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UNBOUNDED LARGEST EIGENVALUE OF LARGE SAMPLE COVARIANCE MATRICES: ASYMPTOTICS, FLUCTUATIONS AND APPLICATIONS

FLORENCE MERLEVÈDE, JAMAL NAJIM, AND PENG TIAN

ABSTRACT. Given a large sample covariance matrix $S_N = \frac{1}{n} \Gamma_N^{1/2} Z_N Z_N^* \Gamma_N^{1/2}$, where Z_N is a $N \times n$ matrix with i.i.d. centered entries, and Γ_N is a $N \times N$ deterministic Hermitian positive semidefinite matrix, we study the location and fluctuations of $\lambda_{\max}(S_N)$, the largest eigenvalue of S_N as $N, n \rightarrow \infty$ and $Nn^{-1} \rightarrow r \in (0, \infty)$ in the case where the empirical distribution μ^{Γ_N} of eigenvalues of Γ_N is tight (in N) and $\lambda_{\max}(\Gamma_N)$ goes to $+\infty$. These conditions are in particular met when μ^{Γ_N} weakly converges to a probability measure with unbounded support on \mathbb{R}^+ .

We prove that asymptotically $\lambda_{\max}(S_N) \sim \lambda_{\max}(\Gamma_N)$. Moreover when the Γ_N 's are block-diagonal, and the following *spectral gap condition* is assumed:

$$\limsup_{N \rightarrow \infty} \frac{\lambda_2(\Gamma_N)}{\lambda_{\max}(\Gamma_N)} < 1,$$

where $\lambda_2(\Gamma_N)$ is the second largest eigenvalue of Γ_N , we prove Gaussian fluctuations for $\lambda_{\max}(S_N)/\lambda_{\max}(\Gamma_N)$ at the scale \sqrt{n} .

In the particular case where Z_N has i.i.d. Gaussian entries and Γ_N is the $N \times N$ autocovariance matrix of a long memory Gaussian stationary process $(\mathcal{X}_t)_{t \in \mathbb{Z}}$, the columns of $\Gamma_N^{1/2} Z_N$ can be considered as n i.i.d. samples of the random vector $(\mathcal{X}_1, \dots, \mathcal{X}_N)^\top$. We then prove that Γ_N is similar to a diagonal matrix which satisfies all the required assumptions of our theorems, hence our results apply to this case.

1. INTRODUCTION

The model. In this paper we consider the following model of sample covariance matrix

$$(1) \quad S_N = \frac{1}{n} \Gamma_N^{1/2} Z_N Z_N^* \Gamma_N^{1/2}$$

where $Z_N = (Z_{i,j}^{(N)})$ is a $N \times n$ matrix whose entries $Z_{i,j}^{(N)}$ are real or complex random variables identically distributed (i.d.) for all i, j, N and independent across i, j for each N , satisfying

$$(2) \quad \mathbb{E} Z_{i,j}^{(N)} = 0, \quad \mathbb{E} |Z_{i,j}^{(N)}|^2 = 1 \quad \text{and} \quad \mathbb{E} |Z_{i,j}^{(N)}|^4 < \infty,$$

and Γ_N is a $N \times N$ deterministic Hermitian positive semidefinite matrix with eigenvalues

$$0 \leq \lambda_N(\Gamma_N) \leq \dots \leq \lambda_1(\Gamma_N) := \lambda_{\max}(\Gamma_N).$$

We consider the case where $\lambda_{\max}(\Gamma_N)$ goes to infinity as $N \rightarrow \infty$ while the empirical spectral distribution (ESD) μ^{Γ_N} associated with Γ_N ,

$$\mu^{\Gamma_N} := \frac{1}{N} \sum_{k=1}^N \delta_{\lambda_k(\Gamma_N)},$$

forms a tight sequence of probabilities on $\mathbb{R}^+ := [0, \infty)$. These conditions encompass the important case where μ^{Γ_N} converges to a limiting distribution with unbounded support on \mathbb{R}^+ .

In this context, our aim is to study the location and fluctuations of the largest eigenvalue $\lambda_{\max}(S_N)$ in the asymptotic regime where

$$(3) \quad N, n \rightarrow \infty \quad \text{and} \quad \frac{N}{n} \rightarrow r \in (0, \infty).$$

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The regime (3) will be simply referred to as $N, n \rightarrow \infty$ in the sequel.

The model S_N defined in (1) is a classical model of sample covariance matrices in the random matrix theory, and its spectral properties have been intensively studied in the regime (3) in the last several decades.

At a global scale, the limiting spectral distribution (LSD) of the ESD $\mu^{S_N} = N^{-1} \sum_{k=1}^N \delta_{\lambda_k(S_N)}$ has been described in the groundbreaking paper by Marčenko and Pastur [30]. In the important case where $S_N = \frac{1}{n} Z_N Z_N^*$, sometimes referred to as the *white noise* model, the limiting spectral distribution of μ^{S_N} is known as Marčenko-Pastur distribution and admits the following closed-form expression

$$\mathbb{P}_{MP}(d\lambda) := (1 - r^{-1})_+ \delta_0(d\lambda) + \frac{\sqrt{[(\lambda^+ - \lambda)(\lambda - \lambda^-)]_+}}{2\pi r \lambda} d\lambda, \quad \lambda^\pm = (1 \pm \sqrt{r})^2,$$

where $x_+ := \max(x, 0)$. Later, this result was improved by many others, see for instance [41, 26, 42, 35, 34]. In [34], Silverstein proved that for the model S_N defined in (1), if μ^{Γ_N} weakly converges to a certain probability ν supported on \mathbb{R}^+ (not necessarily with compact support), then almost surely, the ESD μ^{S_N} weakly converges to a deterministic distribution μ , whose Stieltjes transform g_μ is the unique solution with positive imaginary part of the equation

$$(4) \quad g_\mu(z) = \int \frac{1}{s(1 - r - rzg_\mu(z)) - z} d\nu(s) \in \mathbb{C}^+, \quad \forall z \in \mathbb{C}^+.$$

Central limit theorems have also been established for linear spectral statistics $\sum_{i=1}^N f(\lambda_i(S_N))$, see for instance [26, 24, 3, 32].

At a local scale, the convergence and fluctuations of individual eigenvalues have been studied, with a special emphasis on the eigenvalues located near each edge of the connected components (bulk) of the LSD of S_N . The spiked eigenvalues, that is those which stay away from the bulk of the LSD, have also attracted a lot of attention.

For the white noise model, the support of Marčenko-Pastur's LSD is $[(1 - \sqrt{r})^2, (1 + \sqrt{r})^2]$, with $\{0\}$ if $r > 1$. Geman [22] showed that $\lambda_{\max}(S_N) \rightarrow (1 + \sqrt{r})^2$ almost surely under moment conditions on the entries. Later, Bai et al. [43, 5, 8] showed that $\lambda_{\max}(S_N)$ almost surely converges to a finite limit if and only if the fourth moment $\mathbb{E}|Z_{1,1}^{(1)}|^4$ of the entries is finite. Concerning the fluctuations of $\lambda_{\max}(S_N)$, they were first studied by Johansson [24] for standard Gaussian complex entries and by Johnstone [25] for standard Gaussian real entries. They both established that

$$(5) \quad \gamma_N n^{2/3} (\lambda_{\max}(S_N) - (1 + \sqrt{r_N})^2) \quad \text{where} \quad r_N = \frac{N}{n} \quad \text{and} \quad \gamma_N = \frac{r_N^{1/6}}{(1 + \sqrt{r_N})^{4/3}}$$

converges in distribution to Tracy-Widom (TW) distributions as $N, n \rightarrow \infty$, introduced in [38, 39], to describe the fluctuations of the largest eigenvalues of GUE and GOE random matrices.

For general sample covariance matrices (1), the condition that the spectral norm of Γ_N is uniformly bounded:

$$\sup_{N \geq 1} \|\Gamma_N\| = \sup_{N \geq 1} \lambda_{\max}(\Gamma_N) < \infty$$

implies that the LSD μ (defined by its Stieltjes transform g_μ which satisfies (4)) has a bounded support. In this case, El Karoui [20] and Lee and Schnelli [29] established Tracy-Widom type fluctuations of the largest eigenvalue in the complex and real Gaussian case respectively. By establishing a local law, Bao et al [11], and Knowles and Yin [28] extended the fluctuations of the largest eigenvalue for general entries.

The case of spiked models has been addressed by Baik et al [9, 10] where some eigenvalues (the spikes) may separate from the bulk. In [9] where the so-called BBP phase transition phenomenon is described, Baik et al. study the case where Γ_N has exactly m non-unit eigenvalues $\ell_1 \geq \dots \geq \ell_m$. For complex Gaussian entries, they fully describe the fluctuations of $\lambda_{\max}(S_N)$ for different configurations of the ℓ_i 's. Assume for instance that ℓ_1 is simple (cf. the original paper for the general conditions) then (a) if $\ell_1 \leq 1 + \sqrt{r}$, $\lambda_{\max}(S_N)$ has asymptotically TW fluctuations at speed

$n^{2/3}$; (b) if $\ell_1 > 1 + \sqrt{r}$, the sequence

$$(6) \quad \frac{\sqrt{n}}{\sqrt{\ell_1^2 - \ell_1^2 r_N / (\ell_1 - 1)^2}} \left(\lambda_{\max}(S_N) - \left(\ell_1 + \frac{\ell_1 r_N}{\ell_1 - 1} \right) \right)$$

is asymptotically Gaussian. In [10] Baik and Silverstein consider general entries and prove the strong convergence of the spiked eigenvalues; Bai and Yao [6] consider the spiked model with supercritical spikes (corresponding to the case (b) above) and general entries and establish Gaussian-type fluctuations for the spiked eigenvalues. Other results are, non exhaustively, [12, 13, 18, 7].

To make a rough conclusion from these results, $\lambda_{\max}(S_N)$ does not in general approach the largest eigenvalue of $\lambda_{\max}(\Gamma_N)$. Moreover, if $\lambda_{\max}(S_N)$ converges to the bulk edge of the LSD of μ^{S_N} , then it often has Tracy-Widom fluctuation at the scale $n^{2/3}$. If $\lambda_{\max}(S_N)$ converges to a point outside the bulk, it often has Gaussian-type fluctuation at the scale $n^{1/2}$.

The previously mentioned results are limited to the case where $\lambda_{\max}(\Gamma_N)$ is uniformly bounded. There are however interesting cases where $\lambda_{\max}(\Gamma_N)$ goes to infinity, see for instance Forni et al. [21] in a context of econometrics, or consider the context of long memory stationary processes where the LSD of μ^{Γ_N} has a non-compact support.

Long memory stationary process. We recall that a process $(\mathcal{X}_t)_{t \in \mathbb{Z}}$ is (second order) stationary if the following conditions are satisfied:

$$\mathbb{E}|\mathcal{X}_t|^2 < \infty \quad \text{and} \quad \mathbb{E}\mathcal{X}_t = \mathbb{E}\mathcal{X}_0, \quad \forall t \in \mathbb{Z},$$

and

$$\text{Cov}(\mathcal{X}_{t+h}, \mathcal{X}_t) = \text{Cov}(\mathcal{X}_h, \mathcal{X}_0) = \gamma(h) \quad \forall t, h \in \mathbb{Z}$$

where $\text{Cov}(\mathcal{X}_{t+h}, \mathcal{X}_t) = \mathbb{E}(\mathcal{X}_{t+h} - \mathbb{E}\mathcal{X}_{t+h})(\mathcal{X}_t - \mathbb{E}\mathcal{X}_t)$ and $\gamma : \mathbb{Z} \rightarrow \mathbb{C}$ is some positive definite function, usually called the autocovariance function of the process. Note that $\gamma(0)$ is positive and $\gamma(-h) = \overline{\gamma(h)}$ for all $h \in \mathbb{Z}$. By stationarity, the covariance matrices of the process are

$$(7) \quad T_N(\gamma) := \text{Cov} \begin{pmatrix} \mathcal{X}_{t+1} \\ \vdots \\ \mathcal{X}_{t+N} \end{pmatrix} = \begin{pmatrix} \gamma(0) & \gamma(-1) & \dots & \gamma(-N+1) \\ \gamma(1) & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \gamma(-1) \\ \gamma(N-1) & \dots & \gamma(1) & \gamma(0) \end{pmatrix}.$$

The $T_N(\gamma)$'s are positive semidefinite Hermitian Toeplitz matrices.

By Herglotz's Theorem, there exists a finite positive measure α on $(-\pi, \pi]$ whose Fourier coefficients are exactly $\gamma(h)$, i.e.

$$\gamma(h) = \frac{1}{2\pi} \int_{(-\pi, \pi]} e^{-ihx} d\alpha(x), \quad \forall h \in \mathbb{Z}.$$

This measure is called the symbol of the Toeplitz matrix $T_N(\gamma)$ that we may also write $T_N[\alpha]$.

Tyrtshnikov and Zamarashkin generalized in [40] a result of Szegő and proved that the following equality holds

$$(8) \quad \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{k=1}^N \varphi(\lambda_k(T_N(\gamma))) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \varphi(f_\alpha(x)) dx,$$

where $\varphi : \mathbb{R} \mapsto \mathbb{R}$ is continuous with compact support and $f_\alpha \in L^1(-\pi, \pi)$ is the density of the absolutely continuous part of α with respect to the Lebesgue measure dx on $(-\pi, \pi]$, called the *spectral density* of $T_N(\gamma)$. The equality (8) can be interpreted as the vague convergence of probability measures $\mu^{T_N(\gamma)}$ to the measure ν defined by the integral formula

$$(9) \quad \int \varphi d\nu = \frac{1}{2\pi} \int_{-\pi}^{\pi} \varphi(f_\alpha(x)) dx \quad \forall \varphi \in C_b,$$

where C_b denotes the space of all bounded continuous functions. The measure ν being a probability, the sequence $\mu^{T_N(\gamma)}$ is tight, and the vague convergence coincides with the weak convergence.

The process is usually said to have *short memory* or *short range dependence* if $\sum_{h \in \mathbb{Z}} |\gamma(h)| < \infty$. Otherwise, if

$$\sum_{h \in \mathbb{Z}} |\gamma(h)| = \infty,$$

the process (\mathcal{X}_t) has *long memory* or *long range dependence*¹.

In this article we require that the autocovariance function γ of a long memory stationary process satisfies

$$(10) \quad \gamma(h) = \frac{L(h)}{(1 + |h|)^{1-2d}}, \quad \forall h \in \mathbb{Z}$$

for some $d \in (0, 1/2)$ and a function $L : \mathbb{R} \rightarrow \mathbb{R}$ slowly varying at ∞ , that is a function such that $L(y) > 0$ for $|y|$ large enough such that

$$\lim_{y \rightarrow \infty} \frac{L(xy)}{L(y)} = 1 \quad \forall x > 0.$$

In this case γ is real and even and L is an even function as well. Matrix $T_N(\gamma)$ is real symmetric and (\mathcal{X}_t) is a long memory process. In addition, $\lambda_{\max}(\Gamma_N) \xrightarrow{N \rightarrow \infty} \infty$, see for instance Theorem 2.3.

Description of the main results. Let S_N be defined in (1) and assume that (μ^{Γ_N}) is tight with $\lim_{N \rightarrow \infty} \lambda_{\max}(\Gamma_N) = \infty$, then we establish in Theorem 2.1 that

$$(11) \quad \frac{\lambda_{\max}(S_N)}{\lambda_{\max}(\Gamma_N)} \xrightarrow{N, n \rightarrow \infty} 1$$

in probability. This convergence can be improved to an almost sure convergence if either the $Z_{i,j}^{(N)}$'s are standard (real or complex) gaussian, or stem from the top left corner of an infinite array $(Z_{i,j}, i, j \in \mathbb{N})$ of i.i.d. random variables.

