)} \frac{r^2 - (\beta - 1)}{r^2 + \beta - 1} + \frac{(2 - \beta)r}{r^2 + \beta - 1} \frac{1}{\sin(\theta)} &\rightarrow +\infty \quad \text{as } \theta \rightarrow \pi^-. \end{aligned}$$

As  $-\cot(n\theta)$  has  $n$  branches in the interval  $[0, \pi]$  and since

$$\begin{aligned} -\cot(n\theta) &\rightarrow -\infty \quad \text{as } \theta \rightarrow 0^+ \\ -\cot(n\theta) &\rightarrow +\infty \quad \text{as } \theta \rightarrow \pi^-, \end{aligned}$$

we conclude that Equation (15) has  $n - 1$  solutions  $\theta_k \in (0, \pi)$  (if  $n$  is large enough, see Lemma II.7). The corresponding eigenvalues  $\lambda_k$  of  $\tilde{X}$  approach 0 exponentially fast, so that for the largest eigenvalue of  $\tilde{X}$  we have  $\lambda^* \rightarrow \text{Tr}(\tilde{X})$ . On the other hand direct consideration of the trace shows that at fixed  $\beta$  and  $r$  we have

$$\text{Tr}(\tilde{X}) \rightarrow \frac{\beta}{1 - r^2} \quad \text{as } n \rightarrow \infty.$$

If  $\beta > 1 + r$  we have only  $n - 2$  real solutions  $\theta_k$  to Equation (15), see Lemma II.7. We consider Equations (16), (17) and Equations (18), (19). As  $n$  gets large  $\frac{\sinh((n+1)\theta)}{\sinh(n\theta)}$  quickly converges to  $e^\theta$  with  $\theta \in [0, \infty)$ . By the intermediate value theorem (17) has a solution for  $\beta > 1 + r$  and sufficiently large  $n$ . Any  $\lambda^2$  as in Equation (16) decays exponentially with  $n$ . Hence, in case  $\beta > 1 + r$  we obtain  $n - 1$  eigenvalues that decay exponentially with  $n$ , as before. In the asymptotic limit of large  $n$  we find that  $e^{(\theta^*)} = 1/r$  becomes a solution of (19) and  $\lambda^*$  in (18) does *not* decay exponentially with  $n$ , which identifies the latter as the largest in magnitude solution for large enough  $n$ . Hence, we have that  $\|X\| \rightarrow \beta/(1 - r^2)$  as  $n \rightarrow \infty$ .

*iii) (second part)* We have already seen that  $\|X_{r,\beta}\|$  grows monotonically with  $n$  if  $\beta > 1$ . Hence, we consider  $1 - r^2 < \beta < 1$ . As outlined in *v)* there are for large enough<sup>2</sup>  $n$ , see

<sup>2</sup> When there are  $n$  solutions to (15), monotonicity of  $\|X_{r,\beta}\|$  can be readily be seen in (14) and (15).

Lemma II.7,  $n-1$  solutions  $\theta_k$  to Equation (15) and the corresponding eigenvalues, see (14), can be bounded as

$$r^{2(n-1)} \left(1 - \frac{\beta}{1+r}\right)^2 \leq |\lambda_k|^2 \leq r^{2(n-1)} \left(1 - \frac{\beta}{1-r}\right)^2. \quad (20)$$

We write  $\tilde{X}^{(n)}$  and  $\tilde{X}^{(n-1)}$  for the matrix  $\tilde{X}$  in  $n$  and  $n-1$  dimensions. Let  $\|\cdot\|_{FR}$  denote the Frobenius norm. Direct computation shows that

$$\left\|\tilde{X}^{(n)}\right\|_{FR}^2 - \left\|\tilde{X}^{(n-1)}\right\|_{FR}^2 = nr^{2(n-1)} + (n-1)\beta^2 r^{2(n-2)} - (n-1)r^{2(n-2)}.$$

