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Asymptotics of eigenvalues and eigenvectors of Toeplitz matrices

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Abstract. Analysis of the asymptotic behaviour of the spectral characteristics of Toeplitz matrices as the dimension of the matrix tends to infinity has a history of over 100 years. For instance, quite a number of versions of Szegő's theorem on the asymptotic behaviour of eigenvalues and of the so-called strong Szegő theorem on the asymptotic behaviour of the determinants of Toeplitz matrices are known. Starting in the 1950s, the asymptotics of the maximum and minimum eigenvalues were actively investigated. However, investigation of the individual asymptotics of all the eigenvalues and eigenvectors of Toeplitz matrices started only quite recently: the first papers on this subject were published in 2009–2010. A survey of this new field is presented here.

Bibliography: 55 titles.

Keywords: Toeplitz matrices, eigenvalues, eigenvectors, asymptotic expansion.

§ 1. Introduction

Let $a\colon \mathbb{T} \to \mathbb{C}$ be a Lebesgue integrable function on the unit circle $\mathbb{T}$ and let $T_n(a) := (a_{j-k})_{j,k=0}^{n-1}$ denote the $n \times n$ Toeplitz matrix formed by the Fourier coefficients of a:

$$a_\ell = \frac{1}{2\pi} \int_0^{2\pi} a(e^{i\varphi}) e^{-i\ell\varphi}\, d\varphi.$$

Then a is called the *symbol of the sequence of matrices* $\{T_n(a)\}_{n=1}^{\infty}$.

The behaviour of various spectral characteristics of Toeplitz matrices (eigenvalues and singular values, eigenvectors, determinants, condition numbers and so on) has been an object of active investigation for a century, starting with Szegő's paper [1] (see also the books [2]–[6] and the references there). First and foremost note the numerous versions of Szegő's theorem on the asymptotic distribution of the eigenvalues and the Avram-Parter-type theorems on the asymptotic behaviour of the singular values (see [7]–[12]). There is extensive literature on the asymptotic behaviour of the determinants of Toeplitz matrices (see the monographs [4]–[6] and

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the papers [13]–[19] and the references there). The asymptotics of the maximum and minimum eigenvalues has also been a focus of research (see [20]–[25]). The shape of the limit set of the eigenvalues and its stability have been investigated (see [26]–[28] and [15]). Note that the latter papers (by contrast with most of the papers cited before them) concern the more complicated case of essentially complex-valued symbols, which has not yet been analyzed in full generality.

This considerable interest in the asymptotic behaviour of the spectral characteristics of large Toeplitz matrices was motivated to a significant extent by many important applications: stochastic processes and time series analysis (see [2]); signal processing [29]; the numerical solution of differential and integral equations [30]; image processing [31]; quantum mechanics [32]. We point out the survey paper [19], which discusses the influence of the Ising model in statistical mechanics on the development of the asymptotic theory of the determinants of Toeplitz matrices.

Despite the considerable interest in this field that many authors have displayed, the individual asymptotic behaviour of all eigenvalues and eigenvectors was hardly investigated before 2008. In this connection we can only mention the well-known case of tridiagonal Toeplitz matrices (for instance, see [2] and [5]) and the case of linearly growing matrix elements considered recently in [33], where the eigenvalues and eigenvectors are calculated explicitly. On the other hand the importance of this problem is beyond doubt. For example, many papers are devoted to numerical methods for finding the spectrum of Toeplitz matrices of large size (see [34], [35] and the references there). For dimensions of order 10^3–10^4 this problem can be solved effectively using modern hardware and the algorithms described in the above papers. However, in statistical physics and some other applied problems we encounter dimensions of order 10^8–10^{12}, when no alternative to the asymptotic method exists. In addition, asymptotic formulae give more precise information on the local structure of the set of eigenvalues, the distances between them, accumulation points, their dependence on physical parameters and so on.

In our opinion, the main difficulties arising in the implementation of the asymptotic method are as follows. First, the distances between successive eigenvalues are small (very small when we are in a neighbourhood of an accumulation point!) and our asymptotic formulae must be able to 'separate' them. Furthermore, in addition to n (the dimension of the matrix) being large, the problem involves another parameter, the index j of the eigenvalue. So the asymptotic expansions with respect to n, as n goes to infinity, which we construct must hold uniformly in j, $1 \leqslant j \leqslant n$. Finally, we stress that the determinants that appear in the eigenvalue problem in a natural way are related to one of the most complicated cases, when the symbol of the Toeplitz matrix has zeros on the unit circle.

In the papers [36]–[38], published in 2009–2010, asymptotic representations were constructed in the case of real-valued polynomial symbols (in other words, for Hermitian Toeplitz matrices with a finite number of nontrivial diagonals) that satisfy the so-called SL (simple loop) condition. This means that the real-valued symbol has precisely one minimum and one maximum on the unit circle (the precise definition is expressed by conditions (i) and (ii) in § 2). The SL condition ensures a certain regularity in the arrangement of the eigenvalues; for instance, there are no multiple eigenvalues. In [36] and [37], based on Widom's well-known formula for the determinant of a Toeplitz matrix with polynomial symbol (see [21] and also [5], § 2.4) we found an equation for the eigenvalues, with an exponentially small remainder term, and performed an asymptotic analysis of this equation. In [38] we also used explicit formulae from [39] to calculate eigenvectors of matrices with polynomial symbols, and on this basis we wrote down asymptotic formulae with a remainder term which is exponentially small in n.

In the paper [40] published in 2012 the authors considered the case of infinitely smooth symbols also satisfying the SL condition. Using the asymptotic formula for determinants with Fisher-Hartwig singularities obtained in [18] the authors obtained the same nonlinear equation as in [36] and [37], but with remainder of the form $o(1)$. Next they deduced two-sided estimates for the distance between arbitrary pairs of successive eigenvalues. Before the statement of this theorem the authors mentioned that the smoothness conditions imposed on the symbol can be relaxed.

In [41] and [42] we considered an SL-symbol whose fourth derivative exists and has a certain regularity. We used a method distinct from [37] and [40]. It is based on a precise equation for the eigenvalues, which we derived, and on an asymptotic analysis of it. This equation is given in terms of the inverse matrix of a certain Toeplitz matrix of dimension $n+2$ with positive symbol equal to the ratio of the difference $a(t)-\lambda$ (where λ is the spectral parameter) and a second-order polynomial with the same zeros as this difference. We also point out [43], where the symbol is only assumed to have a first derivative and to satisfy certain additional conditions near the minimum and maximum points.

In [44] and [45] we abandoned the selfadjoint case and investigated Toeplitz matrices with complex-valued symbols. These symbols have a special feature: the corresponding function takes the unit circle to a curve without interior. In other words, the unit circle covers its image with multiplicity two by going in the 'direct' and 'reverse' direction along it. It is well known that then the limit set of the sequence of spectra coincides with this image curve, so for large n the eigenvalues lie close to this curve. Again, as in [36] and [37], in these papers we used known explicit formulae for determinants and inverse matrices because our symbols were polynomials. The resulting equation for the eigenvalues has the same structure as in the real-valued case; however, it must be considered in the complex domain, rather than on an interval of the real line, which brings in quite a number of significant technical difficulties.

In 2009–2010 Kadanoff and his collaborators published the papers [46] and [47], where they considered a symbol, with power-like singularities, in the Fisher-Hartwig class. They presented formulae for the eigenvalues and eigenvectors. These formulae were deduced using heuristic arguments and justified by numerical experiment. In the same period of time, in 2008–2010 we considered a certain subclass of Fisher-Hartwig symbols. In this way, in [48]–[50] we refined and justified the formulae in [46] and [47] rigorously for symbols in the intersection of the classes under consideration.