In order to describe the fluctuations of $\lambda_{\max}(S_N)$, we assume in addition that (Γ_N) satisfies the following *spectral gap condition*

$$(12) \quad \overline{\lim}_{N \rightarrow \infty} \frac{\lambda_2(\Gamma_N)}{\lambda_{\max}(\Gamma_N)} < 1,$$

where $\lambda_2(\Gamma_N)$ is the second largest eigenvalue of Γ_N , and that either the $Z_{i,j}^{(N)}$'s are standard Gaussian or the Γ_N 's have a *block-diagonal structure*

$$(13) \quad \Gamma_N = \begin{pmatrix} \lambda_{\max}(\Gamma_N) & 0 \\ 0 & \Gamma_{N-1} \end{pmatrix}.$$

In this case, the following fluctuation result, stated in Theorem 2.2, holds:

$$(14) \quad \sqrt{n} \left(\frac{\lambda_{\max}(S_N)}{\lambda_{\max}(\Gamma_N)} - 1 - \frac{1}{n} \sum_{k=2}^N \frac{\lambda_k(\Gamma_N)}{\lambda_{\max}(\Gamma_N) - \lambda_k(\Gamma_N)} \right) \xrightarrow{N, n \rightarrow \infty} \mathcal{N}_{\mathbb{R}}(0, \sigma^2)$$

where “ $\xrightarrow{\mathcal{D}}$ ” denotes the convergence in distribution, $\sigma^2 = \mathbb{E}|Z_{1,1}|^4 - 1$ and $\mathcal{N}_{\mathbb{R}}$ stands for the real Gaussian distribution.

Applications to long memory stationary Gaussian processes. Given a centered stationary process $(\mathcal{X}_t)_{t \in \mathbb{Z}}$ with autocovariance function defined by (10), one can study the spectral properties of the sample covariance matrix

$$(15) \quad Q_N := \frac{1}{n} X_N X_N^* = \frac{1}{n} \sum_{j=1}^n X_{\cdot, j} X_{\cdot, j}^*$$

where X_N is a $N \times n$ random matrix whose columns $(X_{\cdot, j}, 1 \leq j \leq n)$ are i.i.d copies of the random vector $\mathcal{X}_{1:N} = (\mathcal{X}_1, \dots, \mathcal{X}_N)^\top$.

Let $T_N(\gamma)$ be the covariance matrix of (\mathcal{X}_t) , then it has been recalled that $\mu^{T_N(\gamma)}$ weakly converges. If the process is Gaussian, then Q_N can be written in the form of S_N in (1) with $\Gamma_N = T_N(\gamma)$

¹There are several definitions of long range dependence, all strongly related but not always equivalent, see for instance [33, Chapter 2].

and the ESD μ^{Q_N} weakly converges with probability one to a deterministic probability measure μ by [34, Theorem 1.1].

In order to study the behavior of $\lambda_{\max}(Q_N)$ and to apply the results already presented, note that the process being gaussian, the matrix model (1) has the same spectral properties as a model where Γ_N is replaced by the diagonal matrix obtained with Γ_N 's eigenvalues. In particular, the block-diagonal structure condition (13) is automatically satisfied. It remains to verify the spectral gap condition (12) and that $\lambda_{\max}(T_N(\gamma))$ goes to infinity. In Theorem 2.3, we describe the asymptotic behaviour of the individual eigenvalues $\lambda_k(T_N(\gamma))$ and prove that for any $k \geq 1$, there exist nonnegative numbers a_k with $a_1 > 0$ such that

$$\lambda_k(T_N(\gamma)) \sim a_k N \gamma(N) \quad \text{and} \quad \lim_{N \rightarrow \infty} \frac{\lambda_2(T_N(\gamma))}{\lambda_{\max}(T_N(\gamma))} = \frac{a_2}{a_1} < 1,$$

hence the spectral gap condition (12) holds. Moreover, standard properties of slowly varying functions [14, Prop. 1.3.6(v)] yield that $N\gamma(N) \rightarrow \infty$ hence $\lambda_{\max}(T_N(\gamma)) \rightarrow \infty$. As a corollary, we obtain the asymptotics and fluctuations of the largest eigenvalue $\lambda_{\max}(Q_N)$ for Gaussian long memory stationary processes with autocovariance function defined in (10).

We now point out two references of interest: In the (non-Gaussian) case where the symbol α is absolutely continuous with respect to the Lebesgue measure and under additional regularity conditions on (\mathcal{X}_t) , Merlevède and Peligrad [31] have established the convergence of the ESD μ^{Q_N} toward a certain deterministic probability distribution. In a context of a stationary Gaussian field, Chakrabarty et al. [17] studied large random matrices associated to long range dependent processes.

Organization. Our paper is organized as follows. In Section 2 we state the assumptions and main results of the article: Theorem 2.1 and Theorem 2.2 are devoted to the limiting behaviour and fluctuations of $\lambda_{\max}(S_N)$; the spectral gap condition for a Toeplitz matrix Γ_N is studied in Theorem 2.3; finally Corollary 2.4 builds upon the previous results and describes the behaviour and fluctuations of covariance matrices based on samples of stationary long memory Gaussian processes. In Section 3, we provide examples, numerical simulations and mention some open questions. Section 4 and Section 5 are dedicated to the proofs of the main theorems.

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2. NOTATIONS AND MAIN THEOREMS

2.1. Notations and assumptions.

Notations. Given $x \in \mathbb{R}$, denote by $\lfloor x \rfloor$ the integer satisfying $\lfloor x \rfloor \leq x < \lfloor x \rfloor + 1$. For vectors u, v in \mathbb{R}^N or \mathbb{C}^N , $\langle u, v \rangle = \sum_{i=1}^N u_i \bar{v}_i$ denotes the scalar product and $\|u\|$ the Euclidean norm of u .

For a matrix or a vector A , we use A^\top to denote the transposition of A , and A^* the conjugate transposition of A ; if A is a $N \times N$ square matrix with real eigenvalues, we use $\lambda_1(A) \geq \dots \geq \lambda_N(A)$ to denote its eigenvalues, and sometimes denote $\lambda_1(A) = \lambda_{\max}(A)$. The ESD μ^A of A is defined as

$$\mu^A := \frac{1}{N} \sum_{k=1}^N \delta_{\lambda_k(A)},$$

where δ_λ is the Dirac measure at λ . For a $N \times n$ matrix M and integers $a, b \in \{1, \dots, N\}$ and $c, d \in \{1, \dots, n\}$, the following notations are used to deal with submatrices of M :

(16)

$$M_{a,b,\cdot} = (M_{i,j})_{a \leq i \leq b, 1 \leq j \leq n}, \quad M_{\cdot,c,d} = (M_{i,j})_{1 \leq i \leq N, c \leq j \leq d}, \quad M_{a,b,c,d} = (M_{i,j})_{a \leq i \leq b, c \leq j \leq d}.$$

By convention, these subscripts have higher priority than the transposition or conjugate transposition, for example $M_{a,b,c,d}^* := (M_{a,b,c,d})^*$ is the conjugated transposition of the submatrix $M_{a,b,c,d}$.

For a matrix A , we write its operator norm as $\|A\| = \sup_{\|v\|=1} \|Av\|$ and its Frobenius norm

$$\|A\|_F = \sqrt{\sum_{i,j} |A_{i,j}|^2}.$$

If $c = (c_k)_{k \in \mathbb{Z}}$ is a sequence of complex numbers, the $N \times N$ Toeplitz matrix $(c(i-j))$ is denoted by $T_N(c)$. If moreover the sequence (c_k) is a positive-definite function $c : \mathbb{Z} \rightarrow \mathbb{C}$ and admits by Herglotz's theorem the representation

$$c_k = \frac{1}{2\pi} \int_{(-\pi, \pi]} e^{-ikx} d\alpha(x),$$

then α is called the symbol of $T_N(c)$ which will sometimes be written $T_N[\alpha]$. If moreover α admits a density with respect to Lebesgue's measure, i.e. $d\alpha(x) = f(x) dx$, $T_N(c)$ will occasionally be denoted by $T_N[f]$. Notice that if $T_N(c)$ is the covariance matrix of a stationary process as in (7) then $f(x)$ (if it exists) is called the spectral density of the process.

Given two complex sequences x_n, y_n we denote

$$(17) \quad x_n \sim y_n \Leftrightarrow \lim_{n \rightarrow \infty} \left(\frac{x_n}{y_n} \right) = 1 \quad \text{and} \quad x_n \doteq y_n \Leftrightarrow \lim_{n \rightarrow \infty} (x_n - y_n) = 0.$$

The notations $x_n = o(1)$ and $x_n = O(1)$ respectively mean $\lim_{n \rightarrow \infty} x_n = 0$ and $\overline{\lim}_{n \rightarrow \infty} |x_n| < \infty$. These notations are also applicable to functions with continuous arguments. If X_n, X are random variables, the notations $X_n = o(1)$ and $X_n = o_P(1)$ respectively mean that $\lim_{n \rightarrow \infty} X_n = 0$ almost surely and in probability. The notations $X_n \xrightarrow{\mathcal{D}} X$ and $X_n \xrightarrow{\mathcal{P}} X$ respectively denote convergence in distribution and in probability. If μ, μ_n are measures, we denote with a slight abuse of notation $\mu_n \xrightarrow{\mathcal{D}} \mu$ for the weak convergence of μ_n to μ .

Given a random variable Y or a sub-algebra \mathcal{G} , we denote by $\mathbb{E}_Y(X)$ and $\mathbb{E}_{\mathcal{G}}(X)$ the conditional expectation of the random variable X with respect to Y and to \mathcal{G} .

We denote by $\mathcal{N}_{\mathbb{R}}(m, \sigma^2)$ the real Gaussian distribution with mean m and variance σ^2 ; we refer to $\mathcal{N}_{\mathbb{R}}(0, 1)$ as the standard real Gaussian distribution. A complex random variable Z is distributed according to the standard complex Gaussian distribution if $Z = U + iV$ where U, V are independent, each with distribution $\mathcal{N}_{\mathbb{R}}(0, 1/2)$. In this case we denote $Z \sim \mathcal{N}_{\mathbb{C}}(0, 1)$. For a symmetric semidefinite positive matrix T , denote by $\mathcal{N}_{\mathbb{R}}(0, T)$ the distribution of a centered Gaussian vector with covariance matrix T .

In the proofs we use C to denote a constant that may take different values from one place to another.

Assumptions. We state our results under one or several of the following assumptions:

A1 (Model setting) Let S_N be $N \times N$ random matrices defined as

$$S_N = \frac{1}{n} \Gamma_N^{\frac{1}{2}} Z_N Z_N^* \Gamma_N^{\frac{1}{2}}$$

where $Z_N = (Z_{i,j}^{(N)})_{1 \leq i \leq N, 1 \leq j \leq n}$ are $N \times n$ matrix whose entries $Z_{i,j}^{(N)}$ are i.d. random variables for all i, j, N , and independent across i, j for each N , satisfying

$$\mathbb{E} Z_{i,j}^{(N)} = 0, \quad \mathbb{E} |Z_{i,j}^{(N)}|^2 = 1 \quad \text{and} \quad \mathbb{E} |Z_{i,j}^{(N)}|^4 < \infty,$$

and Γ_N are $N \times N$ positive semidefinite Hermitian deterministic matrices.

A2 (Asymptotic spectral structure of Γ_N) Given a sequence of $N \times N$ positive semidefinite deterministic matrices Γ_N , the empirical spectral distribution

$$\mu^{\Gamma_N} := \frac{1}{N} \sum_{k=1}^N \delta_{\lambda_k(\Gamma_N)}$$

forms a tight sequence on \mathbb{R}^+ , and the largest eigenvalue $\lambda_{\max}(\Gamma_N)$ tends to ∞ as $N \rightarrow \infty$.

Example 2.1. If $\mu^{\Gamma_N} \xrightarrow{\mathcal{D}} \nu$ with ν a non-compactly supported probability on \mathbb{R}^+ , then **A2** holds.

Example 2.2. Consider $\Gamma_N = \text{diag}(\ell_1^{(n)}, \dots, \ell_m^{(n)}, 1, \dots, 1)$ where $m = m(n)$ is such that $\frac{m(n)}{n} \rightarrow 0$ and where $\ell_i^{(n)} \nearrow \infty$ ($1 \leq i \leq m$), then **A2** holds. The illustrative and simpler case where $\Gamma_N = \text{diag}(\ell_1^{(n)}, 1, \dots, 1)$ will be used hereafter.

A3 (Subarray assumption on Z_N) For each N , $Z_N = Z_{1:N,1:n}$ is the top-left submatrix of an infinite matrix $Z = (Z_{i,j})_{i,j \geq 1}$, with $Z_{i,j}$ i.i.d random variables satisfying

$$\mathbb{E}Z_{i,j} = 0, \quad \mathbb{E}|Z_{i,j}|^2 = 1 \quad \text{and} \quad \mathbb{E}|Z_{i,j}|^4 < \infty.$$

A4 (Spectral gap condition on Γ_N) The two largest eigenvalues $\lambda_{\max}(\Gamma_N)$ and $\lambda_2(\Gamma_N)$ satisfy

$$\overline{\lim}_{N \rightarrow \infty} \frac{\lambda_2(\Gamma_N)}{\lambda_{\max}(\Gamma_N)} < 1.$$

A5 (Block-diagonal structure of Γ_N) For all N , Γ_N is in the form

$$\Gamma_N = \begin{pmatrix} \lambda_{\max}(\Gamma_N) & 0 \\ 0 & \Gamma_{N-1} \end{pmatrix},$$

where Γ_{N-1} is a $(N-1) \times (N-1)$ semidefinite positive Hermitian matrix.

2.2. Main results. We now present the main results of this article. Theorems 2.1 and 2.2 describe the limiting behaviour and fluctuations of $\lambda_{\max}(S_N)$ under generic assumptions. Theorem 2.3 and Corollary 2.4 specialize the previous results to Toeplitz covariance matrices and Gaussian long memory stationary processes.

Theorem 2.1. *Let S_N be a $N \times N$ matrix given by (1) and assume that **A1** and **A2** hold. Then*

$$\frac{\lambda_{\max}(S_N)}{\lambda_{\max}(\Gamma_N)} \xrightarrow[N, n \rightarrow \infty]{\mathcal{P}} 1.$$

*If moreover either the random variables $Z_{ij}^{(N)}$ are standard (real or complex) Gaussian or Assumption **A3** holds, then the above convergence holds almost surely.*

Remark 1 (consistency with the bounded case $\|\Gamma_N\| < \infty$). Consider the simple case where $\Gamma_N = \text{diag}(\ell_1, 1, \dots, 1)$, where $\ell_1 > 1 + \sqrt{r}$ is fixed - see for instance (6). Then it is well known that

$$\lambda_{\max}(S_N) \xrightarrow[N, n \rightarrow \infty]{\mathcal{P}} \ell_1 + \frac{r \ell_1}{\ell_1 - 1},$$

see for instance [10]. Notice in particular that $\frac{\lambda_{\max}(S_N)}{\ell_1} = 1 + \frac{r}{\ell_1 - 1} + o_P(1)$, which is heuristically consistent with Theorem 2.1 if one lets ℓ_1 go to infinity.

Theorem 2.2. *Let S_N be a $N \times N$ matrix given by (1) and assume that **A1**, **A2** and **A4** hold. Assume moreover that one of the following conditions is satisfied:*

- (i) Assumption **A5** holds,
- (ii) The random variables $Z_{ij}^{(N)}$ are standard complex Gaussian,
- (iii) The random variables $Z_{ij}^{(N)}$ are standard real Gaussian and matrices Γ_N are real symmetric.