On the other hand it is well known that  $\|\tilde{X}^{(n)}\|_{FR}^2 = \sum_{i=1}^n |\lambda_i^{(n)}|^2$ , where the  $\lambda_i^{(n)}$  are the eigenvalues of  $\tilde{X}^{(n)}$ . Writing  $\lambda^{*,(n)}$  for the largest in magnitude eigenvalue of  $\tilde{X}^{(n)}$  and making use of the mentioned properties and the estimates (20) we find that

$$\begin{aligned} & |\lambda^{*,(n)}|^2 - |\lambda^{*,(n-1)}|^2 \\ & \geq nr^{2(n-1)} + (n-1)\beta^2 r^{2(n-2)} - (n-1)r^{2(n-2)} \\ & \quad - (n-1)r^{2(n-1)} \left(1 - \frac{\beta}{1-r}\right)^2 \\ & \quad + (n-2)r^{2(n-2)} \left(1 - \frac{\beta}{1+r}\right)^2. \end{aligned}$$

The lower bound is a degree-2 polynomial in  $\beta$ , which is convex if  $r \in (0, 1/2)$ . Hence, the lower bound is an increasing function of  $\beta \in [1-r^2, 1]$ . As  $\beta = 1-r^2$  implies  $|\lambda^{*,(n)}|^2 - |\lambda^{*,(n-1)}|^2 = 0$  this proves monotonicity in  $n$  if  $r \in (0, 1/2)$ . The range for  $r$  can be extended by using better bounds in (20). Here we note that at the endpoints of the interval for  $\beta$  we already have established monotonicity for any  $r$ . Furthermore the norm is a monotonous, convex functions in  $\beta$ . Any of the branches of  $-\cot(n\theta)$  is convex and the terms

$$\frac{r^2 - (\beta - 1)}{r^2 + \beta - 1} \quad \text{and} \quad \frac{(2 - \beta)r}{r^2 + \beta - 1}$$

in (15) are decreasing in  $\beta \in [1-r^2, 1]$ . It follows that the solutions  $\theta_k^{(n)}$  of (15) satisfy

$$\theta_k^{(n)}(\beta_0) - \theta_k^{(n)}(\beta_1) \leq \theta_k^{(n-1)}(\beta_0) - \theta_k^{(n-1)}(\beta_1)$$

for  $\beta_0 \leq \beta_1$ . In conclusion the quantity

$$nr^{2(n-1)} + (n-1)\beta^2 r^{2(n-2)} - (n-1)r^{2(n-2)} + \sum_{k=1}^{n-2} |\lambda_k^{(n-1)}|^2 - \sum_{k=1}^{n-1} |\lambda_k^{(n)}|^2$$

is increasing in  $\beta$ .

*vi)* is a direct consequence of *iii)* and *v)*. □

*Proof of Lemma II.7.* For fixed  $\beta \in [0, 2]$ ,  $r \in (0, 1]$  we for now focus our attention on real values of  $\theta$  and write shortly

$$\varphi_{r,\beta}(\theta) = \frac{r^2 - (\beta - 1)}{r^2 + (\beta - 1)} \cot(\theta) + \frac{(2 - \beta)r}{\beta - 1 + r^2} \frac{1}{\sin(\theta)}$$

such that Equation (12) becomes

$$\varphi_{r,\beta}(\theta) = -\cot(n\theta), \quad \theta \in [-\pi, \pi).$$

We start with some elementary observations.

1. We restrict to the interval  $[0, \pi)$  as all functions are symmetric with respect to the point  $(\pi, 0)$ .
2.  $\cot(n\theta)$  has poles in  $[0, \pi)$  at  $\theta_k = \frac{k}{n}\pi$ ,  $k = 1, \dots, n - 1$ .
3. The functions  $\frac{1}{\sin(\theta)}$  and  $\cot(\theta)$  have poles at 0 and  $\pi$ ,  $\cot(\theta) \sim \frac{1}{\sin(\theta)}$  as  $\theta$  tends to  $0^+$  and  $\cot(\theta) \sim -\frac{1}{\sin(\theta)}$  as  $\theta$  tends to  $\pi^-$ .
4. Looking at the polynomials:

$$P_\beta(r) = r^2 - (2 - \beta)r - (\beta - 1) = (r - 1)(r - (1 - \beta)),$$

and

$$Q_\beta(r) = r^2 + (2 - \beta)r - (\beta - 1) = (r + 1)(r - (\beta - 1)),$$

we have that  $P_\beta(r) < 0$  for  $r \in (1 - \beta, 1)$  and  $P_\beta(r) \geq 0$  elsewhere, while  $Q_\beta(r) < 0$  for  $r \in (-1, \beta - 1)$  and  $Q_\beta(r) \geq 0$  elsewhere.

5. Taking (c) and (d) into account, we have

$$\varphi_{r,\beta}(\theta) \sim_{\theta \rightarrow 0^+} \frac{r^2 + (2 - \beta)r - (\beta - 1)}{\beta - 1 + r^2} \frac{1}{\sin(\theta)} = \frac{Q_\beta(r)}{\beta - 1 + r^2} \frac{1}{\sin(\theta)},$$

while

$$\varphi_{r,\beta}(\theta) \sim_{\theta \rightarrow \pi^-} -\frac{r^2 - (2 - \beta)r - (\beta - 1)}{\beta - 1 + r^2} \frac{1}{\sin(\theta)} = \frac{-P_\beta(r)}{\beta - 1 + r^2} \frac{1}{\sin(\theta)}.$$

We now prove the points in the lemma.

1. **The case  $r = 1$ .** In this case, the structure of (12) is discussed in [OS, Section B]. We now suppose that  $r \in (0, 1)$ .
2. **The case  $r = |\beta - 1| \notin \{0, 2\}$ .**

(a) **The subcase  $\beta < 1$ .** We have that

$$\varphi_{r,\beta}(\theta) = \frac{(-2 + \beta)(\cos(\theta) + 1)}{\sin(\theta)\beta},$$

and as a consequence,  $\varphi_{r,\beta} < 0$  on  $(0, \pi)$ ,  $\lim_{\theta \rightarrow 0^+} \varphi_{r,\beta}(\theta) = -\infty$ , while  $\lim_{\theta \rightarrow \pi^-} \varphi_{r,\beta}(\theta) = 0$ . Thus, the graph of  $\varphi_{r,\beta}$  intersects  $n - 1$  times with the graph of  $\theta \mapsto -\cot(n\theta)$  on  $[\frac{\pi}{2n}, \pi)$ . Moreover,

$$\frac{\varphi_{r,\beta}(\theta)}{-\cot(n\theta)} = \frac{(2 - \beta)\sin(\theta)\sin(n\theta)}{\beta\cos(n\theta)(1 - \cos(\theta))},$$

and in particular, for any  $\theta \in (0, \frac{\pi}{2n})$ ,  $\frac{\varphi_{r,\beta}(\theta)}{-\cot(n\theta)} > 1$ , which can be seen by computing derivatives with respect to  $\theta$ :  $\theta \mapsto \frac{\varphi_{r,\beta}(\theta)}{-\cot(n\theta)}$  is increasing on  $(0, \frac{\pi}{2n})$ , with

$$\lim_{\theta \rightarrow 0^+} \frac{\varphi_{r,\beta}(\theta)}{-\cot(n\theta)} = \frac{2n(2 - \beta)}{\beta} \geq 2n > 1.$$

The graph of  $\varphi_{r,\beta}$  does not intersect the one of  $\theta \mapsto -\cot(n\theta)$  on  $[0, \frac{\pi}{2n})$ . We conclude that in this case (12) has  $2n - 2$  real solutions  $\theta_k$  in  $[-\pi, \pi)$ .