We also point out the paper [51] close to this field. It looks at the asymptotic behaviour of the eigenvalues and eigenvectors of the Wiener-Hopf integral operator on a finite interval as the length of the interval tends to infinity, and it deals with the case of a symmetric rational (generally speaking, complex-valued) symbol. This problem is related to the same problem for Toeplitz matrices; however, its peculiarity consists in there being an infinite number of eigenvalues and eigenfunctions of the operator for an interval of any length.

Finally, we mention [52] and [53], where we go over from convergence in the sense of distributions (Szegő's theorem) to uniform convergence of the quantile function. For rather wide classes of symbols, approximation of eigenvalues can be expressed in terms of this function.

In § 2 we state results for SL-symbols based on [43] and [42]. Toeplitz matrices with symmetric symbols are the subject of § 3, where we present the main results of [44] and [45]. In § 4 we look at Fisher-Hartwig symbols and discuss results from [48] and [50]. In § 5 we investigate Wiener-Hopf operators on a finite interval (see [51]).

§ 2. SL-symbols

2.1. Eigenvalues. Assume that $\alpha \geqslant 0$ and let W^α denote the weighted Wiener algebra of functions $a\colon \mathbb{T} \to \mathbb{C}$ with representations

$$a(t) = \sum_{j=-\infty}^{\infty} a_j t^j, \qquad t \in \mathbb{T},$$

where the Fourier coefficients satisfy

$$\|a\|_\alpha := \sum_{j=-\infty}^{\infty} |a_j|(1+|j|)^\alpha < \infty.$$

Along with $a \in W^\alpha$ we look at the function $g\colon [0,2\pi] \to \mathbb{R}$ given by $g(\sigma) := a(e^{i\sigma})$.

We define the *class* SL^α as the set of symbols a in W^α such that

(i) a is real-valued;

(ii) the range of g is an interval $[0,\mu]$ where $\mu > 0$; $g(0) = g(2\pi) = 0$, $g''(0) = g''(2\pi) > 0$, and there exists a point $\varphi_0 \in (0,2\pi)$ such that $g(\varphi_0) = \mu$, $g'(\sigma) > 0$ for $\sigma \in (0,\varphi_0)$, $g'(\sigma) < 0$ for $\sigma \in (\varphi_0, 2\pi)$ and $g''(\varphi_0) < 0$.

Note that (i) is equivalent to all the matrices $T_n(a)$, $n \in \mathbb{Z}_+$, being Hermitian (selfadjoint). If $a \in W^\alpha$, then $g \in C^{\lfloor\alpha\rfloor}[0,2\pi]$, where $\lfloor\alpha\rfloor$ is the integer part of α. Thus, if $a \in \mathrm{SL}^\alpha$ with $\alpha \geqslant 1$ then, in particular, g belongs to $C^1[0,2\pi]$. Furthermore, in (ii) we assume that g has second derivatives at the points $\sigma = 0$, φ_0 and 2π.

We will say that the symbol a *belongs to the class* MSL^α with $\alpha \geqslant 1$ if $a \in \mathrm{SL}^\alpha$ and the following additional condition is satisfied:

(iii) there exist functions $q_1, q_2 \in W^\alpha$ such that

$$a(t) = (t-1)q_1(t) \quad \text{and} \quad a(t) - a(e^{i\varphi_0}) = (t - e^{i\varphi_0})q_2(t). \tag{2.1}$$

By Lemma 3.1 in [41], if $a \in \mathrm{SL}^\alpha$, then the functions q_1 and q_2 defined by (2.1) must belong to $W^{\alpha-1}$. In the definition of the *class* MSL^α we impose the stronger condition (iii), that is, we assume that the symbol has additional smoothness at the points where it takes the minimum and maximum values. Using the same lemma we can show that each $a \in \mathrm{MSL}^\alpha$ has the representations

$$a(t) = (t-1)^2 q_3(t) \quad \text{and} \quad a(t) - a(e^{i\varphi_0}) = (t - e^{i\varphi_0})^2 q_4(t), \tag{2.2}$$

with $q_3, q_4 \in W^{\alpha-1}$.

Let $a \in \mathrm{MSL}^\alpha$, $\alpha \geqslant 1$. For each $\lambda \in [0,\mu]$ there exists precisely one point $\varphi_1(\lambda)$ on the interval $[0,\varphi_0]$ such that $g(\varphi_1(\lambda)) = \lambda$ and precisely one point $\varphi_2(\lambda) \in [\varphi_0, 2\pi]$ such that $g(\varphi_2(\lambda)) = \lambda$. In other words φ_1 and φ_2 are the inverse functions of g restricted to $[0,\varphi_0]$ and $[\varphi_0, 2\pi]$, respectively. For each $\lambda \in [0,\mu]$, g takes values not exceeding λ on the intervals $[0,\varphi_1(\lambda)]$ and $[\varphi_2(\lambda), 2\pi]$. Let $\varphi(\lambda)$ denote the arithmetic mean of the lengths of these two intervals:

$$\varphi(\lambda) := \frac{1}{2}(\varphi_1(\lambda) - \varphi_2(\lambda)) + \pi = \frac{1}{2}\big|\{\sigma \in [0,2\pi]\colon\ g(\sigma) \leqslant \lambda\}\big|,$$

where $|\cdot|$ denotes Lebesgue measure on $[0,2\pi]$. Note that $\varphi\colon [0,\mu] \to [0,\pi]$ is continuous and bijective and let $\psi\colon [0,\pi] \to [0,\mu]$ denote its inverse function. Up to a linear change of the argument, φ and ψ are the distribution function and the quantile function of the 'random variable' a on the probability space $[0,2\pi]$ with normalized Lebesgue measure. Set

$$\sigma_1(s) = \varphi_1(\psi(s)) = \varphi_1(\lambda) \quad \text{and} \quad \sigma_2(s) = \varphi_2(\psi(s)) = \varphi_2(\lambda).$$

Note that the derivatives of φ_1 and φ_2 are unbounded in a neighbourhood of 0 and μ, whereas the functions σ_1 and σ_2 have continuous first derivatives on the whole of $[0,\pi]$. In addition, it is easy to see that

$$g(\sigma_1(s)) = g(\sigma_2(s)) = \psi(s) = \lambda.$$

For each $s \in [0,\pi]$ the function $a - \psi(s)$ has two zeros, $t = e^{i\sigma_1(s)}$ and $t = e^{i\sigma_2(s)}$. We can define a positive function b in terms of these:

$$b(t,s) := \frac{(a(t) - \psi(s))e^{is}}{(t - e^{i\sigma_1(s)})(t^{-1} - e^{-i\sigma_2(s)})}, \qquad t \in \mathbb{T}, \quad s \in [0,\pi]. \tag{2.3}$$

Let $\eta\colon [0,\pi] \to \mathbb{R}$ be defined by

$$\eta(s) := \frac{1}{4\pi}\int_0^{2\pi} \frac{\log b(e^{i\sigma}, s)}{\tan\frac{\sigma - \sigma_2(s)}{2}}\, d\sigma - \frac{1}{4\pi}\int_0^{2\pi} \frac{\log b(e^{i\sigma}, s)}{\tan\frac{\sigma - \sigma_1(s)}{2}}\, d\sigma. \tag{2.4}$$

The singular integrals above are taken in the sense of the Cauchy principal value.

Let $\lambda_{1,n}, \ldots, \lambda_{n,n}$ denote the eigenvalues of the matrix $T_n(a)$. We can now state the main results in [43].

Theorem 2.1. *Let $\alpha \geqslant 1$ and $a \in \mathrm{MSL}^\alpha$. Then for each $n \geqslant 1$:*

(i) *all eigenvalues of $T_n(a)$ are distinct, so that $\lambda_{1,n} < \cdots < \lambda_{n,n}$;*

(ii) *the quantities $s_{j,n} := \varphi(\lambda_{j,n})$, $j = 1, \ldots, n$, satisfy the equations*

$$(n+1)s_{j,n} + \eta(s_{j,n}) = \pi j + \Delta^{(1)}_{j,n}, \tag{2.5}$$

where $\Delta^{(1)}_{j,n} = o(1/n^{\alpha-1})$ uniformly in j as $n \to \infty$;

(iii) *for sufficiently large n, equation (2.5) has a unique solution $s_{j,n} \in [0,\pi]$ for each $j = 1, \ldots, n$.*

Set $d_{j,n} = \pi j/(n+1)$.