Consider the quantities

$$(18) \quad \beta_N := \frac{1}{n} \sum_{k=2}^N \frac{\lambda_k(\Gamma_N)}{\lambda_{\max}(\Gamma_N) - \lambda_k(\Gamma_N)} \quad \text{and} \quad F_N := \sqrt{n} \left(\frac{\lambda_{\max}(S_N)}{\lambda_{\max}(\Gamma_N)} - 1 - \beta_N \right).$$

Then

$$(19) \quad F_N \xrightarrow[N, n \rightarrow \infty]{\mathcal{D}} \mathcal{N}_{\mathbb{R}}(0, \sigma^2),$$

where $\sigma^2 = \mathbb{E}|Z_{1,1}^{(1)}|^4 - 1$.

Remark 2. Notice that if $\mathbb{E}|Z_{1,1}^{(1)}|^4 = 1$ then $\sigma^2 = 0$ in the previous theorem, hence $F_N \xrightarrow[N, n \rightarrow \infty]{\mathcal{P}} 0$. Simulation 3 in Section 3.2 (see also Fig. 3(b)) supports this fact.

Remark 3. Under **A2** and **A4**, we have $\beta_N \xrightarrow[N, n \rightarrow \infty]{} 0$. Indeed, by the spectral gap condition **A4** and the fact that $N = O(n)$

$$\beta_N = \frac{1}{n} \sum_{k=2}^N \frac{\lambda_k(\Gamma_N)/\lambda_{\max}(\Gamma_N)}{1 - \lambda_k(\Gamma_N)/\lambda_{\max}(\Gamma_N)} \leq \frac{C}{N} \sum_{k=2}^N \frac{\lambda_k(\Gamma_N)}{\lambda_{\max}(\Gamma_N)}.$$

Since μ^{Γ_N} is tight, for any $\varepsilon \in (0, 1)$ there exists $M > 0$ s.t. $\#\{k, : \lambda_k(\Gamma_N) > M\}/N < \varepsilon$ where $\#\{\cdot\}$ denotes the cardinality of a set. Hence

$$\overline{\lim}_{N, n \rightarrow \infty} \beta_N \leq C \overline{\lim}_N \frac{M}{\lambda_{\max}(\Gamma_N)} + C\varepsilon = C\varepsilon,$$

where we use the fact that $\lambda_{\max}(\Gamma_N) \rightarrow \infty$ as $N \rightarrow \infty$ for the last equality. Notice however that $\sqrt{n}\beta_N$ may not go to zero as $N, n \rightarrow \infty$.

Remark 4 (consistency with the bounded case $\|\Gamma_N\| < \infty$, continued). Consider again the case where $\Gamma_N = \text{diag}(\ell_1, 1, \dots, 1)$ with $\ell_1 > 1 + \sqrt{r}$ then

$$\beta_N = \frac{N-1}{n} \frac{1}{\ell_1 - 1} = \frac{r_N}{\ell_1 - 1} + O\left(\frac{1}{n}\right).$$

In the case where $\ell_1 \rightarrow \infty$, F_N in (18) writes

$$F_N = \sqrt{n} \left(\frac{\lambda_{\max}(S_N)}{\ell_1} - \left(1 + \frac{r_N}{\ell_1 - 1}\right) \right) + O\left(\frac{1}{\sqrt{n}}\right)$$

and has Gaussian fluctuations. This formula is consistent with (6) which can be rewritten

$$\frac{\sqrt{n}}{\sqrt{1 + O(\ell_1^{-2})}} \left(\frac{\lambda_{\max}(S_N)}{\ell_1} - \left(1 + \frac{r_N}{\ell_1 - 1}\right) \right).$$

Example 2.3 (various behaviours of $\sqrt{n}\beta_N$). Consider $\Gamma_N = \text{diag}(\ell_1^{(n)}, 1, \dots, 1)$ where $\ell_1^{(n)} \nearrow \infty$, then

$$\sqrt{n}\beta_N = \sqrt{n} \times \left(\frac{N-1}{n}\right) \times \left(\frac{1}{\ell_1 - 1}\right) \xrightarrow[N, n \rightarrow \infty]{} \begin{cases} \infty & \text{if } \ell_1^{(n)} \ll \sqrt{n}, \\ r/a & \text{if } \ell_1^{(n)} = a\sqrt{n}, \\ 0 & \text{if } \ell_1^{(n)} \gg \sqrt{n}. \end{cases}$$

2.3. Application to large sample covariance matrices associated with long memory processes. In order to apply the above results to Gaussian stationary processes with long memory, we need to verify the spectral gap condition of their autocovariance matrices. We first recall some definitions.

Definition 1 (Regularly/Slowly varying functions). A measurable function $R : \mathbb{R} \rightarrow \mathbb{R}$ is regularly varying at infinity if $R(y) > 0$ for $|y|$ large enough and if there exists a real number ρ s.t. for any $x > 0$,

$$\lim_{y \rightarrow \infty} \frac{R(xy)}{R(y)} = x^\rho.$$

The number ρ is called the index of the regular variation. If $\rho = 0$, then we say that the function (often denoted by L in this case) is slowly varying.

A sequence of real numbers $(c_k)_{k \in \mathbb{Z}}$ is regularly (resp. slowly) varying if $y \mapsto c_{[y]}$ is a regularly (resp. slowly) varying function.

With Definition 1, long memory (long range dependence) stationary processes can be defined as follows.

Definition 2. A stationary process $(\mathcal{X}_t)_{t \in \mathbb{Z}}$ has long memory or long range dependence if its autocovariance function γ is regularly varying with index $\rho \in (-1, 0)$.

Remark 5. Notice that this definition is compatible with the definition of the autocovariance function provided in (10). In fact, assume that $\gamma(h)$ is given by (10) then it is regularly varying with index $\rho = 2d - 1 \in (-1, 0)$. Conversely, assume that $\gamma(h)$ is an even regularly varying sequence with $\rho \in (-1, 0)$. Set $d = \frac{\rho+1}{2}$, then $L(y) = \gamma(|y|)(1 + |y|)^{1-2d}$ is a slowly varying function with $d \in (0, 1/2)$ and

$$\gamma(h) = \frac{L(h)}{(1 + |h|)^{1-2d}}.$$

Remark 6. Notice that definitions 1 and 2 enable to consider complex processes (\mathcal{X}_t) , however the associated autocovariance function is necessarily real and cannot be complex.

Remark 7. The above definition coincides with Condition II in [33] where the autocovariance function γ satisfies (10).

In this context, the spectral gap condition on autocovariance matrices of a long memory stationary process is ensured by the following theorem:

Theorem 2.3. *Suppose that $c = (c_h)_{h \in \mathbb{Z}}$ is an even ($c_h = c_{-h}$ for all $h \in \mathbb{Z}$) regularly varying sequence of index $\rho \in (-1, 0)$, then for any fixed $k \geq 1$ the limit*

$$a_k^{(\rho)} = \lim_{N \rightarrow \infty} \frac{\lambda_k(T_N(c))}{Nc_N}$$

exists and is finite. Moreover, $a_1^{(\rho)} > a_2^{(\rho)} \geq 0$. In particular,

$$\lambda_{\max}(T_N(c)) \sim a_1^{(\rho)} Nc_N \rightarrow \infty \quad \text{and} \quad \lim_{N \rightarrow \infty} \frac{\lambda_2(T_N(c))}{\lambda_{\max}(T_N(c))} = \frac{a_2^{(\rho)}}{a_1^{(\rho)}} < 1.$$

Definition 3. We say that a complex Gaussian process $(\mathcal{X}_t)_{t \in \mathbb{Z}}$ is circularly symmetric if for any $N \in \mathbb{N}$ the Gaussian vector $\mathcal{X}_{1:N} := (\mathcal{X}_1, \dots, \mathcal{X}_N)^\top$ is circularly symmetric, i.e. for any $\phi \in \mathbb{R}$, the vector $e^{i\phi} \mathcal{X}_{1:N}$ has the same distribution as $\mathcal{X}_{1:N}$.

Remark 8. Notice in particular that such a process is centered and satisfies that $\mathbb{E} \mathcal{X}_{1:N} \mathcal{X}_{1:N}^\top = 0$, for all $N \geq 1$.

As a canonical example, a standard complex Gaussian vector $X = (X_1, \dots, X_N)^\top$ where the X_i 's are i.i.d. and $\mathcal{N}_{\mathbb{C}}(0, 1)$ -distributed is circularly symmetric with

$$\mathbb{E} X X^* = I_N \quad \text{and} \quad \mathbb{E} X X^\top = 0.$$

For such a vector X , we will denote $X \sim \mathcal{N}_{\mathbb{C}}(0, I_N)$.

As a by-product of the above theorems, we have the following result on the largest eigenvalue of sample covariance matrices of a Gaussian long memory stationary process (recall that such a process admits a real autocovariance function).

Corollary 2.4. *Suppose that $(\mathcal{X}_t)_{t \in \mathbb{Z}}$ is a real centered (resp. complex circularly symmetric) Gaussian stationary process with long range dependence in the sense of definition 2. Let*

$$Q_N = \frac{1}{n} X_N X_N^*$$

where X_N are $N \times n$ random matrices whose columns are i.i.d copies of the random vector $\mathcal{X}_{1:N} = (\mathcal{X}_1, \dots, \mathcal{X}_N)^\top$. Then

$$(20) \quad \frac{\lambda_{\max}(Q_N)}{\lambda_{\max}(T_N)} \xrightarrow[N, n \rightarrow \infty]{a.s.} 1$$

and

$$(21) \quad \sqrt{n} \left(\frac{\lambda_{\max}(Q_N)}{\lambda_{\max}(T_N)} - 1 - \frac{1}{n} \sum_{k=2}^N \frac{\lambda_k(T_N)}{\lambda_{\max}(T_N) - \lambda_k(T_N)} \right) \xrightarrow[N, n \rightarrow \infty]{\mathcal{D}} \mathcal{N}_{\mathbb{R}}(0, \sigma^2),$$

where $T_N = T_N(\gamma)$ is the autocovariance matrix of the process defined in (7) and where

$$\sigma^2 = \frac{\mathbb{E} |\mathcal{X}_1^4|}{\gamma^2(0)} - 1 = \begin{cases} 2 & \text{if } \mathcal{X}_1 \text{ is real} \\ 1 & \text{if } \mathcal{X}_1 \text{ is complex} \end{cases}.$$

Corollary 2.4 being an easy consequence of Theorems 2.1, 2.2 and 2.3, we provide its proof hereafter.

Proof. Let X be a centered N -dimensional random vector either real or circularly symmetric complex gaussian with (real) covariance matrix T . Then X writes $X = T^{1/2}Z$ where $Z \sim \mathcal{N}_{\mathbb{R}}(0, I_N)$ or $\mathcal{N}_{\mathbb{C}}(0, I_N)$ depending on whether X is real or complex. In fact, if T is invertible then $Z = T^{-1/2}X$ has the required properties.

If not, $T = O \operatorname{diag}(d_1^2, \dots, d_p^2, 0 \dots) O^\top$ with O orthogonal and $d_i > 0$. Let $Y = (0, \dots, 0, Y_{p+1}, \dots, Y_N)^\top$ with Y_k i.i.d. standard Gaussian random variables, either real or complex (depending on X), and independent from X . Let

$$Z = O \operatorname{diag}(d_1^{-1}, \dots, d_p^{-1}, 0 \dots) O^\top X + OY$$

then $\operatorname{Cov}(Z) = I_N$ and if X is complex, then $\mathbb{E}ZZ^\top = 0$. In particular, Z is a standard gaussian random vector and a covariance computation yields

$$\operatorname{Cov}(X - T^{1/2}Z) = 0,$$

which implies that $X = T^{1/2}Z$ almost surely.

Then for any N and almost surely, the representation $Q_N = \frac{1}{n} T_N^{1/2} Z_N Z_N^* T_N^{1/2}$ holds with (T_N) the autocovariance matrices of process $(\mathcal{X}_t)_{t \in \mathbb{Z}}$. In Section 1 we have noticed that μ^{T_N} converges weakly, and by Theorem 2.3, $\lambda_{\max}(T_N) \rightarrow \infty$ and (T_N) satisfy the spectral gap condition. By Theorems 2.1 and 2.2, the results follow. \square

3. ADDITIONAL APPLICATIONS AND SIMULATIONS

3.1. Additional applications to Gaussian stationary processes. Although Definition 2 is a common definition of long memory, it can seem restrictive as it requires that the autocovariance function has at most a finite number of nonpositive values. In the first example hereafter we consider Gaussian processes with autocovariance functions either complex or with alternate signs. In the two subsequent examples, we relate our results with other definitions of long memory, via linear representation or via the autocovariance density.

Covariance matrices with alternating signs of entries. Let $(\mathcal{X}_t)_{t \in \mathbb{Z}}$ be a centered Gaussian stationary process with autocovariance function $\gamma^\mathcal{X}$. Let $\theta \in (-\pi, \pi]$, $\theta \neq 0$ be fixed and consider the process $(\mathcal{Y}_t = e^{it\theta} \mathcal{X}_t)_{t \in \mathbb{Z}}$. This process is a Gaussian stationary process with autocovariance function $\gamma^\mathcal{Y}(t) = e^{it\theta} \gamma^\mathcal{X}(t)$ and

$$\mathcal{Y}_{1:N} = \Sigma^\theta \mathcal{X}_{1:N}$$

where $\Sigma^\theta = \operatorname{diag}(e^{ik\theta}, 1 \leq k \leq N)$ is a unitary matrix. Notice that if (\mathcal{X}_t) is complex circularly symmetric, then so is (\mathcal{Y}_t) but if (\mathcal{X}_t) is real then (\mathcal{Y}_t) is either complex Gaussian but not circularly symmetric if $\theta \neq \pi$ or real Gaussian with alternate signs if $\theta = \pi$.

Let $X_N^\mathcal{X}$ (resp. $X_N^\mathcal{Y}$) a $N \times n$ matrix whose columns are i.i.d. copies of the vector $\mathcal{X}_{1:N}$ (resp. $\mathcal{Y}_{1:N}$) and assume that the process (\mathcal{X}_t) fulfills the assumptions of Corollary 2.4. Then

$$Q_N^\mathcal{Y} = \frac{1}{n} X_N^\mathcal{Y} (X_N^\mathcal{Y})^* = \frac{1}{n} \Sigma^\theta X_N^\mathcal{X} (X_N^\mathcal{X})^* (\Sigma^\theta)^* = \Sigma^\theta Q_N^\mathcal{X} (\Sigma^\theta)^* \quad \text{where} \quad Q_N^\mathcal{X} = \frac{1}{n} X_N^\mathcal{X} (X_N^\mathcal{X})^*.$$

In particular, $\lambda_{\max}(Q_N^\mathcal{Y}) = \lambda_{\max}(Q_N^\mathcal{X})$ satisfies (20) and (21). In this example the positivity constraint of the autocovariance function is relaxed.

Linear processes with long memory. If the process $(\mathcal{X}_t)_{t \in \mathbb{Z}}$ has a linear representation

$$\mathcal{X}_t = \sum_{j=0}^{\infty} \psi_j \epsilon_{t-j}$$

where $(\epsilon_t)_{t \in \mathbb{Z}}$ is a sequence of i.i.d real valued standard Gaussian r.v.'s and $\psi_j \sim j^{d-1} L(j)$ as $j \rightarrow \infty$ with $d \in (0, 1/2)$ and L a slowly varying function at ∞ , then it is well known (c.f. for example [33,

Corollary 2.2.10]) that its autocovariance function γ is regularly varying with index $\rho = 2d - 1$, and more precisely we have

$$\gamma(h) \sim h^{2d-1} L^2(h) B(1-2d, d)$$

where $B(1-2d, d) = \int_0^1 x^{-2d} (1-x)^{d-1} dx$ is the beta-function. Corollary 2.4 can be applied in this case.