(b) **The subcase  $\beta > 1$ .** We have that

$$\varphi_{r,\beta}(\theta) = \frac{(-2 + \beta)(\cos(\theta) - 1)}{\sin(\theta)\beta},$$

and as a consequence,  $\varphi_{r,\beta}$  is increasing on  $(0, \pi)$ ,  $\varphi_{r,\beta} > 0$  on  $(0, \pi)$ ,

$$\lim_{\theta \rightarrow 0^+} \varphi_{r,\beta}(\theta) = 0,$$

while  $\lim_{\theta \rightarrow \pi^-} \varphi_{r,\beta}(\theta) = +\infty$ . Hence the graph of  $\varphi_{r,\beta}$  intersects  $n - 1$  times the one of  $-\cot(n\theta)$  on  $(0, \frac{(2n-1)\pi}{2n}]$ . Moreover,

$$\frac{\varphi_{r,\beta}(\theta)}{-\cot(n\theta)} = \frac{(2 - \beta)\sin(\theta)\sin(n\theta)}{\beta\cos(n\theta)(1 + \cos(\theta))},$$

and in particular, for any  $\theta \in (\frac{(2n-1)\pi}{2n}, \pi)$ ,  $\frac{\varphi_{r,\beta}(\theta)}{-\cot(n\theta)} > \frac{2n(2-\beta)}{\beta}$  using the fact (as above) that  $\theta \mapsto \frac{\varphi_{r,\beta}(\theta)}{-\cot(n\theta)}$  is this time decreasing on  $(\frac{(2n-1)\pi}{2n}, \pi)$ , with

$$\lim_{\theta \rightarrow \pi^-} \frac{\varphi_{r,\beta}(\theta)}{-\cot(n\theta)} = \frac{2n(2 - \beta)}{\beta}.$$

Adding the positivity and the continuity of  $\theta \mapsto \frac{\varphi_{r,\beta}(\theta)}{-\cot(n\theta)}$  on  $(\frac{(2n-1)\pi}{2n}, \pi)$ , and

$$\lim_{\theta \rightarrow \frac{(2n-1)\pi}{2n}} \frac{\varphi_{r,\beta}(\theta)}{-\cot(n\theta)} = +\infty,$$

the intermediate value theorem guarantees that the graph of  $\varphi_{r,\beta}$  does not intersect the one of  $\theta \mapsto -\cot(n\theta)$  on  $(\frac{(2n-1)\pi}{2n}, \pi)$  if and only if  $\frac{2n(2-\beta)}{\beta} > 1$  (i.e  $n > \frac{\beta}{2(2-\beta)}$ ). We conclude that in this case (12) has  $2n - 2$  real solutions  $\theta_k$  in  $[-\pi, \pi)$  if and only if  $n > \frac{\beta}{2(2-\beta)}$ .

From now on, we suppose that  $r \neq 1 - \beta$ , and  $r \neq \beta - 1$ . Let us first notice that in case  $\beta - 1 + r^2 \neq 0$ , we have

$$\lim_{\theta \rightarrow 0^+} \frac{\varphi_{r,\beta}(\theta)}{-\cot(n\theta)} = \frac{n(1+r)(\beta-1-r)}{\beta-1+r^2},$$

and

$$\lim_{\theta \rightarrow \pi^-} \frac{\varphi_{r,\beta}(\theta)}{-\cot(n\theta)} = \frac{n(1-r)(r+\beta-1)}{\beta-1+r^2}.$$

Below, we repeat the reasonings of (2) for the remaining cases (3), (4) and (5).

3. **The case  $\beta > 1$ , and  $r \notin \{1, \beta - 1\}$ .** With (e),  $P_\beta(r) < 0$ , for any  $r \in [0, 1)$ . In particular, for any  $r \in [0, 1)$ ,

$$\lim_{\theta \rightarrow \pi^-} \varphi_{r,\beta}(\theta) = +\infty,$$

while

$$\lim_{\theta \rightarrow 0^+} \varphi_{r,\beta}(\theta) = \begin{cases} -\infty & \text{if } r \in [0, \beta - 1) \\ +\infty & \text{if } r \in (\beta - 1, 1) \end{cases},$$

because of the property of  $Q_\beta(r)$  in (d).