Theorem 2.2. *If all the assumptions of Theorem 2.1 are fulfilled, then*

$$s_{j,n} = d_{j,n} + \sum_{k=1}^{\lfloor\alpha\rfloor} \frac{p_k(d_{j,n})}{(n+1)^k} + \Delta^{(2)}_{j,n},$$

where $\Delta^{(2)}_{j,n} = o(1/n^\alpha)$ *uniformly in* j *as* $n \to \infty$. *The coefficients* p_k *can be calculated explicitly; in particular,*

$$p_1(s) = -\eta(s) \quad \text{and} \quad p_2(s) = \eta(s)\eta'(s).$$

Theorem 2.3. *If all the assumptions of Theorem 2.1 are fulfilled, then*

$$\lambda_{j,n} = \psi(d_{j,n}) + \sum_{k=1}^{\lfloor\alpha\rfloor} \frac{r_k(d_{j,n})}{(n+1)^k} + \Delta^{(3)}_{j,n},$$

where $\Delta^{(3)}_{j,n} = o\big(\frac{1}{n^\alpha}(d_{j,n}(\pi - d_{j,n}))^{\alpha-1}\big)$ *for* $1 \leqslant \alpha < 2$ *and* $o\big(\frac{1}{n^\alpha} d_{j,n}(\pi - d_{j,n})\big)$ *for* $\alpha \geqslant 2$ *uniformly in* j *as* $n \to \infty$. *The coefficients* r_k *can be calculated explicitly; in particular,*

$$r_1(s) = -\psi'(s)\eta(s) \quad \text{and} \quad r_2(s) = \frac{1}{2}\psi''(s)\eta^2(s) + \psi'(s)\eta(s)\eta'(s).$$

Remark 2.1. Let $a \in \mathrm{MSL}^\alpha$ and $\alpha \in [1,2)$. Then the eigenvalues (for which $\epsilon \leqslant d_{j,n} \leqslant \pi - \epsilon$) have the following asymptotics:

$$\lambda_{j,n} = \psi(d_{j,n}) - \frac{\psi'(d_{j,n})\eta(d_{j,n})}{n+1} + o\left(\frac{1}{n^\alpha}\right).$$

This means that the distance between two successive eigenvalues has the two-sided estimate

$$\frac{c}{n+1} < \lambda_{j+1,n} - \lambda_{j,n} < \frac{C}{n+1}, \tag{2.6}$$

where the constants c and C are independent of j and n. On the other hand the difference $\lambda_{j,n} - \psi(d_{j,n})$ also has order $O(1/n)$. In this connection an approximation

$$\lambda_{j,n} \approx \psi(d_{j,n}) \tag{2.7}$$

is often not sufficient for computations because the approximate formula (2.7) does not 'separate' eigenvalues: a point $\psi(d_{j,n})$ need not lie closest to the jth eigenvalue, but perhaps to some other eigenvalue, for instance, $\lambda_{j+2,n}$.

The assertion of Theorem 2.3 holds for all eigenvalues of $T_n(a)$. However, bearing in mind the behaviour of $\psi(s)$ and $\eta(s)$ close to the endpoints of $[0,\pi]$ (see Lemmas 4.2 and 4.6 in [43]) we can refine the asymptotic formulae for the extreme eigenvalues (cf. Corollary 2.5 in [41]).

Theorem 2.4. *Let* $a \in \mathrm{MSL}^{\alpha}$ *for some* $\alpha \geqslant 2$.

(i) *If* $j/(n+1) \to 0$, *then*

$$\lambda_{j,n} = g(0) + \frac{c_1 j^2}{(n+1)^2} + \frac{c_2 j^2}{(n+1)^3} + \Delta_{j,n}^{(4)}, \tag{2.8}$$

where $c_1 = \pi^2 g''(0)/2$, $c_2 = -\pi^2 g''(0)\eta'(0)$ *and* $\Delta_{j,n}^{(4)} = o((j/n)^3)$ *as* $n \to \infty$.

(ii) *If* $j/(n+1) \to 1$, *then*

$$\lambda_{j,n} = g(\pi) + \frac{c_3 (n+1-j)^2}{(n+1)^2} + \frac{c_4 (n+1-j)^2}{(n+1)^3} + \Delta_{j,n}^{(5)}, \tag{2.9}$$

where $c_3 = \pi^2 g''(\phi_0)/2$, $c_4 = -\pi^2 g''(\phi_0)\eta'(\pi)$ *and* $\Delta_{j,n}^{(5)} = o(((n+1-j)/n)^3)$ *as* $n \to \infty$.

Theorem 2.1 and, as a consequence, also Theorems 2.2 and 2.3 are based on the following result, which provides an exact equation for the eigenvalues. We introduce some further notation. As functions of the form (2.3) are positive, the operator $T_n(b)$ is invertible for each $n \geqslant 1$. Let $\Theta_k \colon \mathbb{T} \times [0,\pi] \to \mathbb{C}$ be defined by

$$\Theta_k(t,s) := [T_k^{-1}(b(\,\cdot\,,s))\chi_0](t).$$

Here the Toeplitz matrix and the inverse matrix are realized as operators in the space

$$\ell_2^{(n)} := \left\{ p(t) \colon p(t) = \sum_{j=0}^{n-1} p_k t^k,\ t \in \mathbb{T} \right\},$$

of polynomials of degree at most $n-1$ and the function χ_0 is identically equal to one: $\chi_0(t) \equiv 1$. In other words, $\Theta_k(t,s)$ is a polynomial of degree at most $n-1$ constructed from the entries in the zeroth column of $T_k^{-1}(b(\,\cdot\,,s))$. For brevity we set $z_k(s) = e^{i\sigma_k(s)}$, $k = 1,2$, so that we take $z_k^m(s)$ to be treated as $e^{im\sigma_k(s)}$.

Theorem 2.5. *Assume that* $\alpha \geqslant 1$, *and let* $a \in \mathrm{MSL}^{\alpha}$ *and* $n \geqslant 1$. *Then* $\lambda = \psi(s)$ *is an eigenvalue of the operator* $T_n(a)$ *if and only if*

$$z_2^{n+1}(s)\Theta_{n+2}(z_1(s),s)\overline{\Theta_{n+2}(z_2(s),s)} = z_1^{n+1}(s)\Theta_{n+2}(z_2(s),s)\overline{\Theta_{n+2}(z_1(s),s)}. \tag{2.10}$$

Note that (2.10) involves the action of the inverse operator $T_{n+2}^{-1}(b(\,\cdot\,,s))$, so it is rather difficult to analyze directly. However, it can be analyzed asymptotically as $n \to \infty$, when we replace $T_{n+2}^{-1}(b(\,\cdot\,,s))$ by the function $\Theta(t,s) := [T^{-1}(b(\,\cdot\,,s))\chi_0](t)$, where $T^{-1}(b)$ is the inverse of the (infinite) Toeplitz operator. As $\Theta(t,s)$ is easy to calculate in terms of the Wiener-Hopf factorization of b, we obtain equation (2.5) in this way.

We conclude this subsection by observing that the formulae in Theorem 2.3 have proved to be numerically highly efficient and yield nice results for $n = 40, \ldots, 100$ (see [37], [41] and [43]).