Long range dependence defined through spectral density. Among the various definitions of long range dependence, there is an important one which defines the long range dependence through the spectral density, that is, if the symbol of the autocovariance matrices T_N has a density $f : (-\pi, \pi] \rightarrow \mathbb{R}^+$ satisfying

$$(22) \quad f(x) = |x|^{-2d} L \left(\frac{1}{|x|} \right), \quad x \in (-\pi, 0) \cup (0, \pi],$$

with $d \in (0, 1/2)$, and L a slowly varying function defined on $[1/\pi, +\infty)$. (cf. Condition IV in [33]). If a (real centered or complex circularly) Gaussian stationary process $(\mathcal{X}_t)_{t \in \mathbb{Z}}$ has long memory in this sense, then the LSD of the covariance matrices $T_N[f]$ is not compactly supported and in particular $\lambda_{\max}(T_N[f]) \rightarrow \infty$ and (20) in Corollary 2.4 holds. Moreover if L in (22) is quasi-monotone, then the process is also a long memory process in the sense of Definition 2 (see for instance [33, Corollary 2.2.17]) with index $\rho = 2d - 1$. More precisely we have

$$\gamma(h) \sim 2h^{2d-1} L(h) \Gamma(1-2d) \sin(d\pi) \text{ as } h \rightarrow \infty$$

where $\Gamma(t) := \int_0^\infty x^{t-1} e^{-x} dx$ denotes the gamma-function. Hence by Theorem 2.3, T_N satisfies the spectral gap condition, and applying Theorem 2.2 we get the same result as Corollary 2.4.

3.2. Numerical simulations.

Simulation 1: Limiting behaviour of $\lambda_{\max}(S_N)$. To illustrate Theorem 2.1, we take

$$S_N = \frac{1}{n} \Gamma_N^{\frac{1}{2}} Z_N Z_N^\top \Gamma_N^{\frac{1}{2}}$$

with Z_N a $N \times n$ matrix having i.i.d standard real Gaussian entries, and $\Gamma_N = T_N(\gamma)$ is the Toeplitz matrix determined by $\gamma(h) = \frac{1}{(1+|h|)^{3/4}}$. Let N take all the values in the finite sequence $\{100, 150, 200, \dots, 3000\}$, and let $n = \lfloor 5N/4 \rfloor$. We plot the simulation results in Figure ??.

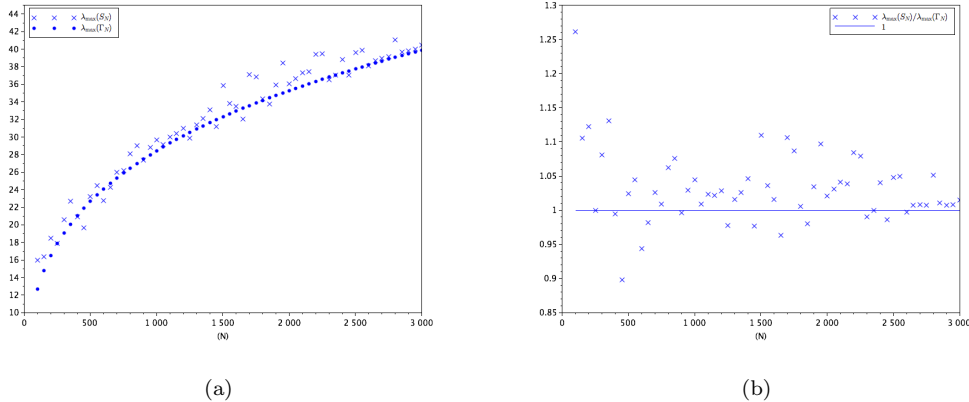


FIGURE 1. Convergence of $\lambda_{\max}(S_N)/\lambda_{\max}(\Gamma_N)$ to 1. In 1(a), the values $\lambda_{\max}(S_N)$ and $\lambda_{\max}(\Gamma_N)$ are plotted as crosses and solid points respectively; in 1(b) the values of the ratio $\lambda_{\max}(S_N)/\lambda_{\max}(\Gamma_N)$ are plotted as crosses, compared with the constant 1.

Simulation 2: Fluctuations of $\lambda_{\max}(S_N)$. To illustrate the fluctuations of $\lambda_{\max}(S_N)$, we fix $N = 1000$ and $n = 1250$ and let $\Gamma_N = \text{diag}(\lambda_k(T_{1000}(\gamma)))$ with γ as in the previous simulation. We take 900 independent samples of S_{1000} , plot the histogram of F_{1000} defined in (18) and compare with the density of the theoretical limiting law. In Figure 2(a) we simulate the model S_{1000} with Z_{1000} having i.i.d. real Gaussian entries, the limiting law, according to Theorem 2.2, is $\mathcal{N}_{\mathbb{R}}(0, 2)$; while in Figure 2(b), Z_{1000} has i.i.d. standardized exponential entries, i.e. $Z_{i,j}^{(1000)} \sim \mathcal{E}(1) - 1$. The limiting law is $\mathcal{N}_{\mathbb{R}}(0, 8)$.

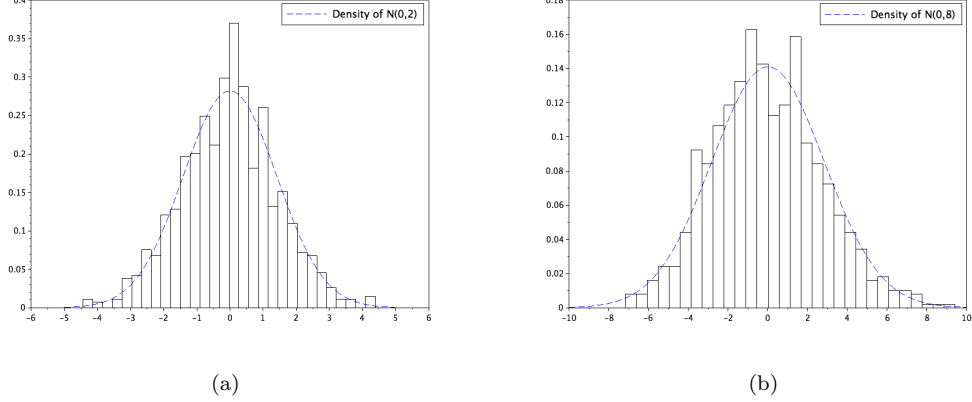


FIGURE 2. Fluctuations of $\lambda_{\max}(S_{1000})$, with Z_{1000} having Gaussian entries in 2(a) and standardized exponential entries in 2(b). Simulation with 900 samples.

Simulation 3: Concentration. We now address the case $\mathbb{E}|Z_{1,1}^{(N)}|^4 = 1$. Consider a matrix Z_N with i.i.d. symmetric Bernoulli variables taking values in $\{-1, 1\}$. As previously we take $\Gamma_N = \text{diag}(\lambda_k(T_N(\gamma)))$ with $\gamma(h) = \frac{1}{(1+|h|)^{3/4}}$. In this case, Theorem 2.2 asserts that

$$\sqrt{n} \left(\frac{\lambda_{\max}(S_N)}{\lambda_{\max}(\Gamma_N)} - 1 - \frac{1}{n} \sum_{k=2}^N \frac{\lambda_k(\Gamma_N)}{\lambda_{\max}(\Gamma_N) - \lambda_k(\Gamma_N)} \right) \xrightarrow[N, n \rightarrow \infty]{\mathcal{P}} 0.$$

In Figure 3(a) we plot the fluctuations of $\lambda_{\max}(S_{1000})$ with $n = 1250$ and notice that the corresponding F_{1000} are far more concentrated around 0 than the previous simulations, as predicted by the theorem.

An interesting phenomenon occurs in Figure 3(b), where the same matrix Z_{1000} is considered while we do not diagonalize Γ_{1000} and just take $\Gamma_{1000} = T_{1000}(\gamma)$. In this case, the concentration phenomenon disappears, and the obtained histogram is very close to that in Figure 2(a). This simulation suggests that some universality holds in the fluctuations of $\lambda_{\max}(S_N)$ if the (Γ_N) 's are Toeplitz matrices. This will be explored in a forthcoming work.

3.3. Open questions.

At the border between long memory and short memory. An interesting regime is when $\rho = -1$. In this case, the autocovariance function $\gamma(h) = (1 + |h|)^{-1}L(h)$ can be summable or not depending on the slowly varying function L . For example if $L(h) = \log^{-1-\varepsilon}(2 + |h|)$ with $\varepsilon > 0$ then γ is absolutely summable and the process has short memory. If $L(\cdot) = 1$ then one can prove that $\lambda_{\max}(T_N(\gamma)) = O(\log N)$, and that the spectral gap condition no longer holds. In this case, the asymptotics (20) remains true as Theorem 2.1 does not rely on the spectral gap condition but only on the condition $\lambda_{\max}(T_N(\gamma)) \rightarrow \infty$. The question whether the fluctuations (21) together with their normalization and the limiting distribution hold remains open.

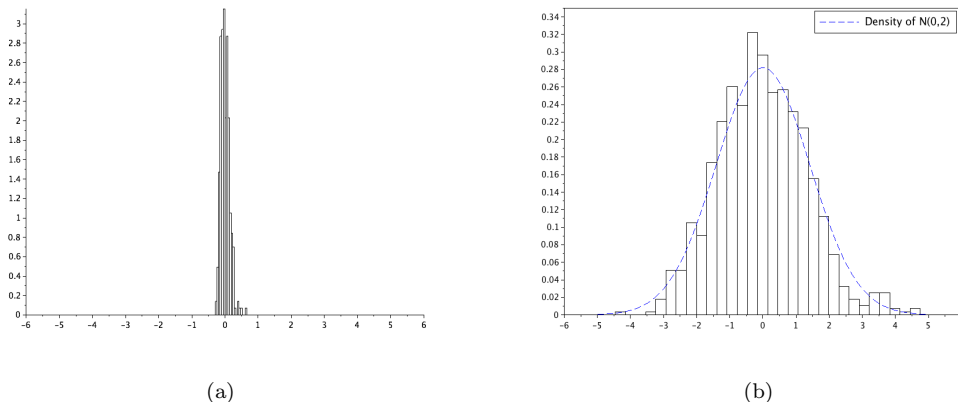


FIGURE 3. Fluctuations of $\lambda_{\max}(S_N)$ in the case of symmetric Bernoulli entries. Γ_N is diagonal in 3(a) and nondiagonal in 3(b).

Non-Gaussian long memory stationary processes. A Gaussian long memory stationary process admits a linear representation $\mathcal{X}_{1:N} = T_N(\gamma)Z_{1:N}$, where $T_N(\gamma)$ is a hermitian Toeplitz matrix and $Z_{1:N}$ is a standard Gaussian vector. This representation is key in the analysis of the top eigenvalue of the corresponding large covariance matrix of samples of the process but does not hold anymore if the process is not Gaussian. The question whether it is possible to perform the same eigenvalue analysis in the case of non-Gaussian long memory stationary process is open.

Correlation structure of the top eigenvalues. Beyond the top eigenvalue $\lambda_{\max}(S_N)$, it would be interesting to understand the asymptotic correlation structure and the fluctuations of the (many) largest eigenvalues $(\lambda_{\max}(S_N), \lambda_2(S_N), \dots, \lambda_k(S_N))$ for a fixed $k \geq 1$.

Behaviour of the eigenvectors associated to the top eigenvalues. For bounded spiked models (by bounded we mean $\sup_N \|\Gamma_N\| < \infty$) the structure of the eigenvectors associated to the top eigenvalues has been studied and carries interesting information, see for example [13]. A similar study would be interesting in the general context of unbounded population covariance matrices where $\lambda_{\max}(\Gamma_N) \rightarrow \infty$ and of (Gaussian) long memory stationary processes. In this latter case, one needs to have a good understanding of the Toeplitz matrix' $T_N(\gamma)$ eigenvectors.

Universality for non-Gaussian linear stationary processes with long memory. In the case where Γ_N is required to be (block-)diagonal, the variance of the limiting distribution depends on the fourth moment of the entries $Z_{i,j}^N$ and may be equal to zero if $\mathbb{E}|Z_{1,1}^{(1)}|^4 = 1$. However when Γ_N is a Toeplitz matrix (7) with γ satisfying (10), this dependence is weakened and Simulation 3 in Section 3.2 strongly suggests that some universality occurs depending on the population covariance matrix Γ_N , see in particular Figures 3(a) and 3(b). This question will be addressed in a forthcoming work.

4. PROOFS OF THEOREM 2.1 AND THEOREM 2.2

4.1. A short reminder of results related to large covariance matrices. Given a probability measure μ on \mathbb{R} , define its Cauchy-Stieltjes transform as

$$m_\mu(z) := \int \frac{d\mu(s)}{z-s}, \quad \forall z \in \mathbb{C}^+ := \{z \in \mathbb{C} : \Im z > 0\}$$

Notice that $m_\mu(z)$ is the opposite of the Stieltjes transform $g_\mu(z) = \int \frac{d\mu(s)}{s-z}$.

For a random matrix S_N given by (1), we will often consider its companion matrix

$$(23) \quad \underline{S}_N = \frac{1}{n} Z_N^* \Gamma_N Z_N,$$

which shares the same non-zero eigenvalues with S_N . In particular, $\lambda_{\max}(\underline{S}_N) = \lambda_{\max}(S_N)$. Recall that $r_N := \frac{N}{n}$ and let $\mu^{S_N}, \mu^{\underline{S}_N}$ be the ESD of S_N and \underline{S}_N respectively, then the following relation holds:

$$(24) \quad \mu^{\underline{S}_N} = (1 - r_N)\delta_0 + r_N\mu^{S_N}.$$

Limiting spectral distribution. We recall results from [34, Theorem 1.1]. For any probability ν in \mathbb{R}^+ and any $r \in (0, +\infty)$, there exists a unique probability measure $\mu = \mu(r, \nu)$ whose Cauchy-Stieltjes transform m_μ satisfies the equation:

$$m_\mu(z) = \int \frac{d\nu(s)}{z - s(1 - r + rzm_\mu(z))} \quad \text{for any } z \in \mathbb{C}^+.$$

If the probability measure ν is the ESD μ^A associated with a matrix A , we simply write $\mu = \mu(r, A)$ instead of $\mu = \mu(r, \mu^A)$. Similarly, there exists a unique probability measure $\underline{\mu} = \underline{\mu}(r, \nu)$ with Cauchy-Stieltjes transform $m_{\underline{\mu}}$ satisfying

$$(25) \quad z = \frac{1}{m_{\underline{\mu}}(z)} + r \int \frac{s d\nu(s)}{1 - sm_{\underline{\mu}}(z)} \quad \text{for any } z \in \mathbb{C}^+.$$

As previously, we will write $\underline{\mu}(r, A)$ instead of $\underline{\mu}(r, \mu^A)$. If moreover $\mu^{\Gamma_N} \xrightarrow[N \rightarrow \infty]{\mathcal{D}} \nu$, then

$$(26) \quad \mu^{S_N} \xrightarrow[N, n \rightarrow \infty]{\mathcal{D}} \mu \quad \text{a.s.} \quad \text{and} \quad \mu^{\underline{S}_N} \xrightarrow[N, n \rightarrow \infty]{\mathcal{D}} \underline{\mu} \quad \text{a.s.}$$

Spectrum confinement. By "spectrum confinement", we refer to the phenomenon where the empirical spectrum of the eigenvalues "concentrates" near the support of the limiting spectral distribution. In the specific case of model (1) under assumption $\sup_N \|\Gamma_N\| < \infty$ and the convergence (26), spectrum confinement can be roughly expressed (in the absence of spikes) as: for every $\varepsilon > 0$, almost surely,

$$\text{supp}(\mu^{S_N}) \subset \text{supp}(\mu) + (-\varepsilon, \varepsilon)$$

for N large enough.