- (a) **The subcase  $1 < \beta < 1 + r$ .** In this case,  $\varphi_{r,\beta} > 0$  on  $(0, \pi)$  and

$$\lim_{\theta \rightarrow 0^+} \varphi_{r,\beta}(\theta) = \lim_{\theta \rightarrow \pi^-} \varphi_{r,\beta}(\theta) = +\infty.$$

Moreover,  $\varphi_{r,\beta}$  has a global minimum at some point  $\theta_0 \in (0, \pi)$  such that  $\varphi_{r,\beta}$  is decreasing on  $(0, \theta_0]$  and increasing on  $[\theta_0, \pi)$ . Thus, the curve of  $\varphi_{r,\beta}$  intersects the one of  $\theta \mapsto -\cot(n\theta)$  exactly  $n - 1$  times on  $(0, \frac{(2n-1)\pi}{2n}]$ . On the interval  $(\frac{(2n-1)\pi}{2n}, \pi)$ , the curve of  $\varphi_{r,\beta}$  does not intersect the one of  $\theta \mapsto -\cot(n\theta)$  if and only if  $\lim_{\theta \rightarrow \pi^-} \frac{\varphi_{r,\beta}(\theta)}{-\cot(n\theta)} > 1$ , (else, the number of real intersections on  $[0, \pi)$  is  $n$ ). Indeed as before,  $\theta \mapsto \frac{\varphi_{r,\beta}(\theta)}{-\cot(n\theta)}$  is (positive, continuous and) decreasing on  $(\frac{(2n-1)\pi}{2n}, \pi)$ . We conclude that in this case (12) has  $2n - 2$  real solutions  $\theta_k$  in  $[-\pi, \pi)$  if and only if  $n > \frac{\beta-1+r^2}{(1-r)(r+\beta-1)}$ .

- (b) **The subcase**  $\beta > 1 + r$ . In this case,  $\varphi_{r,\beta}$  is increasing on  $(0, \pi)$ , and  $\lim_{\theta \rightarrow 0^+} \varphi_{r,\beta}(\theta) = -\infty$ , while  $\lim_{\theta \rightarrow \pi^-} \varphi_{r,\beta}(\theta) = +\infty$ . Thus, the curve of  $\varphi_{r,\beta}$  intersects the one of  $\theta \mapsto -\cot(n\theta)$  exactly  $n - 2$  times on  $[\frac{\pi}{2n}, \frac{(2n-1)\pi}{2n}]$ . Moreover, on  $(0, \frac{\pi}{2n}) \cup (\frac{(2n-1)\pi}{2n}, \pi)$ ,  $\theta \mapsto \frac{\varphi_{r,\beta}(\theta)}{-\cot(n\theta)}$  is positive and continuous; it is increasing on  $(0, \frac{\pi}{2n})$  and decreasing on  $(\frac{(2n-1)\pi}{2n}, \pi)$ . Thus, the curve of  $\varphi_{r,\beta}$  does not intersect the one of  $\theta \mapsto -\cot(n\theta)$  on  $(0, \frac{\pi}{2n})$  (resp. on  $(\frac{(2n-1)\pi}{2n}, \pi)$ ) if and only if  $\lim_{\theta \rightarrow 0^+} \frac{\varphi_{r,\beta}(\theta)}{-\cot(n\theta)} > 1$  (resp.  $\lim_{\theta \rightarrow \pi^-} \frac{\varphi_{r,\beta}(\theta)}{-\cot(n\theta)} > 1$ ). We conclude that in this case (12) has  $2n - 4$  real solutions  $\theta_k$  in  $[-\pi, \pi)$  if and only if  $n > \frac{\beta-1+r^2}{(1-r)(r+\beta-1)}$ , since  $\frac{\beta-1+r^2}{(1+r)(\beta-1-r)} < \frac{\beta-1+r^2}{(1-r)(r+\beta-1)}$ .