2.2. Eigenvectors. The arguments resulting in the exact equation (2.10) enable us to deduce exact formulae for the components of the eigenvectors too. The results presented in this subsection were published in [42]. Keeping the notation used in § 2.1, for brevity we write

$$\theta(t) := \Theta(t, s_{j,n}) = [T_{n+2}^{-1}(b(\,\cdot\,, s_{j,n}))\chi_0](t),$$

where we recall that $s_{j,n}$ is related to the jth eigenvalue of the matrix $T_n(a)$ by $\lambda_{j,n} = \psi(s_{j,n})$.

Theorem 2.6. *Assume that $\alpha \geqslant 1$ and let $a \in \mathrm{MSL}^\alpha$, $n \geqslant 1$ and $1 \leqslant j \leqslant n$. Then the vector*

$$X^{(j,n)} = M^{(j,n)} + L^{(j,n)} + R^{(j,n)} \tag{2.11}$$

whose pth component, $p = 0, 1, \dots, n-1$, is given by

$$\begin{aligned} M_p^{(j,n)} &:= z_1^{(n-1)/2-p}|\theta(z_1)| + (-1)^{n-j} z_2^{(n-1)/2-p}|\theta(z_2)|, \\ L_p^{(j,n)} &:= -\frac{z_1^{(n+1)/2}\,\overline{\theta(z_1)}}{2\pi i|\theta(z_1)|}\int_{\mathbb{T}}\biggl(\frac{\theta(t)-\theta(z_1)}{t-z_1} - \frac{\theta(t)-\theta(z_2)}{t-z_2}\biggr)\frac{dt}{t^{p+1}}, \\ R_p^{(j,n)} &:= \overline{L_{n-p-1}^{(j,n)}}, \end{aligned}$$

is an eigenvector corresponding to the eigenvalue $\lambda_{j,n}$. In addition, $M^{(j,n)}$ is conjugation symmetric: $M_p^{(j,n)} = \overline{M_{n-p-1}^{(j,n)}}$.

That is, the eigenvector $X^{(j,n)}$ can be represented as a sum of three vectors: the leading term $M^{(j,n)}$, the term $L^{(j,n)}$, concentrated in a neighbourhood of the left-hand endpoint (for small p its components $L_p^{(j,n)}$ exceed significantly the other terms in absolute value) and the term $R^{(j,n)}$, concentrated in a neighbourhood of the right-hand endpoint. In other words, $M^{(j,n)}$ yields a rough approximation of the eigenvector, which is satisfactory for central components, while $L^{(j,n)}$ and $R^{(j,n)}$ play the roles of left- and right-hand corrections, respectively.

In the symmetric case, that is, when the symbol has the property $a(t) = a(t^{-1})$ (which is equivalent to $g(\sigma) = g(2\pi - \sigma)$), the statement of Theorem 2.6 can be simplified slightly.

Corollary 2.1. *Assume that $\alpha \geqslant 1$ and let $a \in \mathrm{MSL}^\alpha$ be a function with real Fourier coefficients (so that $a(t) = a(t^{-1})$). Then for each $s \in [0, 2\pi]$*

$$\varphi_0 = \pi, \qquad \varphi(\lambda) = [g|_{[0,\pi]}]^{-1}(\lambda), \qquad \psi(s) = g|_{[0,\pi]}(s),$$

$$\sigma_1(s) = s, \qquad \sigma_2(s) = 2\pi - s, \qquad b(e^{i\sigma}, s) = \frac{g(\sigma) - g(s)}{2(\cos s - \cos\sigma)},$$

and the formulae in Theorem 2.6 can be written as follows:

$$\begin{aligned} M_p^{(j,n)} &= 2i^{j+1}|\theta(z_1)|\sin\biggl(\biggl(p - \frac{n-1}{2}\biggr)s_j^{(n)} - \frac{j\pi}{2}\biggr), \\ L_p^{(j,n)} &= \frac{z_1^{(n+1)/2}\,\overline{\theta(z_1)}}{2\pi i|\theta(z_1)|}\int_{\mathbb{T}}\biggl(\frac{\theta(t)-\theta(z_1)}{t-z_1} - \frac{\theta(t)-\overline{\theta(z_1)}}{t-\overline{z}_1}\biggr)\frac{dt}{t^{p+1}}, \\ R_p^{(j,n)} &:= \overline{L_{n-p-1}^{(j,n)}}. \end{aligned} \tag{2.12}$$

Theorem 2.6 reveals the structure of eigenvectors, but can only be implemented if we calculate the exact eigenvalues and can invert $(n+2)\times(n+2)$-matrices. To simplify the formulae in Theorem 2.6 we look at the 'basic' approximation (see Theorem 2.1) of the equation for the eigenvalues,

$$(n+1)s+\eta(s)=\pi j. \tag{2.13}$$

Note that if it has roots $\widehat{s}_{j,n}$, then

$$|s_{j,n}-\widehat{s}_{j,n}|=o\biggl(\frac{1}{n^{\alpha-1}}\biggr), \qquad n\to\infty,$$

uniformly in j. Equation (2.13) is easy to solve numerically. In addition, asymptotic approximations to its solution are given by the formulae in Theorem 2.3. For $s\in[0,\pi]$ we have the Wiener-Hopf factorization

$$b(t,s)=b_+(t,s)b_-(t,s),$$

where

$$b_\pm(t,s)=\exp\biggl(\frac{1}{2}\log b(t,s)\pm\frac{1}{2\pi i}\int_{\mathbb{T}}\frac{\log b(\tau,s)}{\tau-t}\,d\tau\biggr). \tag{2.14}$$

Theorem 2.7. *Let $a\in\mathrm{MSL}^\alpha$, $\alpha\geqslant 3$. Let $\widehat{z}_k:=e^{i\sigma_k(s_{j,n})}$, $k=1,2$, and for $p=0,1,\dots,n-1$ set*

$$\widehat{M}_p^{(j,n)}:=\frac{\widehat{z}_1^{\,(n-1)/2-p}}{|b_+(\widehat{z}_1)|}+(-1)^{n-j}\frac{\widehat{z}_2^{\,(n-1)/2-p}}{|b_+(\widehat{z}_2)|},$$

$$\widehat{L}_p^{(j,n)}:=-\frac{\widehat{z}_1^{\,(n+1)/2}b_+(\widehat{z}_1)}{2\pi i|b_+(\widehat{z}_1)|}\int_{\mathbb{T}}\biggl(\frac{b_+^{-1}(t)-b_+^{-1}(\widehat{z}_1)}{t-\widehat{z}_1}-\frac{b_+^{-1}(t)-b_+^{-1}(\widehat{z}_2)}{t-\widehat{z}_2}\biggr)\frac{dt}{t^{p+1}},$$

$$\widehat{R}_p^{(j,n)}:=\overline{\widehat{L}_{n-p-1}^{(j,n)}}.$$

Let $\Omega^{(j,n)}$ be the vector defined as the remainder term in the formula

$$X^{(j,n)}=\widehat{M}^{(j,n)}+\widehat{L}^{(j,n)}+\widehat{R}^{(j,n)}+\Omega^{(j,n)}. \tag{2.15}$$

Then $\Omega_p^{(j,n)}=o(1/n^{\alpha-3})$ as $n\to\infty$ and this relation holds uniformly in j and p.

The integral involved in Theorem 2.7 can often be simplified. For example, if the symbol is rational, then the integral can be calculated using residue theory. In fact, in this case the function $b(\,\cdot\,,s)$ given by (2.3) can be expressed by

$$b(t,s)=\frac{P(t,s)}{Q(t,s)},$$

where P and Q are polynomials in t. It is easy to see that the symbol $b(\,\cdot\,,s)$ has a Wiener-Hopf factorization $b(t,s)=b_-(t,s)b_+(t,s)$, where

$$b_-(t,s)=\frac{\prod_{j=1}^{\rho}\bigl(1-\frac{1}{\overline{v}_j(s)t}\bigr)}{\prod_{j=1}^{q}\bigl(1-\frac{1}{\overline{u}_j(s)t}\bigr)}, \qquad b_+(t,s)=\beta_0(s)\frac{\prod_{j=1}^{\rho}\bigl(1-\frac{t}{v_j(s)}\bigr)}{\prod_{j=1}^{q}\bigl(1-\frac{t}{u_j(s)}\bigr)};$$

here ρ and q are positive integers, $v_j(s)$ and $\overline{v}_j^{\,-1}(s)$ are formed from the 2ρ zeros of $P(\,\cdot\,,s)$, $u_j(s)$ and $\overline{u}_j^{\,-1}(s)$ are formed from the $2q$ zeros of $Q(\,\cdot\,,s)$, and $\beta_0(s)$ is a constant. Again, for brevity we write $b_\pm(t)$ instead of $b_\pm(t,s_{j,n})$.