A more accurate description of spectrum confinement relies on the deterministic equivalent of $\mu^{\underline{S}_N}$ defined as $\underline{\mu}_N := \underline{\mu}(r_N, \Gamma_N)$ (cf. (25) with $\nu = \mu^{\Gamma_N}$). Assume that **A3** holds. By [1, Theorem 1.1], if there exists $\varepsilon > 0$ and an interval $[a, b]$ such that

$$[a, b] \cap \left(\text{supp}(\underline{\mu}_N) + (-\varepsilon, \varepsilon) \right) = \emptyset$$

for N large enough, then almost surely

$$(27) \quad \text{supp}(\mu^{\underline{S}_N}) \cap [a, b] = \emptyset$$

for N large enough. In particular, if $a > 0$ there is no eigenvalue of S_N in $[a, b]$ for N large enough.

The description of the support of a probability distribution defined via a fixed-point equation (25) is given in [36, Theorems 4.1 and 4.2]. Based on these results, we now state a necessary and sufficient condition for which a real number x lies outside the support of $\underline{\mu}_N = \underline{\mu}(r_N, \Gamma_N)$. Let

$$(28) \quad B_N := \{y \in \mathbb{R} : y \neq 0, y^{-1} \neq \lambda_k(\Gamma_N), \forall k = 1, \dots, N\},$$

and define

$$(29) \quad x_N(y) := \frac{1}{y} + r_N \int \frac{s d\mu^{\Gamma_N}(s)}{1 - sy} \quad \text{for } y \in B_N.$$

A real number $x \in \mathbb{R}$ lies outside the support of $\underline{\mu}_N$ if and only if

$$\exists y \in B_N, \quad x = x_N(y) \quad \text{and} \quad x'_N(y) = -\frac{1}{y^2} + r_N \int \frac{s^2 d\mu^{\Gamma_N}(s)}{(1 - sy)^2} < 0.$$

Exact separation. Let $[a, b]$ be an interval eventually outside the support of $\underline{\mu}_N = \underline{\mu}(r_N, \Gamma_N)$, assume that $\mu^{\Gamma_N} \rightarrow \nu$ and let $\underline{\mu} = \underline{\mu}(r, \nu)$. "Exact separation" is a phenomenon that expresses the fact that (almost surely and eventually) the interval $[a, b]$ separates the empirical eigenvalues of matrix S_N exactly in the same proportions as $[1/m_{\underline{\mu}}(a), 1/m_{\underline{\mu}}(b)]$ separates those of matrix Γ_N .

This expression has been coined in the article [2] by Bai and Silverstein, from which we recall the result of interest to us, that is mainly [2, Theorem 1.2(2)]: Assume in addition to the assumptions of [1, Theorem 1.1] (and in particular to assumption **A3**) that the conditions $m_{\underline{\mu}}(b) > 0$ and $r(1 - \nu(\{0\})) \leq 1$ hold. For N large enough, let i_N be an integer such that

$$\lambda_{i_N}(\Gamma_N) > \frac{1}{m_{\underline{\mu}}(b)} \quad \text{and} \quad \lambda_{i_N+1}(\Gamma_N) < \frac{1}{m_{\underline{\mu}}(a)}.$$

Then almost surely, $\lambda_{i_N}(S_N) > b$ and $\lambda_{i_N+1}(S_N) < a$ for N large enough. This result will be used in the particular case where $\nu = \delta_0$. In this case, $m_{\underline{\mu}}(x) = \frac{1}{x}$ and $r(1 - \delta_0(0)) = 0$.

4.2. Reduction to the bounded model. When studying $\lambda_{\max}(S_N)$ under **A2**, the main difficulty is to handle the unboundedness of $\lambda_{\max}(\Gamma_N)$. In order to circumvent this issue, we define

$$\tilde{S}_N = \frac{1}{n} \tilde{\Gamma}_N^{1/2} Z_N Z_N^* \tilde{\Gamma}_N^{1/2} \quad \text{where} \quad \tilde{\Gamma}_N := \frac{\Gamma_N}{\lambda_{\max}(\Gamma_N)}.$$

In particular, notice that $\lambda_{\max}(\tilde{S}_N) = \frac{\lambda_{\max}(S_N)}{\lambda_{\max}(\Gamma_N)}$. Thus, in order to establish the results stated in Theorems 2.1 and 2.2, we only need to prove the corresponding results for \tilde{S}_N .

Using the definition of $\tilde{\Gamma}_N$, the tightness of (μ^{Γ_N}) and the fact that $\lambda_{\max}(\Gamma_N) \rightarrow \infty$, we immediately deduce the following properties for $\tilde{\Gamma}_N$:

$$\lambda_{\max}(\tilde{\Gamma}_N) = 1 \quad \text{and} \quad \mu^{\tilde{\Gamma}_N} \xrightarrow[N \rightarrow \infty]{\mathcal{D}} \delta_0.$$

In particular, the spectral norm of $\tilde{\Gamma}_N$ is bounded and many classical results, for instance those of Bai and Silverstein [34, 1] can be applied to \tilde{S}_N . Considering this fact, we state and prove below Theorems 4.1 and 4.2 which are the counterparts of Theorems 2.1 and 2.2.

A2(b) Given a sequence of $N \times N$ positive semidefinite deterministic matrices Γ_N , the following properties hold:

$$\lambda_{\max}(\Gamma_N) = 1 \quad \forall N \geq 1 \quad \text{and} \quad \mu^{\Gamma_N} \xrightarrow[N \rightarrow \infty]{\mathcal{D}} \delta_0.$$

Theorem 4.1. *Let S_N be a $N \times N$ matrix given by (1) and assume that **A1** and **A2(b)** hold. Then*

$$(30) \quad \lambda_{\max}(S_N) \xrightarrow[N, n \rightarrow \infty]{\mathcal{P}} 1.$$

*If moreover either the random variables $Z_{ij}^{(N)}$ are standard (real or complex) Gaussian or Assumption **A3** holds, then the above convergence holds almost surely.*

Theorem 4.2. *Let S_N be a $N \times N$ matrix given by (1) and assume that **A1**, **A2(b)** and **A4** hold. Assume moreover that one of the following conditions is satisfied:*

- (i) Assumption **A5** holds,
- (ii) The random variables $Z_{ij}^{(N)}$ are standard complex Gaussian,
- (iii) The random variables $Z_{ij}^{(N)}$ are standard real Gaussian and matrices Γ_N are real symmetric,

then

$$(31) \quad \sqrt{n} \left(\lambda_{\max}(S_N) - 1 - \frac{1}{n} \sum_{k=2}^N \frac{\lambda_k(\Gamma_N)}{1 - \lambda_k(\Gamma_N)} \right) \xrightarrow[N, n \rightarrow \infty]{\mathcal{D}} \mathcal{N}_{\mathbb{R}}(0, \sigma^2),$$

where $\sigma^2 = \mathbb{E}|Z_{1,1}^{(1)}|^4 - 1$.

In order to prove Theorem 2.1 and 2.2, we only need to apply the above theorems to \tilde{S}_N .

4.3. Proof of Theorem 4.1. We first prove the theorem under assumption **A3**. We first establish that

$$(32) \quad \overline{\lim}_{N,n \rightarrow \infty} \lambda_{\max}(\underline{S}_N) \leq 1 \quad \text{a.s.}$$

Recall the definition of the set B_N in (28). Due to the spectrum confinement property (27), we only need to prove that for any $\varepsilon > 0$, the interval $[1 + \varepsilon, +\infty)$ eventually stays outside the support of $\underline{\mu}_N = \underline{\mu}(r_N, \Gamma_N)$. Relying on the characterization of a point x outside $\text{supp}(\underline{\mu}_N)$, this will be the consequence of the following property

$$\forall x \in [1 + \varepsilon, \infty), \quad \exists y \in B_N, \quad x = x_N(y) \quad \text{and} \quad x'_N(y) < 0$$

that we now prove.

Since $\lambda_{\max}(\Gamma_N) = 1$ under **A2(b)**, notice that $(0, 1) \subset B_N$. Consider a real number η such that

$$\eta \in \left(\frac{1}{1 + \varepsilon}, 1 \right).$$

For $s \leq 1$, we have $|1 - s\eta| \geq 1 - \eta > 0$, therefore by the definition (29) of x_N , and by the fact that $\mu^{\Gamma_N} \xrightarrow[N \rightarrow \infty]{} \delta_0$, we have

$$x_N(\eta) \xrightarrow[N,n \rightarrow \infty]{} \frac{1}{\eta} < 1 + \varepsilon \quad \text{and} \quad x'_N(\eta) \xrightarrow[N,n \rightarrow \infty]{} -\frac{1}{\eta^2} < 0.$$

So for N large enough, we have $x_N(\eta) < 1 + \varepsilon$, and $x'_N(\eta) < 0$. For such N 's, note that x_N is continuous on $(0, \eta)$ and that $x_N(y) \rightarrow +\infty$ as $y \rightarrow 0^+$. We have proved so far that $[1 + \varepsilon, \infty) \subset x_N((0, \eta))$. Notice finally that x'_N is increasing on $(0, \eta)$, in particular $x'_N(y) \leq x'_N(\eta) < 0$ for all $y \in (0, \eta)$. Therefore $x_N((0, \eta))$ and thus $[1 + \varepsilon, \infty)$ eventually lie outside the support of $\underline{\mu}_N$. Equation (32) is established.

We now prove that

$$(33) \quad \underline{\lim}_{N,n \rightarrow \infty} \lambda_{\max}(\underline{S}_N) \geq 1, \quad \text{a.s.}$$

by an exact separation argument.

As $\underline{\mu} = \delta_0$, we have $1/m_{\underline{\mu}}(a) = a$, $1/m_{\underline{\mu}}(b) = b$ for any $a, b > 0$. We intend to find some constant interval of the form $[a, 1 - \varepsilon]$, for small $\varepsilon > 0$ which separates the eigenvalues of matrix Γ_N into two non-empty parts. This is not always possible because even if $\lambda_{\max}(\Gamma_N) = 1$ and $\mu^{\Gamma_N} \rightarrow \delta_0$, there might be some intermediate eigenvalues among the $(\lambda_i(\Gamma_N))$'s for $i \geq 2$ eventually lying in $(0, 1)$. In order to circumvent this issue, we introduce the auxiliary matrices

$$\hat{\underline{S}}_N := \frac{1}{n} Z_N^* \Theta_N Z_N \quad \text{and} \quad \hat{S}_N := \frac{1}{n} \Theta_N^{\frac{1}{2}} Z_N Z_N^* \Theta_N^{\frac{1}{2}},$$

where Θ_N is obtained from the spectral decomposition of Γ_N as:

$$\Theta_N := U_N \text{diag}(1, 0, \dots) U_N^* \quad \text{where} \quad \Gamma_N = U_N \text{diag}(1, \lambda_2(\Gamma_N), \dots) U_N^*.$$

Using [36, Theorems 4.1 and 4.2], we conclude that for any $0 < \varepsilon < 1/2$, the interval $[\varepsilon, 1 - \varepsilon]$ is eventually outside the support of probability $\underline{\mu}(r_N, \Theta_N)$, obtained from (25) with parameters r_N and Θ_N . Notice in particular that

$$\lambda_{\max}(\Theta_N) = 1 \quad \text{and} \quad \lambda_i(\Theta_N) = 0 \quad \text{for} \quad i = 2 : N.$$

Applying [2, Theorem 1.2] to $\hat{\underline{S}}_N$ with separating interval $[\varepsilon, 1 - \varepsilon]$ for arbitrary $\varepsilon \in (0, 1/2)$, we conclude that almost surely, $\lambda_{\max}(\hat{\underline{S}}_N) > 1 - \varepsilon$ for N large enough. We have proved so far that

$$\underline{\lim}_{N,n \rightarrow \infty} \lambda_{\max}(\hat{\underline{S}}_N) \geq 1$$

almost surely. Now, since

$$\underline{S}_N - \hat{\underline{S}}_N = \frac{1}{n} Z_N^* U_N \text{diag}(0, \lambda_2(\underline{S}_N), \dots, \lambda_N(\underline{S}_N)) U_N^* Z_N$$

is nonnegative definite, we have $\underline{\lim}_{N,n \rightarrow \infty} \lambda_{\max}(\underline{S}_N) \geq \underline{\lim}_{N,n \rightarrow \infty} \lambda_{\max}(\hat{\underline{S}}_N) \geq 1$. Therefore Theorem 4.1 with assumption **A3** is proved.

As a byproduct of the above proof, we can easily prove $\lambda_{\max}(S_N) \xrightarrow{\mathcal{P}} 1$ without imposing **A3**. Suppose that $S_N = \frac{1}{n}\Gamma_N^{1/2}Z_N Z_N^* \Gamma_N^{1/2}$ satisfies **A1** and **A2(b)** and construct $\check{Z} = (\check{Z}_{i,j})_{i,j \geq 1}$ with $\check{Z}_{i,j}$ i.i.d random variables identically distributed as the entries of Z_N . Let $S'_N = \frac{1}{n}\Gamma_N^{1/2}Z'_N Z'^*_N \Gamma_N^{1/2}$ with Z'_N the top-left $N \times n$ submatrix of \check{Z} . Then according to the above proof, $\lambda_{\max}(S'_N)$ converges to 1 almost surely, hence in probability. Since $\lambda_{\max}(S_N)$ and $\lambda_{\max}(S'_N)$ have the same distribution, we have also $\lambda_{\max}(S_N) \xrightarrow{\mathcal{P}} 1$.

Finally, we prove that if the entries $Z_{i,j}^{(N)}$ are i.d standard Gaussian variables, and i.i.d for all $1 \leq i, j \leq N$, the convergence (30) holds almost surely without the need of assumption **A3**. This mainly relies on a concentration argument. Recall that we already have $\lambda_{\max}(S_N) \xrightarrow{\mathcal{P}} 1$. Using [16, Theorem 5.6], we prove the following concentration inequality: for all $N \geq 1$ and all $\varepsilon > 0$,

$$(34) \quad \mathbb{P}(|\sqrt{\lambda_{\max}(S_N)} - \mathbb{E}\sqrt{\lambda_{\max}(S_N)}| > \varepsilon) < 2e^{-CN\varepsilon^2}$$

where $C > 0$ is a proper fixed constant. Indeed it suffices to show that the function s defined by

$$s : Z_N \mapsto \sqrt{\lambda_{\max}(S_N)} = \sqrt{\lambda_{\max}\left(\frac{1}{n}\Gamma_N^{\frac{1}{2}}Z_N Z_N^* \Gamma_N^{\frac{1}{2}}\right)}$$

is $\frac{1}{\sqrt{CN}}$ -lipschitz, where we consider the $N \times n$ matrix Z_N as a vector in Euclidean space \mathbb{R}^{Nn} when $Z_{i,j}^{(N)}$ are real Gaussian, and in \mathbb{R}^{2Nn} when the entries are complex Gaussian. Note that the Euclidean norm of the vector Z_N is the same as the Frobenius norm $\|Z_N\|_F$ of the matrix Z_N . So for any two matrices Z_N and \hat{Z}_N , we have

$$\begin{aligned} |s(Z_N) - s(\hat{Z}_N)| &= \frac{1}{\sqrt{n}} \left| \|\Gamma_N^{1/2}Z_N\| - \|\Gamma_N^{1/2}\hat{Z}_N\| \right| \leq \frac{1}{\sqrt{n}} \|\Gamma_N^{1/2}(Z_N - \hat{Z}_N)\| \\ &\leq \frac{1}{\sqrt{n}} \|\Gamma_N^{1/2}(Z_N - \hat{Z}_N)\|_F \stackrel{(a)}{\leq} \frac{1}{\sqrt{n}} \|\Gamma_N^{1/2}\| \|Z_N - \hat{Z}_N\|_F \stackrel{(b)}{=} \frac{1}{\sqrt{n}} \|Z_N - \hat{Z}_N\|_F, \end{aligned}$$

where (a) follows from the Frobenius norm inequality $\|AB\|_F \leq \|A\| \|B\|_F$, and (b) from the fact that $\|\Gamma_N^{1/2}\| = \sqrt{\lambda_{\max}(\Gamma_N)} = 1$. Thus s is $1/\sqrt{n}$ -lipschitz, and the concentration inequality (34) is proved. Using Borel-Cantelli lemma, we have

$$(35) \quad \sqrt{\lambda_{\max}(S_N)} - \mathbb{E}\sqrt{\lambda_{\max}(S_N)} \rightarrow 0 \quad \text{a.s.}$$

Together with $\sqrt{\lambda_{\max}(S_N)} \xrightarrow{\mathcal{P}} 1$, we then obtain that $\mathbb{E}\sqrt{\lambda_{\max}(S_N)} \rightarrow 1$. By (35) again, it follows that

$$\lambda_{\max}(S_N) \xrightarrow{N, n \rightarrow \infty} 1 \quad \text{a.s.}$$

The proof of Theorem 4.1 is complete.