4. **The case**  $\beta < 1$  and  $r \notin \{1, 1 - \beta\}$ . With (e),  $Q_\beta(r) \geq 0$ , for any  $r \in [0, 1)$ . In particular, for any  $r \in [0, 1)$ ,

$$\lim_{\theta \rightarrow 0^+} \varphi_{r,\beta}(\theta) = \begin{cases} +\infty & \text{if } \beta - 1 + r^2 > 0 \\ -\infty & \text{if } \beta - 1 + r^2 < 0 \end{cases},$$

while

$$\lim_{\theta \rightarrow \pi^-} \varphi_{r,\beta}(\theta) = \begin{cases} +\infty & \text{if } \beta - 1 + r^2 > 0 \\ +\infty & \text{if } \beta - 1 + r^2 < 0 \text{ and } r \in [0, 1 - \beta) \\ -\infty & \text{if } \beta - 1 + r^2 < 0 \text{ and } r \in (1 - \beta, 1) \end{cases},$$

because of the property of  $P_\beta(r)$  in (d).

- (a) **The subcase**  $1 - r^2 < \beta < 1$ . In this case,  $\varphi_{r,\beta} > 0$  on  $(0, \pi)$ , and  $\lim_{\theta \rightarrow 0^+} \varphi_{r,\beta}(\theta) = \lim_{\theta \rightarrow \pi^-} \varphi_{r,\beta}(\theta) = +\infty$ . Moreover,  $\varphi_{r,\beta}$  has a global minimum at some point  $\theta_0 \in (0, \pi)$  such that  $\varphi_{r,\beta}$  is decreasing on  $(0, \theta_0]$  and increasing on  $[\theta_0, \pi)$ . We conclude as in (3)-(a) that in this case, (12) has  $2n - 2$  real solutions  $\theta_k$  in  $[-\pi, \pi)$  if and only if  $n > \frac{\beta-1+r^2}{(1-r)(r+\beta-1)}$ .
- (b) **The subcase**  $0 < \beta < 1 - r^2$ .
- i. If  $0 < \beta < 1 - r$ ,  $\varphi_{r,\beta}$  is increasing on  $(0, \pi)$ ,  $\lim_{\theta \rightarrow 0^+} \varphi_{r,\beta}(\theta) = -\infty$ , and  $\lim_{\theta \rightarrow \pi^-} \varphi_{r,\beta}(\theta) = +\infty$ . We conclude by a similar reasoning as the one in (3)-(b) that in this case also (12) has  $2n - 4$  real solutions  $\theta_k$  in  $[-\pi, \pi)$  if and only if  $n > \frac{\beta-1+r^2}{(1-r)(r+\beta-1)}$ , since  $\frac{\beta-1+r^2}{(1+r)(\beta-1-r)} < \frac{\beta-1+r^2}{(1-r)(r+\beta-1)}$ .
  - ii. If  $1 - r < \beta < 1 - r^2$ ,  $\varphi_{r,\beta}(\theta) < 0$ ,  $\forall \theta \in (0, \pi)$ , and  $\lim_{\theta \rightarrow 0^+} \varphi_{r,\beta}(\theta) = \lim_{\theta \rightarrow \pi^-} \varphi_{r,\beta}(\theta) = -\infty$ . Moreover,  $\varphi_{r,\beta}$  has a global maximum  $\theta_0 \in (0, \pi)$  such that  $\varphi_{r,\beta}$  is increasing on  $(0, \theta_0]$  and decreasing on  $[\theta_0, \pi)$ . Thus, the curve of  $\varphi_{r,\beta}$  intersects the one of  $\theta \mapsto -\cot(n\theta)$  exactly  $n - 1$  times on  $[\frac{\pi}{2n}, \pi)$ . In the interval  $(0, \frac{\pi}{2n})$ , the curve of  $\varphi_{r,\beta}$  does not intersect the one of  $\theta \mapsto -\cot(n\theta)$  if and only if  $\lim_{\theta \rightarrow 0^+} \frac{\varphi_{r,\beta}(\theta)}{-\cot(n\theta)} > 1$ . The latter condition is always satisfied since  $\frac{n(1+r)(\beta-1-r)}{\beta-1+r^2} = \frac{n(1+r)(1-\beta+r)}{1-\beta-r^2} > n$ . We conclude that in this case, (12) has  $2n - 2$  real solutions  $\theta_k$  on  $[-\pi, \pi)$ .