Theorem 2.8. *Let a be a rational symbol in* MSL^α. *Assume further that $b(\,\cdot\,,s)$ has only simple poles. Then an eigenvector can be expressed in the following form*:

$$X^{(j,n)}=\widehat{M}^{(j,n)}+\widehat{L}^{(j,n)}+\widehat{R}^{(j,n)}+\Omega^{(j,n)},$$

where, for $p=0,1,\dots,n-1$,

$$\begin{aligned}\widehat{M}_p^{(j,n)}&:=\frac{\widehat{z}_1^{\,(n-1)/2-p}}{|b_+(\widehat{z}_1)|}+(-1)^{n-j}\,\frac{\widehat{z}_2^{\,(n-1)/2-p}}{|b_+(\widehat{z}_2)|},\\ \widehat{L}_p^{(j,n)}&:=\frac{\widehat{z}_1^{\,(n+1)/2}(\widehat{z}_1-\widehat{z}_2)b_+(\widehat{z}_1)}{|b_+(\widehat{z}_1)|}\sum_{m=1}^{q}\frac{v_m^{-p-1}(s_{j,n})}{\frac{\partial b_+}{\partial t}(v_m(s_{j,n}))(v_m(s_{j,n})-\widehat{z}_1)(v_m(s_{j,n})-\widehat{z}_2)},\\ \widehat{R}_p^{(j,n)}&:=\overline{\widehat{L}_{n-p-1}^{(j,n)}},\end{aligned}$$

and for each $\gamma>0$ the limit relation $\Omega_p^{(j,n)}=o(1/n^\gamma)$ holds uniformly in j and p as $n\to\infty$.

Note that if some of the poles of $b(\,\cdot\,,s)$ are multiple, then we can also find an expression for $\widehat{L}_p^{(j,n)}$ using residue theory.

In [42] we presented numerical experiments validating the formulae in Theorems 2.7 and 2.8 and revealing the meaning of the different terms in these formulae.

§ 3. Symmetric symbols

In this section we consider complex-valued polynomial symbols of the form

$$a(t)=\sum_{k=-r}^{r}a_kt^k,\qquad a_k=a_{-k},\quad t\in\mathbb{T},\tag{3.1}$$

where $r\geqslant 1$ and $a_r\neq 0$. Such a polynomial is an even function of the angle φ:

$$a(e^{i\varphi})=a(e^{-i\varphi}),\qquad \varphi\in[0,\pi].\tag{3.2}$$

Let $\mathscr{R}(a)$ denote the set of values of a, that is, the curve on the complex plane formed by the points $a(e^{i\varphi})$:

$$\mathscr{R}(a):=a(\mathbb{T}).$$

Then (for instance, see Theorems 5.28 and 5.32 in [3]) the limit as $n\to\infty$ of the sequence of spectra of the $T_n(a)$ coincides with $\mathscr{R}(a)$. Thus, for sufficiently large n the eigenvalues of the matrix $T_n(a)$ lie in a small neighbourhood of $\mathscr{R}(a)$.

3.1. Eigenvalues of symmetric Toeplitz matrices. Consider a symbol of the form (3.1) and assume that

1) the curve $\mathscr{R}(a)$ does not intersect itself; in particular, $a(1)\neq a(-1)$;
2) $a'(t)\neq 0$ for $t\in\mathbb{T}\setminus\{-1,1\}$;
3) $a''(\pm1)\neq 0$.

As usual, set $g(\varphi):=a(e^{i\varphi})$. Then it follows from (3.2) that

$$\mathscr{R}(a)=\{z\in\mathbb{C}\colon\ z=g(\varphi),\ \varphi\in[0,\pi]\},\qquad g'(0)=g'(\pi)=0,\quad a'(\pm1)=0.$$

For sufficiently small $\delta > 0$ set $\mathscr{R}_\delta(a) := g(\Omega_\delta)$, where

$$\Omega_\delta := \{\varphi \in \mathbb{C}\colon 0 < \operatorname{Re}\varphi < \pi,\ |\operatorname{Im}\varphi| < \delta\}.$$

First we look at the equation $a(z) - \lambda = 0$ for $\lambda \in \mathscr{R}(a) \setminus \{a(1), a(-1)\}$. It has $2r$ roots in the complex plane, which we arrange in the order of ascending absolute values. Taking the symmetry (3.2) into account we can represent this set of roots as follows:

$$\left\{u_1, u_2, \ldots, u_{r-1}, u_r, \frac{1}{u_r}, \frac{1}{u_{r-1}}, \ldots, \frac{1}{u_2}, \frac{1}{u_1}\right\}. \tag{3.3}$$

Thus, the root u_k, $1 \leqslant k \leqslant r-1$, which lies outside the unit circle $\mathbb{T}$, corresponds to the root $1/u_k$ inside $\mathbb{T}$. By conditions 1) and 2) precisely two roots lie on $\mathbb{T}$:

$$u_r = e^{i\varphi} \quad \text{and} \quad \frac{1}{u_r} = e^{-i\varphi}, \qquad \varphi \in (0, \pi). \tag{3.4}$$

The other $2r-2$ roots are separated from $\mathbb{T}$ uniformly in $\lambda \in \mathscr{R}(a) \setminus \{a(1), a(-1)\}$. Now let $\lambda \in \mathscr{R}_\delta(a)$. It is easy to show that by 2) and 3), for sufficiently small δ the equation $a(z) - \lambda = 0$ has a unique root in a neighbourhood of the upper half-circle, which has the form $z_r = e^{i\varphi}$, where $\varphi := \varphi(\lambda)$ is an analytic function in Ω_δ. In accordance with this definition $g(\varphi(\lambda)) = \lambda$ for $\lambda \in \mathscr{R}_\delta(a)$. We will regard the $u_k := u_k(\lambda) = u_k(g(\varphi))$ as functions of φ and denote them by $u_k := u_k(\varphi)$, where $\varphi \in \Omega_\delta$. Now there exists a positive δ_0 such that

$$\inf_{k=1,2,\ldots,r-1} \inf_{\lambda \in \mathscr{R}_\delta(a)} \operatorname{dist}(u_k, \mathbb{T}) \geqslant e^{\delta_0} - 1 \quad (> \delta_0). \tag{3.5}$$

Consider the functions

$$h(z) = \prod_{k=1}^{r-1} \left(1 - \frac{z}{u_k(\varphi)}\right), \qquad z \in \mathbb{C}, \quad \varphi \in \Omega_\delta, \tag{3.6}$$

and

$$\theta(\varphi) = -i \log \frac{h(e^{i\varphi})}{h(e^{-i\varphi})}, \qquad \varphi \in \Omega_\delta. \tag{3.7}$$

It follows from the definition (3.6) of h that $h(z) \neq 0$ for $z \in \Gamma_\delta := \exp\{i\Omega_\delta\}$. Hence we can take a continuous branch of the function $\theta(\varphi)$ in the domain $\varphi \in \overline{\Omega_\delta}$ such that $\theta(0) = \theta(\pi) = 0$. We introduce the quantities

$$d_{j,n} := \frac{\pi j}{n+1} \quad \text{and} \quad e_{j,n} := d_{j,n} - \frac{\theta(d_{j,n})}{n+1} \tag{3.8}$$

and the domains

$$\Omega_{j,n} := \left\{\varphi \in \mathbb{C}\colon |\varphi - e_{j,n}| \leqslant \frac{c_{j,n}}{(n+1)^2}\right\}, \tag{3.9}$$

where $j = 1, 2, \ldots, n$, $c_{j,n} = 3M'_{j,n}M_{j,n}$,

$$M_{j,n} = \sup_{\varphi \in \Omega_{j,n}} |\theta(\varphi)| \quad \text{and} \quad M'_{j,n} = \sup_{\varphi \in \Omega_{j,n}} |\theta'(\varphi)|. \tag{3.10}$$

Note that $c_{j,n}$ is bounded uniformly in j and n.