4.4. Proof of Theorem 4.2. We first prove the fluctuation of $\lambda_{\max}(S_N)$ under **A1**, **A2(b)**, **A4** and **A5**. Under these assumptions, Γ_N is of the form

$$\Gamma_N = \begin{pmatrix} 1 & 0 \\ 0 & \Gamma_{N-1} \end{pmatrix},$$

where (Γ_{N-1}) is a sequence of semidefinite positive Hermitian matrices satisfying $\mu^{\Gamma_{N-1}} \xrightarrow{\mathcal{D}} \delta_0$, and

$$\overline{\lim}_{N \rightarrow \infty} \lambda_{\max}(\Gamma_{N-1}) = \overline{\lim}_{N \rightarrow \infty} \lambda_2(\Gamma_N) = \overline{\lim}_{N \rightarrow \infty} \frac{\lambda_2(\Gamma_N)}{\lambda_1(\Gamma_N)} < 1$$

by assumption **A4**. We set $d = \overline{\lim}_{N \rightarrow \infty} \lambda_{\max}(\Gamma_{N-1})$. For convenience, in this section we omit all the subscript N of matrices, for example we write $S = n^{-1}\Gamma^{\frac{1}{2}}ZZ^*\Gamma^{\frac{1}{2}}$. In the following of this section we write $\lambda_{\max}(S_N)$ as λ_{\max} if it does not cause any ambiguity.

Recall the submatrix notations introduced in (16) and consider the following block decomposition of matrix S :

$$(36) \quad S = \begin{pmatrix} S_{1,1} & S_{1,2:N} \\ S_{2:N,1} & S_{2:N,2:N} \end{pmatrix} = \frac{1}{n} \begin{pmatrix} Z_{1,\cdot} Z_{1,\cdot}^* & Z_{1,\cdot} Z_{2:N,\cdot}^* \Gamma^{\frac{1}{2}} \\ \Gamma^{\frac{1}{2}} Z_{2:N,\cdot} Z_{1,\cdot}^* & \Gamma^{\frac{1}{2}} Z_{2:N,\cdot} Z_{2:N,\cdot}^* \Gamma^{\frac{1}{2}} \end{pmatrix}.$$

Denote

$$\underline{S}_{2:N,2:N} := \frac{1}{n} Z_{2:N,\cdot}^* \Gamma Z_{2:N,\cdot}, \quad \text{and} \quad r_N = \frac{N-1}{n}.$$

Analog to $\underline{\mu}(r_N, \Gamma_N)$ defined in (25), we define the probability measure $\underline{\mu}(r_N, \Gamma_{N-1})$ whose Cauchy-Stieltjes transform \underline{m} satisfies the equation

$$z = \frac{1}{\underline{m}(z)} + \frac{1}{n} \sum_{k=2}^N \frac{\lambda_k(\Gamma_N)}{1 - \lambda_k(\Gamma_N) \underline{m}(z)}, \quad \forall z \in \mathbb{C}^+.$$

Also, for all $y \in \mathbb{B}_N := \{y \in \mathbb{R} : y \neq 0, y^{-1} \neq \lambda_k(\Gamma_N), \forall k = 2, \dots, N\}$, we define

$$(37) \quad \mathbf{x}_N(y) := \frac{1}{y} + \frac{1}{n} \sum_{k=2}^N \frac{\lambda_k(\Gamma_N)}{1 - \lambda_k(\Gamma_N) y} = \frac{1}{y} + r_N \int \frac{s}{1 - sy} d\mu^{\Gamma_{N-1}}(s).$$

Consider in particular

$$(38) \quad \theta_N = \mathbf{x}_N(1) = 1 + \frac{1}{n} \sum_{k=2}^N \frac{\lambda_k(\Gamma_N)}{1 - \lambda_k(\Gamma_N)}.$$

Let $\varepsilon > 0$ be small enough. Thanks to the assumption $\mu^{\Gamma_{N-1}} \xrightarrow{\mathcal{D}} \delta_0$ and $d = \overline{\lim} \lambda_{\max}(\Gamma_{N-1}) < 1$, one can adapt the first part of the proof of Theorem 4.1 to obtain that eventually

$$\sup \text{supp } \underline{\mu}(r_N, \Gamma_{N-1}) < d + \varepsilon.$$

Let $\varepsilon < \frac{1-d}{2}$ so that $d + \varepsilon < 1 - \varepsilon$ and consider the family of events Ω_N defined as

$$(39) \quad \Omega_N := \{\lambda_{\max}(S_{2:N,2:N}) < d + \varepsilon < 1 - \varepsilon < \lambda_{\max}\}.$$

According to the spectrum confinement property [1, Theorem 1.1] and to Theorem 4.1, one has

$$\mathbb{P}(\Omega_N) \xrightarrow{N, n \rightarrow \infty} 1.$$

In particular, for any sequence of events A_N , we have $\mathbb{P}(A_N) - \mathbb{P}(A_N \cap \Omega_N) \rightarrow_{N \rightarrow \infty} 0$, which can be written

$$\mathbb{P}(A_N) \doteq \mathbb{P}_\Omega(A_N)$$

if one writes $\mathbb{P}_\Omega(\cdot)$ for $\mathbb{P}(\cdot \cap \Omega_N)$ and recall the notation $x \doteq y$ for $x - y \rightarrow 0$. Hence, with no loss of generality, we will assume below that Ω_N holds.

Let $\lambda_{\max} \in \Omega_N$. Using the bloc decomposition (36) of S together with the determinantal formula based on Schur complements (see for instance [23, Section 0.8.5]), the eigenvalue λ_{\max} satisfies the equation:

$$\begin{aligned} \det(\lambda_{\max} I - S) &= (\lambda_{\max} I - S_{1,1} - S_{1,2:N}(\lambda_{\max} I - S_{2:N,2:N})^{-1} S_{2:N,1}) \det(\lambda_{\max} I - S_{2:N,2:N}) = 0. \end{aligned}$$

Since $\det(\lambda_{\max} I - S_{2:N,2:N}) \neq 0$ on Ω_N , we have

$$\begin{aligned} \lambda_{\max} &= S_{1,1} + S_{1,2:N}(\lambda_{\max} I - S_{2:N,2:N})^{-1} S_{2:N,1}, \\ &= \frac{Z_{1,\cdot} Z_{1,\cdot}^*}{n} + \frac{Z_{1,\cdot} Z_{2:N,\cdot}^* \Gamma^{\frac{1}{2}}}{n} \left(\lambda_{\max} I - \frac{1}{n} \Gamma^{\frac{1}{2}} Z_{2:N,\cdot} Z_{2:N,\cdot}^* \Gamma^{\frac{1}{2}} \right) \frac{\Gamma^{\frac{1}{2}} Z_{2:N,\cdot} Z_{1,\cdot}^*}{n}, \\ (40) \quad &= \frac{Z_{1,\cdot}}{n} \left(I + A^* (\lambda_{\max} I - A A^*) A \right) Z_{1,\cdot}^*. \quad \left(A = n^{-1/2} \Gamma^{\frac{1}{2}} Z_{2:N,\cdot} \right) \end{aligned}$$

Using the equality $I + A^*(\lambda I - A A^*)^{-1} A = \lambda(\lambda I - A^* A)^{-1}$ for all scalar λ and all matrix A such that $\lambda I - A A^*$ and $\lambda I - A^* A$ are invertible, the equation (40) is equivalent to

$$(41) \quad 1 = \frac{1}{n} Z_{1,\cdot} (\lambda_{\max} I - \underline{S}_{2:N,2:N})^{-1} Z_{1,\cdot}^*.$$

As $\theta_N = \mathbf{x}_N(1) \geq 1$ lies outside the support of $\underline{\mu}(r_N, \Gamma_{N-1})$ for large N , [36, Theorem 4.2] yields

$$\underline{m}(\theta_N) = \underline{m}(\mathbf{x}_N(1)) = 1.$$

This can be regarded as a “deterministic” version of (41), which indicates that λ_{\max} and θ_N are comparable.

In order to prove the Gaussian fluctuations of λ_{\max} , we need to prove that for all $b \in \mathbb{R}$

$$(42) \quad \mathbb{P}(\lambda_{\max} \leq \eta_N) \xrightarrow[N, n \rightarrow \infty]{} \Phi(b, \sigma)$$

where

$$\eta_N := \theta_N + \frac{b}{\sqrt{n}}, \quad \Phi(x, \sigma) := \frac{1}{\sigma\sqrt{2\pi}} \int_{-\infty}^x e^{-\frac{t^2}{2\sigma^2}} dt \quad \text{and} \quad \sigma^2 = \mathbb{E} \left| Z_{1,1}^{(1)} \right|^4 - 1.$$

Note that on Ω_N the function

$$\Upsilon(\lambda) := \frac{1}{n} Z_{1,\cdot} (\lambda I - \underline{S}_{2:N,2:N})^{-1} Z_{1,\cdot}^*$$

is decreasing on $(d + \varepsilon, +\infty)$. Let N large enough so that $\eta_N > d + \varepsilon$.

Taking into account the fact that $\Upsilon(\lambda_{\max}) = 1$ due to (41), we have

$$(43) \quad \mathbb{P}_\Omega(\lambda_{\max} \leq \eta_N) = \mathbb{P}_\Omega(\Upsilon(\eta_N) \leq 1) = \mathbb{P}_\Omega(\sqrt{n}(\Upsilon(\eta_N) - \underline{\mathbf{m}}(\eta_N)) \leq \sqrt{n}(1 - \underline{\mathbf{m}}(\eta_N))) .$$

We first prove that

$$(44) \quad \sqrt{n}(1 - \underline{\mathbf{m}}(\eta_N)) = b + o(1) .$$

Taking into account the fact that $\underline{\mathbf{m}}(\theta_N) = 1$ and performing a Taylor expansion on $\underline{\mathbf{m}}$ around θ_N yields

$$\sqrt{n}(1 - \underline{\mathbf{m}}(\eta_N)) = \sqrt{n}(\underline{\mathbf{m}}(\theta_N) - \underline{\mathbf{m}}(\eta_N)) = -b \underline{\mathbf{m}}'(\theta_N) - \underline{\mathbf{m}}''(\xi_N) \frac{b^2}{\sqrt{n}}$$

where ξ_N is between $\theta_N = x_N(1)$ and η_N . The assumptions $\mu^{\Gamma_{N-1}} \xrightarrow{\mathcal{D}} \delta_0$ and $d = \overline{\lim} \lambda_{\max}(\Gamma_{N-1}) < 1$ yield

$$\theta_N, \eta_N \xrightarrow[N, n \rightarrow \infty]{} 1 .$$

Similarly, one proves that $x'_N(1) \xrightarrow[N, n \rightarrow \infty]{} -1$. By [36, Theorem 4.2], equality $\underline{\mathbf{m}}(x_N(y)) = y$ holds for any $y \notin \text{supp } \mu^{\Gamma_{N-1}}$. Differentiating, we get

$$\underline{\mathbf{m}}'(x_N(y)) x'_N(y) = 1 \quad \text{and} \quad \underline{\mathbf{m}}'(x_N(1)) = \frac{1}{x'_N(1)} \xrightarrow[N, n \rightarrow \infty]{} -1 .$$

Finally, for large N , we have $\sup_N \text{supp } \mu(r_N, \Gamma_{N-1}) < d + \varepsilon < 1 - \varepsilon < \min(\eta_N, \theta_N)$ which implies

$$|\underline{\mathbf{m}}''(\xi_N)| = 2 \left| \int \frac{d\mu(r_N, \Gamma_{N-1})(s)}{(\xi_N - s)^3} \right| \leq \frac{2}{(1 - d - 2\varepsilon)^3} .$$

Plugging this into the Taylor expansion finally yields (44).

We now go back to (43) and handle the quantity $\sqrt{n}(\Upsilon(\eta_N) - \underline{\mathbf{m}}(\eta_N))$. More precisely, we prove in the sequel that

$$(45) \quad \sqrt{n}(\Upsilon(\eta_N) - \underline{\mathbf{m}}(\eta_N)) = \sqrt{n} \left(\frac{1}{n} Z_{1,\cdot} Z_{1,\cdot}^* - 1 \right) + o_P(1) .$$

In order to proceed, we need the following estimates, valid under the assumptions of Theorem 4.2.