5. **The case  $\beta = 1$ .** In this case,

$$\varphi_{r,\beta}(\theta) = \frac{1 + r\cos(\theta)}{r\sin(\theta)},$$

and thus  $\varphi_{r,\beta}(\theta) > 0$ ,  $\forall \theta \in (0, \pi)$ , and  $\lim_{\theta \rightarrow 0^+} \varphi_{r,\beta}(\theta) = \lim_{\theta \rightarrow \pi^-} \varphi_{r,\beta}(\theta) = +\infty$ . Moreover,  $\varphi_{r,\beta}$  has a global minimum at some point  $\theta_0 \in (0, \pi)$  such that  $\varphi_{r,\beta}$  is decreasing on  $(0, \theta_0]$  and increasing on  $[\theta_0, \pi)$ . In particular, the graph of  $\varphi_{r,\beta}$  intersects the one of  $\theta \mapsto -\cot(n\theta)$  exactly  $n - 1$  times on  $(0, \frac{(2n-1)\pi}{2n}]$ . On the interval  $(\frac{(2n-1)\pi}{2n}, \pi)$ , the function  $\theta \mapsto \frac{\varphi_{r,\beta}(\theta)}{-\cot(n\theta)}$  is decreasing and thus the curve of  $\varphi_{r,\beta}$  does not intersect the one of  $\theta \mapsto -\cot(n\theta)$  if and only if  $\lim_{\theta \rightarrow \pi^-} \frac{\varphi_{r,\beta}(\theta)}{-\cot(n\theta)} > 1$ . We conclude that in this case, (12) has  $2n - 2$  real solutions  $\theta_k$  on  $[-\pi, \pi)$  if and only if  $n > \frac{r}{1-r}$  (else (12) has  $2n$  real solutions in  $[-\pi, \pi)$ ).

□

## V. APPENDIX

The columns  $C_i$ ,  $i = 1, \dots, n$  of the  $n \times n$  matrix  $\tilde{X} - \lambda^2$  are:

$$C_1 = \begin{bmatrix} -\lambda^2 + \beta^2(1 + r^2 + \dots + r^{2 \cdot (n-2)}) + r^{2 \cdot (n-1)} \\ \beta^2 r(1 + r^2 + r^{2 \cdot (n-3)}) + \beta r^{2 \cdot (n-1)-1} \\ \beta^2 r^2(1 + r^2 + r^{2 \cdot (n-4)}) + \beta r^{2 \cdot (n-1)-2} \\ \vdots \\ \beta^2 r^{n-3}(1 + r^2) + \beta r^{n+1} \\ \beta^2 r^{n-2} + \beta r^n \\ \beta r^{n-1} \end{bmatrix},$$

$$C_2 = \begin{bmatrix} \beta^2 r(1 + r^2 + r^{2 \cdot (n-3)}) + \beta r^{2 \cdot (n-1)-1} \\ -\lambda^2 + \beta^2 r^2(1 + r^2 + \dots + r^{2 \cdot (n-3)}) + r^{2 \cdot (n-1)} \\ \beta^2 r^3(1 + r^2 + r^{2 \cdot (n-4)}) + \beta r^{2 \cdot (n-1)-1} \\ \vdots \\ \beta^2 r^{n-2}(1 + r^2) + \beta r^{n+2} \\ \beta^2 r^{n-1} + \beta r^{n+1} \\ \beta r^n \end{bmatrix},$$