Now we state the main result of this subsection.

Theorem 3.1. *Let a be a function of the form (3.1) such that conditions 1)–3) are satisfied. Then the following results hold for sufficiently large n.*

(i) *All the eigenvalues of $T_n(a)$ are simple and $\lambda_{j,n} \in g(\Omega_{j,n})$ for $j = 1, 2, \ldots, n$.*

(ii) *The points $\varphi_{j,n}$ $(\in \Omega_\delta)$ such that $\lambda_{j,n} = g(\varphi_{j,n})$ satisfy*

$$(n+1)\varphi_{j,n} + \theta(\varphi_{j,n}) = \pi j + \Delta_n(\varphi_{j,n}), \qquad j = 1, 2, \ldots, n, \tag{3.11}$$

where $|\Delta_n(\varphi)| = O(e^{-\Delta \cdot n})$ and $|\Delta_n'(\varphi)| = O(ne^{-\Delta \cdot n})$ for some positive constant Δ, uniformly in $\varphi \in \Omega_{j,n}$ and j as $n \to \infty$. Equation (3.11) has a unique solution in the domain $\Omega_{j,n}$.

(iii) *Each equation of the form*

$$(n+1)\varphi_{j,n}^* + \theta(\varphi_{j,n}^*) = \pi j, \qquad j = 1, 2, \ldots, n, \tag{3.12}$$

has a unique solution in $\Omega_{j,n}$, and $\lambda_{j,n} = g(\varphi_{j,n}^*) + O(e^{-\Delta \cdot n}/n)$ for some positive constant Δ uniformly in j as $n \to \infty$.

(iv) *The function*

$$H_{j,n}(\varphi) := d_{j,n} - \frac{\theta(\varphi)}{n+1} \tag{3.13}$$

is a contraction mapping of $\Omega_{j,n}$ into itself; if

$$\varphi_{j,n}^{(1)} = e_{j,n} \quad \textit{and} \quad \varphi_{j,n}^{(k)} = H_{j,n}(\varphi_{j,n}^{(k-1)}), \quad k \geqslant 2, \tag{3.14}$$

then

$$|\varphi_{j,n}^* - \varphi_{j,n}^{(k)}| = 6\biggl(\frac{M_{j,n}'}{n+1}\biggr)^k \biggl(\frac{M_{j,n}}{n+1}\biggr), \tag{3.15}$$

$$|\lambda_{j,n}^* - g(\varphi_{j,n}^{(k)})| = 6\biggl(\frac{M_{j,n}'}{n+1}\biggr)^k \biggl(\frac{M_{j,n}K_{j,n}'}{n+1}\biggr), \tag{3.16}$$

where $M_{j,n}$ and $M_{j,n}'$ are defined by (3.10) and $K_{j,n}' = \sup_{\varphi \in \Omega_j} |g(\varphi)|$.

Setting $k = 2$ in (3.15) and (3.16) we obtain the following asymptotic expansions for $\varphi_{j,n}$ and $\lambda_{j,n}$.

Theorem 3.2. *Let $a(t)$ be a symbol of the form (3.1) such that conditions 1)–3) are satisfied. Then*

(i)

$$\varphi_{j,n} = d_{j,n} - \frac{\theta(d_{j,n})}{n+1} + \frac{\theta(d_{j,n})\theta'(d_{j,n})}{(n+1)^2} + \Delta_{j,n}^{(6)}, \tag{3.17}$$

where $\Delta_{j,n}^{(6)} = O(1/n^3)$ as $n \to \infty$ uniformly in $j = 1, 2, \ldots, n$;

(ii)

$$\lambda_{j,n} = g(d_{j,n}) + \frac{c_1(d_{j,n})}{n+1} + \frac{c_2(d_{j,n})}{(n+1)^2} + \Delta_{j,n}^{(7)}, \tag{3.18}$$

where $\Delta_{j,n}^{(7)} = O(d_{j,n}(\pi - d_{j,n})/n^3)$ uniformly in $j = 1, 2, \ldots, n$ as $n \to \infty$,

$$c_1(d) = -g'(d)\theta(d) \quad \textit{and} \quad c_2(d) = \frac{1}{2}g''(d)\theta^2(d) + g'(d)\theta(d)\theta'(d).$$

We have given the asymptotic formulae (3.17) and (3.18) as examples. Using estimates (3.15) and (3.16) for $k > 2$ we can find arbitrarily many terms of the expansions for $\lambda_{j,n}$ and $\varphi_{j,n}$.

As a consequence of Theorem 3.2, we obtain a result on the extreme eigenvalues.

Theorem 3.3. *Let a be a symbol of the form* (3.1) *and assume that conditions* 1)–3) *are satisfied. Then the following results hold*:

(i) *if* $j^2/(n+1) \to 0$, *then*

$$\lambda_{j,n} = g(0) + \frac{c_3 j^2}{(n+1)^2} + \frac{c_4 j^2}{(n+1)^3} + \Delta^{(8)}_{j,n}, \tag{3.19}$$

where $c_3 = \pi^2 g''(0)/2$, $c_4 = -\pi^2 g''(0)\theta'(0)$ *and* $\Delta^{(8)}_{j,n} = O(j^4/n^4)$ *as* $n \to \infty$;

(ii) *if* $(n+1-j)^2/(n+1) \to 0$, *then*

$$\lambda_{j,n} = g(\pi) + \frac{c_5 (n+1-j)^2}{(n+1)^2} + \frac{c_6 (n+1-j)^2}{(n+1)^3} + \Delta^{(9)}_{j,n}, \tag{3.20}$$

where $c_5 = \pi^2 g''(\pi)/2$, $c_6 = -\pi^2 g''(\pi)\theta'(\pi)$ *and* $\Delta^{(9)}_{j,n} = O((n+1-j)^4/n^4)$ *as* $n \to \infty$.

Remark 3.1. The leading term of the asymptotic expansion (3.18) corresponds to a point $g(d)$ on the curve $\mathscr{R}(a)$. This approximation to the eigenvalue $\lambda_{j,n} \approx g(d)$ has accuracy $O(1/n)$ and cannot be considered satisfactory: the distance between successive eigenvalues also has order $O(1/n)$. Thus, this approximation 'does not separate' eigenvalues (see Remark 2.1). On the other hand the approximation $\lambda_{j,n} \approx g(e_{j,n})$ has accuracy $O(1/n^2)$ (see (3.16) for $k = 1$) and can be treated as an individual approximation to the eigenvalue $\lambda_{j,n}$. In particular, the expression $g(e_{j,n})$ can be used to analyze the position of $\lambda_{j,n}$ relative to the curve $\mathscr{R}(a)$. In fact,

$$g(e_{j,n}) = g\biggl(d - \frac{\theta(d)}{n+1}\biggr) = g\biggl(d - \frac{\operatorname{Re}\theta(d)}{n+1} - i\,\frac{\operatorname{Im}\theta(d)}{n+1}\biggr),$$

where

$$\operatorname{Re}\theta(d) = \arg\frac{h(e^{id})}{h(e^{-id})}, \qquad \operatorname{Im}\theta(d) = -\log\frac{|h(e^{id})|}{|h(e^{-id})|}.$$

Setting

$$\widetilde{e}_{j,n} := d - \frac{\operatorname{Re}\theta(d)}{n+1} = \frac{\pi j - \operatorname{Re}\theta(d)}{n+1}$$

we obtain

$$g(e_{j,n}) = g(\widetilde{e}_{j,n}) - i\,\frac{g'(\widetilde{e}_{j,n})\operatorname{Im}\theta(d)}{n+1} + O\biggl(\frac{1}{n^2}\biggr).$$

That is, to within $O(1/n^2)$ the eigenvalue $\lambda_{j,n}$ lies on the normal to $\mathscr{R}(a)$ at the point $g(\widetilde{e}_{j,n})$. The distance from $\lambda_{j,n}$ along the normal has order $O(1/n)$, provided that $\operatorname{Im}\theta(d) \neq 0$. Note that depending on the sign of $\operatorname{Im}\theta(d)$ the point $\lambda_{j,n}$ lies to the right or the left of $\mathscr{R}(a)$ in the plane.