Proposition 4.3. *Assume that A1, A2(b), A4 and A5 hold, then*

$$(a) \quad \sqrt{n} \left(\frac{1}{n} \text{tr}(\eta_N I - \underline{S}_{2:N,2:N})^{-1} - \underline{\mathbf{m}}(\eta_N) \right) \xrightarrow[N, n \rightarrow \infty]{\mathcal{P}} 0 ,$$

$$(b) \quad \frac{\sqrt{n}}{\eta_N} \left(\frac{1}{n} Z_{1,\cdot} (\eta_N I - \underline{S}_{2:N,2:N})^{-1} \underline{S}_{2:N,2:N} Z_{1,\cdot}^* - \frac{1}{n} \text{tr}(\eta_N I - \underline{S}_{2:N,2:N})^{-1} \underline{S}_{2:N,2:N} \right) \xrightarrow[N, n \rightarrow \infty]{\mathcal{P}} 0 .$$

Proof of Proposition 4.3 is postponed to Section 4.4.1. We have

$$(46) \quad \begin{aligned} & \sqrt{n}(\Upsilon(\eta_N) - \underline{\mathbf{m}}(\eta_N)) \\ &= \sqrt{n} \left(\Upsilon(\eta_N) - \frac{1}{n} \text{tr}(\eta_N I - \underline{S}_{2:N,2:N})^{-1} + \frac{1}{n} \text{tr}(\eta_N I - \underline{S}_{2:N,2:N})^{-1} - \underline{\mathbf{m}}(\eta_N) \right) \\ &= \sqrt{n} \left(\Upsilon(\eta_N) - \frac{1}{n} \text{tr}(\eta_N I - \underline{S}_{2:N,2:N})^{-1} \right) + o_P(1) \end{aligned}$$

by the first part of Proposition 4.3. We now apply the resolvent identity $A^{-1} - B^{-1} = A^{-1}(B - A)B^{-1}$ to $A = \eta_N - \underline{S}_{2:N,2:N}$ and $B = \eta_N I$ and obtain

$$\begin{aligned}
& \sqrt{n} \left(\Upsilon(\eta_N) - \frac{1}{n} \operatorname{tr}(\eta_N I - \underline{S}_{2:N,2:N})^{-1} \right) \\
&= \frac{\sqrt{n}}{\eta_N} \left(\frac{1}{n} Z_{1,\cdot} (\eta_N I - \underline{S}_{2:N,2:N})^{-1} \underline{S}_{2:N,2:N} Z_{1,\cdot}^* - \frac{1}{n} \operatorname{tr}(\eta_N I - \underline{S}_{2:N,2:N})^{-1} \underline{S}_{2:N,2:N} \right) \\
&\quad + \frac{\sqrt{n}}{\eta_N} \left(\frac{1}{n} Z_{1,\cdot} Z_{1,\cdot}^* - 1 \right) \\
(47) \quad &= \frac{\sqrt{n}}{\eta_N} \left(\frac{1}{n} Z_{1,\cdot} Z_{1,\cdot}^* - 1 \right) + o_P(1)
\end{aligned}$$

where the last equality follows from the second estimate of Proposition 4.3. Notice that by the standard Central Limit theorem,

$$\sqrt{n} \left(\frac{1}{n} Z_{1,\cdot} Z_{1,\cdot}^* - 1 \right) = \sqrt{n} \left(\frac{1}{n} \sum_{j=1}^n |Z_{1,j}|^2 - 1 \right) \xrightarrow[n \rightarrow \infty]{\mathcal{D}} \mathcal{N}_{\mathbb{R}}(0, \operatorname{Var} |Z_{1,1}|^2)$$

where $\operatorname{Var} |Z_{1,1}|^2 = \mathbb{E}|Z_{1,1}|^4 - 1$. Since $\eta_N \rightarrow 1$, one has

$$\frac{\sqrt{n}}{\eta_N} \left(\frac{1}{n} Z_{1,\cdot} Z_{1,\cdot}^* - 1 \right) = \sqrt{n} \left(\frac{1}{n} Z_{1,\cdot} Z_{1,\cdot}^* - 1 \right) + o_P(1).$$

Plugging this last estimate into (47) and (46) finally yields (45). We can now conclude the proof of the CLT:

$$\begin{aligned}
\mathbb{P}(\lambda_{\max} \leq \eta_N) &\doteq \mathbb{P}_{\Omega}(\lambda_{\max} \leq \eta_N) \\
&\stackrel{(a)}{=} \mathbb{P}_{\Omega}(\sqrt{n}(\Upsilon(\eta_N) - \underline{\mathbf{m}}(\eta_N)) \leq b + o(1)) \\
&\stackrel{(b)}{=} \mathbb{P}_{\Omega}\left(\sqrt{n}\left(\frac{1}{n} Z_{1,\cdot} Z_{1,\cdot}^* - 1\right) + o_P(1) \leq b\right) \\
(48) \quad &\doteq \mathbb{P}\left(\sqrt{n}\left(\frac{1}{n} Z_{1,\cdot} Z_{1,\cdot}^* - 1\right) + o_P(1) \leq b\right)
\end{aligned}$$

where (a) follows from (43) and (44) and (b) follows from (45). We can now get rid of the term $o_P(1)$ in (48) by Slutsky's theorem and finally obtain the desired result:

$$\mathbb{P}(\sqrt{n}(\lambda_{\max} - \theta_N) \leq b) = \mathbb{P}(\lambda_{\max} \leq \eta_N) \xrightarrow[N, n \rightarrow \infty]{} \Phi(b, \sigma), \quad \sigma^2 = \mathbb{E}|Z_{1,1}|^4 - 1.$$

This completes the proof of Theorem 4.2 under condition (i).

Assume now that $Z_{ij}^{(N)} \sim \mathcal{N}_{\mathbb{C}}(0, 1)$ and consider the eigen-decomposition $\Gamma_N = U_N D_N U_N^*$, where U_N is unitary and $D_N = \operatorname{diag}(\lambda_1(\Gamma_N), \dots, \lambda_N(\Gamma_N))$. Then S_N can be written as

$$S_N = \frac{1}{n} U_N D_N^{\frac{1}{2}} (U_N^* Z_N) (Z_N^* U_N) D_N^{\frac{1}{2}} U_N^* = \frac{1}{n} U_N D_N^{\frac{1}{2}} \tilde{Z}_N \tilde{Z}_N^* D_N^{\frac{1}{2}} U_N^* \quad \text{where} \quad \tilde{Z}_N = U_N^* Z_N$$

and has the same eigenvalues as the matrix $R_N = n^{-1} D_N^{\frac{1}{2}} \tilde{Z}_N \tilde{Z}_N^* D_N^{\frac{1}{2}}$. It remains to notice that \tilde{Z}_N has i.i.d. $\mathcal{N}_{\mathbb{C}}(0, 1)$ entries. In particular, R_N satisfies **A1**, **A2(b)**, **A4** and **A5**, and the desired result follow for S_N . Theorem 4.2 is established under condition (ii).

Assume now that $Z_{ij}^{(N)} \sim \mathcal{N}_{\mathbb{R}}(0, 1)$ and that Γ_N is real symmetric. In this case, Γ_N 's eigen-decomposition writes $\Gamma_N = O_N D_N O_N^{\top}$, where matrix O_N is orthogonal. It remains to notice that $O_N^{\top} Z_N$ has i.i.d. $\mathcal{N}_{\mathbb{R}}(0, 1)$ entries and to proceed as in the complex case to prove Theorem 4.2 under condition (iii).

Proof of Theorem 4.2 is completed.

4.4.1. *Proof of Proposition 4.3.* We first establish item (a). Denote by

$$\Delta_N(x) = \frac{1}{n} \operatorname{tr} (xI - \underline{S}_{2:N,2:N})^{-1} - \underline{m}(x) .$$

We will first establish that $n\Delta_n(\eta_N)$ is tight and then, as an easy consequence, we will deduce the desired convergence: $\sqrt{n}\Delta_N(\eta_N) \xrightarrow[N, n \rightarrow \infty]{\mathcal{P}} 0$.

If $x \geq 1 - \varepsilon$ is fixed with $1 - \varepsilon > d + \varepsilon$, then the tightness of $n\Delta_N(x)$ is a consequence of Bai and Silverstein's peripheral results of their CLT paper [3], see also [4, Chapter 9]. In fact,

$$\Delta_N(x) = \int f(x, \lambda) \mu^{\underline{S}_{2:N,2:N}}(d\lambda) - \int f(x, \lambda) \underline{\mu}(r_N, \Gamma_{N-1})(d\lambda) \quad \text{where} \quad f(x, \lambda) = \frac{1}{x - \lambda} .$$

Notice that for any $x \geq 1 - \varepsilon$, $\lambda \mapsto f(x, \lambda)$ is analytic in a neighbourhood of $[0, d + \varepsilon]$ which contains the support of $\underline{\mu}(r_N, \Gamma_{N-1})$. According to [4, Theorem 9.10(1)] and to the remark at the end of page 265 in [4] which tightens the interval where the function $f(x, \cdot)$ needs to be analytic, we immediatly obtain the tightness of $(n\Delta_N(x))$.

The case where $x = \eta_N \geq 1 - \varepsilon$ for N large necessitates some adaptation. We closely follow [4, Chapter 9]. Denote by

$$M_N(z) = n (m^{\underline{S}_{2:N,2:N}}(z) - \underline{m}(z))$$

and by \mathcal{C}^+ the contour defined by ($\delta, u > 0$ fixed)

$$\mathcal{C}^+ = \mathcal{C}_\ell \cup \mathcal{C}_{\text{up}} \cup \mathcal{C}_r \quad \text{where} \quad \begin{cases} \mathcal{C}_\ell & = \{z = (-\delta, y), y \in [0, u]\} \\ \mathcal{C}_{\text{up}} & = \{z = (x, u), x \in [-\delta, d + \varepsilon]\} \\ \mathcal{C}_r & = \{z = (d + \varepsilon, y), y \in [0, u]\} \end{cases} .$$

Consider the truncated version $\hat{M}_N(z)$ of $M_N(z)$ as defined in [4, (9.8.2)] then

$$\int_{\mathcal{C}} \frac{1}{\eta_N - z} (\hat{M}_N(z) - M_N(z)) dz \xrightarrow[N, n \rightarrow \infty]{\text{a.s.}} 0 \quad \text{where} \quad \mathcal{C} = \mathcal{C}^+ \cup \overline{\mathcal{C}^+}$$

and $\{\hat{M}_N(\cdot)\}$ forms a tight sequence on \mathcal{C} . Consider now the mapping

$$\Gamma_N : \hat{M}_N(\cdot) \mapsto \frac{1}{2i\pi} \int_{\mathcal{C}} \frac{1}{\eta_N - z} \hat{M}_N(z) dz .$$

Γ_N is a continuous mapping from $C(\mathcal{C}, \mathbb{R}^2)$ to \mathbb{C} . Applying Prohorov's theorem (see for instance [27, Theorem 16.3]) and the continuous mapping theorem [27, Theorem 4.27], we conclude that $\Gamma_N(\hat{M}_N)$ is tight. It remains to notice that

$$n\Delta_N(\eta_N) = \Gamma_N(\hat{M}_N) + \underbrace{(\Gamma_N(\hat{M}_N) - \Gamma_N(M_N))}_{\xrightarrow{\text{a.s.}} 0}$$

to conclude that $n\Delta_N(\eta_N)$ is tight. Now let $\delta > 0$ be fixed, then

$$\mathbb{P}(|\sqrt{n}\Delta_N(\eta_N)| > \delta) = \mathbb{P}(|n\Delta_N(\eta_N)| > \sqrt{n}\delta) \xrightarrow[N, n \rightarrow \infty]{} 0$$

by tightness, hence the convergence of $\sqrt{n}\Delta_N(\eta_N)$ to zero in probability. Part (a) of Proposition 4.3 is proved.

We now prove part (b) of Proposition 4.3 and rely on the lemma on quadratic forms [4, Lemma B.26]. Denote by

$$P_N = \sqrt{n} \left(\frac{1}{n} Z_{1,\cdot} (\eta_N I - \underline{S}_{2:N,2:N})^{-1} \underline{S}_{2:N,2:N} Z_{1,\cdot}^* - \frac{1}{n} \operatorname{tr} \{ (\eta_N I - \underline{S}_{2:N,2:N})^{-1} \underline{S}_{2:N,2:N} \} \right)$$

and apply the lemma on quadratic forms with $p = 2$: There exists a constant C such that

$$\mathbb{E}_{Z_{2:N,\cdot}} (|P_N|^2) \leq \frac{C}{n} \mathbb{E}(|Z_{1,1}^{(1)}|^4) \operatorname{tr} \{ (\eta_N I - \underline{S}_{2:N,2:N})^{-2} \underline{S}_{2:N,2:N}^2 \} .$$

Taking into account the facts that

$$\lim_{n \rightarrow \infty} \eta_N = 1, \quad \overline{\lim}_N \lambda_{\max}(\underline{S}_{2:N,2:N}) \stackrel{\mathcal{P}}{\leq} d \quad \text{and} \quad \mu^{\underline{S}_{2:N,2:N}} \xrightarrow[N, n \rightarrow \infty]{\mathcal{D}} \delta_0 \quad \text{a.s.} ,$$

we obtain that

$$\frac{1}{n} \operatorname{tr} \{ (\eta_N - \underline{S}_{2:N,2:N})^{-2} \underline{S}_{2:N,2:N}^2 \} = \int \frac{s^2}{(\eta_N - s)^2} \mu^{\underline{S}_{2:N,2:N}}(ds) \xrightarrow[N, n \rightarrow \infty]{\mathcal{P}} 0.$$

Thus $\mathbb{E}_{Z_{2:N, \cdot}}(|P_N|^2)$ converges to zero in probability, from which we deduce that for $\delta > 0$,

$$\mathbb{E}_{Z_{2:N, \cdot}}(\mathbb{1}_{|P_N|^2 > \delta}) \leq \frac{1}{\delta} \mathbb{E}_{Z_{2:N, \cdot}}(|P_N|^2 \mathbb{1}_{|P_N|^2 > \delta}) \xrightarrow[N, n \rightarrow \infty]{\mathcal{P}} 0.$$

Finally

$$\mathbb{P}(|P_N|^2 > \delta) = \mathbb{E} \mathbb{E}_{Z_{2:N, \cdot}}(\mathbb{1}_{|P_N|^2 > \delta}) \xrightarrow[N, n \rightarrow \infty]{} 0,$$

which completes the proof of Proposition 4.3.

5. PROOF OF THEOREM 2.3

In order to study the spectral gap associated to the family of Toeplitz matrices and to prove Theorem 2.3, we follow the method used in [15]. The main idea is to interpret the eigenvalues of the Toeplitz matrix T_N as eigenvalues of an operator \mathcal{K}_N using Widom-Shampine's Lemma, and then analyse the convergence of this operator, correctly normalized.

In this section, for $p \in [1, \infty]$, the L^p norm of a function f is denoted by $\|f\|_p$, and the $L^p \rightarrow L^p$ norm of an operator \mathcal{K} is denoted by $\|\mathcal{K}\|_p$. Recall that $\|\mathcal{K}\|_p := \sup_{\|f\|_p=1} \|\mathcal{K}f\|_p$.

5.1. Widom-Shampine's Lemma and convergence of operators. We first recall Widom-Shampine's Lemma, see [15] for a proof.

Lemma 5.1 (Widom-Shampine). *Let $A = (a_{i,j})_{i,j=0}^{N-1}$ be a matrix with complex entries $a_{i,j}$, and let G be the integral operator on $L^2(0,1)$ defined by*

$$(Gf)(x) = \int_0^1 a_{\lfloor Nx \rfloor \lfloor Ny \rfloor} f(y) dy, \quad x \in (0,1).$$

Then a nonzero complex number λ is an eigenvalue of A of a certain algebraic multiplicity if and only if λ/N is an eigenvalue of G of the same algebraic multiplicity.

Let $c = (c_k)_{k \in \mathbb{Z}}$ be the sequence in Theorem 2.3, and $\rho \in (-1, 0)$ be the index, then the function $R(h) := c_{\lfloor h \rfloor}$ is even and regularly varying and $R(k) = c_k$. By Definition 1, $R(N) \neq 0$ for large enough $N \in \mathbb{N}$, for convenience we can suppose that $R(N) \neq 0$ for all $N \in \mathbb{N}$ without loss of generality. By Widom-Shampine's Lemma, for each N , the matrix $T_N(c)/(NR(N))$ has the same nonzero eigenvalues (with the same multiplicities) as the integral operator $\mathcal{K}_N^{(\rho)}$ defined on $L^2(0,1)$ by

$$(49) \quad (\mathcal{K}_N^{(\rho)} f)(x) = \int_0^1 \frac{R(\lfloor Nx \rfloor - \lfloor Ny \rfloor)}{R(N)} f(y) dy.$$

We will prove that the operators $\mathcal{K}_N^{(\rho)}$ converge in the operator norm to the operator $\mathcal{K}^{(\rho)}$ defined on $L^2(0,1)$ by

$$(50) \quad (\mathcal{K}^{(\rho)} f)(x) = \int_0^1 |x - y|^\rho f(y) dy.$$

For this we need the following Lemma 5.2 which is a special case of the uniform convergence theorem of regularly varying functions.

Lemma 5.2 ([14, Theorem 1.5.2]). *If R is regularly varying with index $\rho < 0$, then for every $a > 0$*

$$\sup_{x > a} \left| \frac{R(xy)}{R(y)} - x^\rho \right| \xrightarrow[y \rightarrow \infty]{} 0.$$

The following description of the asymptotic integral of regularly varying functions will also be useful in the sequel.