$$\begin{aligned}
C_3 &= \begin{bmatrix} \beta^2 r^2(1 + r^2 + r^{2 \cdot (n-4)}) + \beta r^{2 \cdot (n-1)-2} \\ \beta^2 r^3(1 + r^2 + r^{2 \cdot (n-4)}) + \beta r^{2 \cdot (n-1)-1} \\ -\lambda^2 + \beta^2 r^4(1 + r^2 + \dots + r^{2 \cdot (n-4)}) + r^{2 \cdot (n-1)} \\ \beta^2 r^5(1 + r^2 + \dots + r^{2 \cdot (n-5)}) + \beta r^{2 \cdot (n-1)-1} \\ \vdots \\ \beta^2 r^{n-1}(1 + r^2) + \beta r^{n+3} \\ \beta^2 r^n + \beta r^{n+2} \\ \beta r^{n+1} \end{bmatrix}, \\
C_4 &= \begin{bmatrix} \beta^2 r^3(1 + r^2 + r^{2 \cdot (n-5)}) + \beta r^{2 \cdot (n-1)-3} \\ \beta^2 r^4(1 + r^2 + r^{2 \cdot (n-5)}) + \beta r^{2 \cdot (n-1)-2} \\ \beta^2 r^5(1 + r^2 + r^{2 \cdot (n-5)}) + \beta r^{2 \cdot (n-1)-1} \\ -\lambda^2 + \beta^2 r^6(1 + r^2 + \dots + r^{2 \cdot (n-5)}) + r^{2 \cdot (n-1)} \\ \beta^2 r^7(1 + r^2 + r^{2 \cdot (n-6)}) + \beta r^{2 \cdot (n-1)-1} \\ \vdots \\ \beta^2 r^n(1 + r^2) + \beta r^{n+4} \\ \beta^2 r^{n+1} + \beta r^{n+3} \\ \beta r^{n+2} \end{bmatrix}, \dots \\
\dots C_{n-3} &= \begin{bmatrix} \beta^2 r^{n-4}(1 + r^2 + r^4) + \beta r^{n+2} \\ \beta^2 r^{n-3}(1 + r^2 + r^4) + \beta r^{n+3} \\ \beta^2 r^{n-2}(1 + r^2 + r^4) + \beta r^{n+4} \\ \vdots \\ \beta^2 r^{2n-10}(1 + r^2 + r^4) + r^{2n-4} \\ \beta^2 r^{2n-9}(1 + r^2 + r^4) + r^{2n-3} \\ -\lambda^2 + \beta^2 r^{2n-8}(1 + r^2 + r^4) + r^{2n-2} \\ \beta^2 r^{2n-7}(1 + r^2) + \beta r^{2n-3} \\ \beta^2 r^{2n-6} + \beta r^{2n-4} \\ \beta r^{2n-5} \end{bmatrix}, \\
C_{n-2} &= \begin{bmatrix} \beta^2 r^{n-3}(1 + r^2) + \beta r^{n+1} \\ \beta^2 r^{n-2}(1 + r^2) + \beta r^{n+2} \\ \vdots \\ \vdots \\ \beta^2 r^{2n-9}(1 + r^2) + \beta r^{2n-5} \\ \beta^2 r^{2n-8}(1 + r^2) + \beta r^{2n-4} \\ \beta^2 r^{2n-7}(1 + r^2) + \beta r^{2n-3} \\ -\lambda^2 + \beta^2 r^{2n-6}(1 + r^2) + r^{2n-2} \\ \beta^2 r^{2n-5} + \beta r^{2n-3} \\ \beta r^{2n-4} \end{bmatrix},
\end{aligned}$$

$$C_{n-1} = \begin{bmatrix} \beta^2 r^{n-2} + \beta r^n \\ \beta^2 r^{n-1} + \beta r^{n+1} \\ \beta^2 r^n + \beta r^{n+2} \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \beta^2 r^{2n-5} + \beta r^{2n-3} \\ -\lambda^2 + \beta^2 r^{2n-4} + r^{2n-2} \\ \beta r^{2n-3} \end{bmatrix},$$

and

$$C_n = \begin{bmatrix} \beta r^{n-1} \\ \beta r^n \\ \beta r^{n+1} \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \beta r^{2n-4} \\ \beta r^{2n-3} \\ -\lambda^2 + r^{2n-2} \end{bmatrix}.$$

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