The numerical gain from the formulae in Theorems 3.1–3.3 was fairly comprehensively analyzed in [44].

3.2. Eigenvectors of symmetric Toeplitz matrices.

Theorem 3.4. *Let $a(t)$ be a symbol of the form (3.1) and assume that conditions 1)–3) are satisfied. Then eigenvectors $X^{(j,n)} = (X_p^{(j,n)})_{p=1}^n$ associated with the eigenvalues $\lambda_{j,n}$ can be chosen so that the following asymptotic expressions (putting $\lambda := \lambda_{j,n}$ for brevity) hold:*

$$X_p^{(j,n)} = a_{j,p}(\lambda) + b_{j,p}(\lambda) + c_{j,p}(\lambda) + O(e^{-\delta_1 n}), \qquad p = 1, 2, \dots, n, \tag{3.21}$$

where the remainder estimate is uniform with respect to λ, and δ_1 is independent of n, j and p. Furthermore,

$$a_{j,p}(\lambda) = \frac{(-1)^j e^{-ip\varphi(\lambda)}}{h_\lambda(e^{i\varphi(\lambda)})} - \frac{(-1)^j e^{ip\varphi(\lambda)}}{h_\lambda(e^{-i\varphi(\lambda)})}, \tag{3.22}$$

$$b_{j,p}(\lambda) = (-1)^j \sum_{\nu=1}^{r-1} \biggl[\frac{2i\sin(\varphi(\lambda))}{u_\nu^p(\lambda)} \cdot \frac{1}{(u_\nu(\lambda) - e^{i\varphi(\lambda)})(u_\nu(\lambda) - e^{-i\varphi(\lambda)})h'_\lambda(u_\nu(\lambda))}\biggr] \tag{3.23}$$

and

$$c_{j,p}(\lambda) = (-1)^{j-1} b_{j,n+1-p}(\lambda). \tag{3.24}$$

Remark 3.2. Theorem 3.4 was established as Theorem 2.3 in [45], albeit under the additional assumption that the function $a(t) - \lambda$ has only simple zeros for each λ in $\mathscr{R}_\delta(a)$. Now, after [42], we can drop this technical condition.

Remark 3.3. Let us analyze the formulae in Theorem 3.4. As the root $u_\nu(\lambda)$ lies outside the unit circle, the term $b_{j,p}(\lambda)$ is small for components with large index p, and the term $c_{j,p}(\lambda)$ is small when $n - p$ is large. In addition, it is easy to see that, as n grows, the contribution of these terms can be significant for a few of the first and last components, respectively. Note however, that the number of these components does not depend significantly on n. Components in the middle part of the vector $X^{(j,n)}$ are mostly well approximated by $a_{j,p}(\lambda)$ from (3.22). A numerical illustration of this observation can be found in [45].

Remark 3.4. In (3.22)–(3.24) we can replace the exact eigenvalues by their approximations (asymptotic expressions), for instance, the ones given by (3.18).

Remark 3.5. Formulae (3.22)–(3.24) become much simpler for eigenvectors corresponding to the extreme eigenvalues (see Theorem 2.4 in [45]).

§ 4. Eigenvalues and eigenvectors of Hessenberg Toeplitz matrices and a problem of Dai, Geary and Kadanoff's

4.1. Eigenvalues. Dai, Geary and Kadanoff [46] and Kadanoff [47] considered symbols of the form

$$a(t) = \left(2 - t - \frac{1}{t}\right)^\gamma (-t)^\beta, \qquad t \in \mathbb{T}, \tag{4.1}$$

where $0 < \gamma < -\beta < 1$. They conjectured that for large n the corresponding eigenvalues $\lambda = \lambda_{j,n}$ satisfy

$$\lambda_{j,n} \approx a\biggl(n^{(2\gamma+1)/n} \exp\biggl\{-i\biggl(\frac{2\pi j}{n}\biggr) - \frac{i}{n} d\biggl(\frac{2\pi j}{n}\biggr)\biggr\} + o\biggl(\frac{1}{n}\biggr)\biggr), \tag{4.2}$$

where d is some function (unknown to them). This conjecture was supported by numerical experiment and a certain heuristic argument.

Now we state the main results of [48] and compare these with (4.2).

As usual, let H^∞ be the Hardy space of bounded analytic functions in the unit disc $\mathbb{D}$. For a fixed function $a \in C(\mathbb{T})$ let $\operatorname{wind}_\lambda(a)$ denote the number of windings of the image of a, that is, the curve $\mathscr{R}(a) := \{z \in \mathbb{C}\colon\ z = a(t),\ t \in \mathbb{T}\}$, about the point $\lambda \in \mathbb{C} \setminus \mathscr{R}(a)$, and let $\mathscr{D}(a)$ be the set of points $\lambda \in \mathbb{C}$ for which $\operatorname{wind}_\lambda(a) \neq 0$. In this subsection we treat matrices $T_n(a)$ with symbols of the form $a(t) = t^{-1}h(t)$, where

1) $h \in H^\infty$ and $h_0 := h(0) \neq 0$;
2) $h(t) = (1-t)^\alpha f(t)$, where $\alpha \in [0,\infty) \setminus \mathbb{Z}$ and $f \in C^\infty(\mathbb{T})$;
3) h extends analytically to an open neighbourhood W of the set $\mathbb{T} \setminus \{1\}$ which does not contain 1;
4) $\mathscr{R}(a)$ is a Jordan curve in $\mathbb{C}$ and $\operatorname{wind}_\lambda(a) = -1$ for each $\lambda \in \mathscr{D}(a)$.

Note that if we set $\gamma = \alpha/2$ and $\beta = \gamma - 1$ in (4.1), then the symbol satisfies conditions 1)–4), with $f(t) \equiv (-1)^{2\gamma-1}$.

Let $D_n(a)$ denote the determinant of $T_n(a)$. Then the eigenvalues of the matrix $T_n(a)$ are the roots of the equation $D_n(a-\lambda) = 0$. By our assumptions $T_n(a)$ is a Hessenberg matrix, that is, it can be obtained from a lower triangular matrix by adding one nontrivial diagonal. In combination with the Baxter-Schmidt formula (see [5], § 2.3, for instance) this enables us to represent $D_n(a-\lambda)$ as a Fourier integral. Its value depends significantly on the pole at λ and the singularity of the term $(1-t)^\alpha$ at 1. Let W_0 be a small neighbourhood of zero in $\mathbb{C}$. We can show that for each $\lambda \in \mathscr{D}(a) \cap (a(W) \setminus W_0)$ there exists a unique point $t_\lambda \notin \overline{\mathbb{D}}$ such that $a(t_\lambda) = \lambda$. An asymptotic analysis of the Fourier integral just mentioned yields an asymptotic representation for $D_n(a-\lambda)$.