Lemma 5.3 ([14, Proposition 1.5.8]). *If R is regularly varying with index $\rho > -1$, and suppose that R is locally bounded, then*

$$\int_0^y R(x) dx \sim \frac{yR(y)}{1+\rho} \quad (y \rightarrow +\infty).$$

Recall that for an operator defined by $(\mathcal{K}f)(x) = \int_0^1 K(x, y)f(y) dy$, we have

$$\|\mathcal{K}\|_1 \leq M_1 \quad \text{and} \quad \|\mathcal{K}\|_\infty \leq M_\infty,$$

where

$$(51) \quad M_1 := \operatorname{ess\,sup}_{y \in [0,1]} \int_0^1 |K(x, y)| dx, \quad M_\infty := \operatorname{ess\,sup}_{x \in [0,1]} \int_0^1 |K(x, y)| dy.$$

If the kernel K is symmetric for x and y , then $M_1 = M_\infty$. In this case and if $M_1 = M_\infty < \infty$, then by the Riesz–Thorin interpolation theorem (cf. [19, Theorem 2.2.14], taking $p_0 = q_0 = 1, p_1 = q_1 = \infty$), for all $p \in [1, +\infty]$, we have

$$(52) \quad \|\mathcal{K}\|_p \leq M_1 = M_\infty.$$

We are now ready to prove the theorem. As mentioned above, we first prove the following convergence of operators.

Lemma 5.4. *Let $\rho \in (-1, 0)$, then for any $p \in [1, \infty]$ and any $N \in \mathbb{N}$, the formulas (49) and (50) define bounded operators $\mathcal{K}_N^{(\rho)}$ and $\mathcal{K}^{(\rho)}$ on $L^p(0, 1)$. Moreover we have*

$$\lim_{N \rightarrow \infty} \|\mathcal{K}_N^{(\rho)} - \mathcal{K}^{(\rho)}\|_p = 0$$

for any $p \in [1, \infty]$.

Proof. Let $K_N^{(\rho)} : [0, 1]^2 \rightarrow \mathbb{R}$ and $K_\rho : [0, 1]^2 \rightarrow \mathbb{R}$ be the integral kernels defining respectively $\mathcal{K}_N^{(\rho)}$ and $\mathcal{K}^{(\rho)}$, that is,

$$K_N^{(\rho)}(x, y) = \frac{R(\lfloor Nx \rfloor - \lfloor Ny \rfloor)}{R(N)}, \quad K^{(\rho)}(x, y) = |x - y|^\rho.$$

Recall that since R is even, the considered kernels are symmetric and the two essential supremums in (51) of each kernel are equal. Moreover, for each N , $K_N^{(\rho)}$ is bounded on $[0, 1]^2$ as it takes only a finite number of values, hence

$$\operatorname{ess\,sup}_{x \in [0,1]} \int_0^1 |K_N^{(\rho)}(x, y)| dy = \operatorname{ess\,sup}_{y \in [0,1]} \int_0^1 |K_N^{(\rho)}(x, y)| dx < \infty.$$

For $\rho \in (-1, 0)$, easy calculations yield

$$\operatorname{ess\,sup}_{x \in [0,1]} \int_0^1 |x - y|^\rho dy = \operatorname{ess\,sup}_{y \in [0,1]} \int_0^1 |x - y|^\rho dx = \frac{2^{-\rho}}{(1+\rho)} < \infty.$$

So by (52), for all $p \in [1, +\infty]$ we have

$$\|\mathcal{K}_N^{(\rho)}\|_p < \infty \quad \text{and} \quad \|\mathcal{K}^{(\rho)}\|_p \leq \frac{2^{-\rho}}{(1+\rho)}.$$

Also by (52), we have

$$(53) \quad \|\mathcal{K}_N^{(\rho)} - \mathcal{K}^{(\rho)}\|_p \leq \operatorname{ess\,sup}_{y \in [0,1]} \int_0^1 \left| \frac{R(\lfloor Nx \rfloor - \lfloor Ny \rfloor)}{R(N)} - |x - y|^\rho \right| dx.$$

We now prove that $\|\mathcal{K}_N^{(\rho)} - \mathcal{K}^{(\rho)}\|_p \rightarrow 0$ by showing that the RHS of (53) goes to 0 as $N \rightarrow \infty$. Taking an arbitrary $\varepsilon \in (0, 1)$, we set $A_\varepsilon := \{(x, y) \in [0, 1]^2 : |x - y| > \varepsilon\}$ and for $y \in [0, 1]$, we set $A_\varepsilon(y) := \{x \in [0, 1] : (x, y) \in A_\varepsilon\} = \{x \in [0, 1] : |x - y| > \varepsilon\}$.

By the inequality

$$(54) \quad |x - y| - \frac{1}{N} \leq \frac{|\lfloor Nx \rfloor - \lfloor Ny \rfloor|}{N} \leq |x - y| + \frac{1}{N}$$

and the uniform continuity of the function $x \mapsto x^\rho$ on $[\frac{\varepsilon}{2}, +\infty)$, we can take $N_1 = N_1(\varepsilon) \in \mathbb{N}$ such that for $N > N_1$ and $(x, y) \in A_\varepsilon$ we have

$$(55) \quad \frac{|\lfloor Nx \rfloor - \lfloor Ny \rfloor|}{N} > \frac{\varepsilon}{2}$$

and

$$(56) \quad \left| \frac{|\lfloor Nx \rfloor - \lfloor Ny \rfloor|^\rho}{N^\rho} - |x - y|^\rho \right| < \frac{\varepsilon}{2}.$$

Then applying Lemma 5.2 with $a = \varepsilon/2$, we can find $N_2 = N_2(\varepsilon) \in \mathbb{N}$ such that for $N > N_2$ and for all c satisfying $|c| \geq \varepsilon/2$, we have

$$(57) \quad \left| \frac{R(cN)}{R(N)} - |c|^\rho \right| < \frac{\varepsilon}{2}.$$

For all $N > \max(N_1, N_2)$ and $(x, y) \in A_\varepsilon$, let $c = \frac{\lfloor Nx \rfloor - \lfloor Ny \rfloor}{N}$ then by (55) we have $|c| > \varepsilon/2$. Moreover

$$(58) \quad \left| \frac{R(\lfloor Nx \rfloor - \lfloor Ny \rfloor)}{R(N)} - \frac{|\lfloor Nx \rfloor - \lfloor Ny \rfloor|^\rho}{N^\rho} \right| < \frac{\varepsilon}{2}$$

by (57). Combining (56), (58) and the triangle inequality, we have

$$\left| \frac{R(\lfloor Nx \rfloor - \lfloor Ny \rfloor)}{R(N)} - |x - y|^\rho \right| < \varepsilon$$

for all $N > \max(N_1, N_2)$ and $(x, y) \in A_\varepsilon$. Then for N large enough, we have

$$(59) \quad \operatorname{ess\,sup}_{y \in [0,1]} \int_{A_\varepsilon(y)} \left| \frac{R(\lfloor Nx \rfloor - \lfloor Ny \rfloor)}{R(N)} - |x - y|^\rho \right| dx < \varepsilon.$$

On the other hand, for all $y \in [0, 1]$, we have

$$(60) \quad \int_{[0,1] \setminus A_\varepsilon(y)} |x - y|^\rho dx \leq \int_{-\varepsilon}^\varepsilon |x|^\rho dx = \frac{2\varepsilon^{1+\rho}}{1+\rho}.$$

Hence we just need to control the integral

$$\int_{[0,1] \setminus A_\varepsilon(y)} \left| \frac{R(\lfloor Nx \rfloor - \lfloor Ny \rfloor)}{R(N)} \right| dx.$$

Notice that both R and $|R|$ are even, locally bounded and regularly varying with index ρ . By Lemma 5.3, we have

$$(61) \quad \begin{aligned} \int_{[0,1] \setminus A_\varepsilon(y)} \left| \frac{R(\lfloor Nx \rfloor - \lfloor Ny \rfloor)}{R(N)} \right| dx &\leq \int_{y-\varepsilon}^{y+\varepsilon} \left| \frac{R(\lfloor Nx \rfloor - \lfloor Ny \rfloor)}{R(N)} \right| dx \\ &\stackrel{(a)}{=} \int_{-\varepsilon}^\varepsilon \left| \frac{R(\lfloor Nx + (Ny - \lfloor Ny \rfloor)\rfloor)}{R(N)} \right| dx \\ &= \int_{-N\varepsilon}^{N\varepsilon} \left| \frac{R(\lfloor x + (Ny - \lfloor Ny \rfloor)\rfloor)}{NR(N)} \right| dx \\ &\leq \int_{-N\varepsilon-1}^{N\varepsilon+1} \left| \frac{R(\lfloor x \rfloor)}{NR(N)} \right| dx \\ &\stackrel{(b)}{\approx} 2 \left| \frac{R(N\varepsilon+1)}{R(N)} \right| \frac{\varepsilon}{1+\rho} \stackrel{(c)}{\approx} \frac{2\varepsilon^{1+\rho}}{1+\rho} \end{aligned}$$

as $N \rightarrow \infty$, where (a) follows from a change of variable and the fact that $\lfloor x \rfloor + h = \lfloor x + h \rfloor$ for every $h \in \mathbb{Z}$, (b) follows from Lemma 5.3 and (c) from Lemma 5.2. Notice that the controls (60) and (61) are independent of y , hence for N large enough, we have

$$(62) \quad \operatorname{ess\,sup}_{y \in [0,1]} \int_{[0,1] \setminus A_\varepsilon(y)} \left| \frac{R(\lfloor Nx \rfloor - \lfloor Ny \rfloor)}{R(N)} - |x - y|^\rho \right| dx < \frac{5\varepsilon^{1+\rho}}{1+\rho}.$$

Combining (59) and (62), and taking $\varepsilon \rightarrow 0$, we finally obtain

$$\|\mathcal{K}_N^{(\rho)} - \mathcal{K}^{(\rho)}\|_p \xrightarrow{N \rightarrow \infty} 0$$

for all $p \in [1, \infty]$. \square

As a consequence of Lemma 5.4, we conclude that $\mathcal{K}^{(\rho)}$ is compact on $L^p(0, 1)$ for all $p \in [1, \infty]$, because it is the limit in operator norm of finite dimensional operators $\mathcal{K}_N^{(\rho)}$.

We will complete the proof of Theorem 2.3 in the next section.

5.2. Convergence of eigenvalues and simplicity of the largest eigenvalue. For a fixed $k = 1, 2, \dots$, let $a_k^{(\rho)}$ be the k -th largest eigenvalue of $\mathcal{K}^{(\rho)}$ and $a_{N,k}^{(\rho)} = \lambda_k(T_N(c))/(NR(N))$ be the k -th largest eigenvalue of $\mathcal{K}_N^{(\rho)}$. From the convergence $\|\mathcal{K}_N^{(\rho)} - \mathcal{K}^{(\rho)}\|_2 \rightarrow 0$ we deduce that $a_{N,k}^{(\rho)} \rightarrow a_k^{(\rho)}$ as $N \rightarrow \infty$. In fact, as $\mathcal{K}_N^{(\rho)}$ and $\mathcal{K}^{(\rho)}$ are compact and self-adjoint, by the Min-Max Formula (see also [37, Theorem 4.12]) we have

$$\begin{aligned} a_{N,k}^{(\rho)} &= \min_{\dim U = k-1} \max_{\substack{u \in U^\perp \\ \|u\|_2 = 1}} \langle u, \mathcal{K}_N^{(\rho)} u \rangle \\ &\leq \min_{\dim U = k-1} \max_{\substack{u \in U^\perp \\ \|u\|_2 = 1}} \langle u, \mathcal{K}^{(\rho)} u \rangle + \|\mathcal{K}_N^{(\rho)} - \mathcal{K}^{(\rho)}\|_2 = a_k^{(\rho)} + \|\mathcal{K}_N^{(\rho)} - \mathcal{K}^{(\rho)}\|_2. \end{aligned}$$

Symmetrically, we also have $a_k^{(\rho)} \leq a_{N,k}^{(\rho)} + \|\mathcal{K}_N^{(\rho)} - \mathcal{K}^{(\rho)}\|_2$, from which we deduce

$$|a_{N,k}^{(\rho)} - a_k^{(\rho)}| \leq \|\mathcal{K}_N^{(\rho)} - \mathcal{K}^{(\rho)}\|_2$$

for all N and k . This implies the convergence of each eigenvalue $a_{N,k}^{(\rho)}$ toward $a_k^{(\rho)}$.

We now prove that $a_1^{(\rho)}$ is a simple eigenvalue of $\mathcal{K}^{(\rho)}$. Let $u \in L^2(0, 1)$ be an eigenfunction of $a_1^{(\rho)}$, then by the mini-max formula $a_1^{(\rho)} = \max_{f \in L^2, \|f\|_2 = 1} \langle f, \mathcal{K}^{(\rho)} f \rangle$, we have

$$a_1^{(\rho)} = \int_0^1 \int_0^1 |x - y|^\rho u(x) \overline{u(y)} dx dy \leq \int_0^1 \int_0^1 |x - y|^\rho |u(x)u(y)| dx dy \leq a_1^{(\rho)}$$

which implies

$$\int_0^1 \int_0^1 |x - y|^\rho (|u(x)u(y)| - u(x)\overline{u(y)}) dx dy = 0.$$

Hence $|u(x)u(y)| = u(x)\overline{u(y)}$ for $(x, y) \in [0, 1]^2$ dx dy-a.e. This implies that for almost all $y \in [0, 1]$, the equality $|u(x)u(y)| = u(x)\overline{u(y)}$ holds for almost all $x \in [0, 1]$. Let y_0 be such that $u(y_0) \neq 0$ and $c = u(y_0)/|u(y_0)| = e^{i\varphi_0}$. Then for almost every $x \in [0, 1]$, we have

$$u(x) = \frac{|u(x)u(y_0)|}{u(y_0)} = c|u(x)|.$$

So up to a nonzero constant multiplier we can suppose that $u \geq 0$ on $[0, 1]$. Therefore

$$a_1^{(\rho)} u(x) = \int_0^1 |x - y|^\rho u(y) dy \geq \int_0^1 u(y) dy > 0.$$

This implies that $a_1^{(\rho)} > 0$ and $u(x) > 0$ for all $x \in [0, 1]$. Then for any other function $v \in L^2(0, 1)$ s.t. $\langle u, v \rangle = 0$, v cannot be an eigenfunction of the eigenvalue $a_1^{(\rho)}$. Otherwise following the same line of reasoning as previously we may write $v = |v|e^{i\tilde{\varphi}_0}$ where $|v|$ is also an eigenfunction associated to $a_1^{(\rho)}$, $|v| > 0$ on $[0, 1]$ and $\langle u, |v| \rangle = e^{-i\tilde{\varphi}_0} \langle u, v \rangle = 0$. But $u, |v| > 0$ contradict the orthogonality

$$\langle u, |v| \rangle = \int_0^1 u(x)|v(x)| dx = 0.$$

Finally recall that if R is regularly varying of index $\rho \in (-1, 0)$, then $NR(N) \rightarrow \infty$ as $N \rightarrow \infty$ by [14, Prop. 1.3.6(v)]. Combining Widom-Shampine's lemma and the convergence of eigenvalues, we obtain

$$a_{N,1}^{(\rho)} = \frac{\lambda_{\max}(T_N(c))}{NR(N)} \xrightarrow{N \rightarrow \infty} a_1^{(\rho)} \quad \text{and} \quad a_{N,2}^{(\rho)} = \frac{\lambda_2(T_N(c))}{NR(N)} \xrightarrow{N \rightarrow \infty} a_2^{(\rho)}.$$

Hence $\lambda_{\max}(T_N(c)) \sim a_1^{(\rho)} NR(N) \rightarrow \infty$ and

$$\frac{\lambda_2(T_N(c))}{\lambda_{\max}(T_N(c))} \xrightarrow{N \rightarrow \infty} \frac{a_2^{(\rho)}}{a_1^{(\rho)}} < 1.$$

Proof of Theorem 2.3 is now completed.

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