In all the statements in this subsection we take

$$\alpha_0 := \min\{\alpha, 1\} \quad \text{and} \quad c_\alpha := \frac{\pi}{f(1)\Gamma(\alpha+1)\sin(\alpha\pi)}.$$

Theorem 4.1. *Let $a(t) = t^{-1}h(t)$ be a symbol satisfying conditions 1)–4). Then for each small open neighbourhood W_0 of zero in $\mathbb{C}$ and points $\lambda \in \mathscr{D}(a) \cap (a(W) \setminus W_0)$*

$$D_n(a-\lambda) = (-h_0)^{n+1}\biggl(\frac{1}{t_\lambda^{n+2} a'(t_\lambda)} - \frac{1}{c_\alpha \lambda^2 n^{\alpha+1}} + R_1(n,\lambda)\biggr), \tag{4.3}$$

where $R_1(n,\lambda) = O(1/n^{\alpha+\alpha_0+1})$ as $n \to \infty$ uniformly in $\lambda \in a(W) \setminus W_0$.

We now turn to the main results in this subsection. Set $\omega_n := \exp(-2\pi i/n)$. For the values of n under consideration there exist positive integers n_1 and n_2 such that $\omega_n^{n_1}, \omega_n^{n-n_2} \in a^{-1}(W_0)$, but $\omega_n^{n_1+1}, \omega_n^{n-n_2-1} \notin a^{-1}(W_0)$. Recall that $a(t_\lambda) = \lambda$.

Theorem 4.2. *Let $a(t) = t^{-1}h(t)$ be a symbol with properties 1)–4). Then for each small open neighbourhood W_0 of zero and for each j between n_1 and $n - n_2$,*

$$t_{\lambda_{j,n}} = n^{(\alpha+1)/n}\omega_n^j\left(1 + \frac{1}{n}\log\left(\frac{c_\alpha a^2(\omega_n^j)}{a'(\omega_n^j)\omega_n^{2j}}\right) + R_2(n,j)\right), \tag{4.4}$$

where $R_2(n,j) = O(1/n^{\alpha_0+1}) + O(\log n/n^2)$ as $n \to \infty$ uniformly in j.

Thus formula (4.4) proves the conjecture (4.2) in the special case when $\beta = \gamma - 1$. In addition, we have found the function

$$d(t) := t\log\left(\frac{c_\alpha a^2(t)}{a'(t)t^2}\right)$$

and have refined the order of the error term.

Taking the value of a at the point (4.4) we obtain the following asymptotic expression for $\lambda_{j,n}$.

Theorem 4.3. *Let $a(t) = t^{-1}h(t)$ be a symbol with properties 1)–4). Then for each small open neighbourhood W_0 of zero in $\mathbb{C}$ and j between n_1 and $n - n_2$,*

$$\lambda_{j,n} = a(\omega_n^j) + (\alpha+1)\omega_n^j a'(\omega_n^j)\frac{\log n}{n} + \frac{\omega_n^j a'(\omega_n^j)}{n}\log\left(\frac{c_\alpha a^2(\omega_n^j)}{a'(\omega_n^j)\omega_n^{2j}}\right) + R_3(n,j), \tag{4.5}$$

where $R_3(n,j) = O(1/n^{\alpha_0+1}) + O(\log^2 n/n^2)$ as $n \to \infty$ uniformly for j between n_1 and $n - n_2$.

Remark 4.1. Here we have written out only a few of the first terms of the asymptotic expansion. Note however that using our method an arbitrary number of terms in this expansion can be obtained.

A numerical illustration of Theorem 4.3 can be found in [48].

4.2. Eigenvectors. To present the formulae for eigenvectors we define a function $b^{(j,n)}$ on $\mathbb{T}$ by

$$b^{(j,n)}(t) := \frac{1}{h(t) - \lambda_{j,n}t}$$

and let $b_p^{(j,n)}$ denote its pth Fourier coefficient.

Theorem 4.4. *If $b_{n-1}^{(j,n)} \neq 0$, then*

$$X^{(j,n)} := (b_p^{(j,n)})_{p=0}^{n-1} \tag{4.6}$$

is an eigenvector of $T_n(a)$ corresponding to the eigenvalue $\lambda_{j,n}$.

The next result describes the asymptotic behaviour of $b_p^{(j,n)}$ for large p and n.

Theorem 4.5. *The relation*

$$b_p^{(j,n)} = \frac{D_2(\omega_n^j)\omega_n^{-jp}}{(D_1(\omega_n^j)n^{\alpha+1})^{p/n}}(1 + R_1(j,n,p)) + \frac{D_3(\omega_n^j)}{p^{\alpha+1}}(1 + R_2(j,n,p)) \tag{4.7}$$

holds, where

$$D_1(u) := \frac{c_\alpha a^2(u)}{u^2 a'(u)}, \qquad D_2(u) := \frac{-1}{u^2 a'(u)}, \qquad D_3(u) := \frac{1}{c_\alpha a^2(u)},$$
$$R_1(j,n,p) = O\biggl(\frac{p}{n^{\alpha_0+1}}\biggr) + O\biggl(\frac{\log n}{n}\biggr) \quad \textit{uniformly in } j \textit{ as } p,n\to\infty,$$
$$R_2(j,n,p) = O\biggl(\frac{\log n}{n}\biggr) + O\biggl(\frac{1}{p}^{\alpha_0}\biggr) \quad \textit{uniformly in } n \textit{ and } j.$$

We stress that we only consider points ω_n^j in $W\setminus a^{-1}(W_0)$. In this domain the functions a and a' are bounded and separated away from zero. Hence the D_ℓ, $\ell=1,2,3$, are also bounded and separated away from zero there. Note also that since $p<n$, R_1 tends to zero as $n\to\infty$.

Remark 4.2. We compare the above results on the asymptotics of eigenvectors and the results in [46] and [47] concerning symbols of the form (4.1).

We have already mentioned that for $\beta=\gamma-1$ the function (4.1) becomes 'our' symbol of the form $a(t)=t^{-1}h(t)$, with $h(t)=(-1)^{2\gamma-1}(1-t)^{2\gamma}$. In [46] the authors conjectured that an eigenvector has the form

$$X^{(j,n)} \approx \biggl(\frac{1+O(1/n)}{t^p_{\lambda_{j,n}}}\biggr)_{p=0}^{n-1}, \quad \text{where} \quad t_{\lambda_{j,n}} \approx n^{(\alpha+1)/n}\omega_n^j \tag{4.8}$$

as $n\to\infty$. Theorem 4.2 refines this conjecture and proves it while giving a rigorous estimate for the error term. Note that

$$D_1^{p/n}(\omega_n^j) = \exp\biggl(\frac{p}{n}\log D_1(\omega_n^j)\biggr) = \exp\biggl(\frac{p}{n}\,O(1)\biggr) = 1+O\biggl(\frac{p}{n}\biggr).$$

This shows that (4.8) corresponds to the first term on the right-hand side of (4.7) in the case when the ratio p/n is close to zero. Otherwise the representation (4.8) can give a large error: the corresponding numerical examples were presented in [50].

Remark 4.3. Our asymptotic expansion (4.7) holds for $\lambda_{j,n}$ outside a small neighbourhood W_0 of zero and for large p. For small p, for instance, $p=0,1,\dots,m-1$, $m\ll n$, the values of $b_p^{(j,n)}$ can be calculated using the relation between the Fourier coefficients of $b^{(j,n)}=1/(h(t)-\lambda_{j,n}t)$ and $h(t)=(1-t)^\alpha f(t)$. Here we obtain a triangular system of equations, which can be solved by $O(m^2)$ operations, and taking $m=[\sqrt{n}]$ we need $O(n)$ operations. We can calculate the remaining components using asymptotic formulae (4.7), which also have order of complexity $O(n)$ from a numerical standpoint.

§ 5. Spectral theory of Wiener-Hopf operators with symmetric complex kernels and rational symbols on a large interval

A truncated Wiener-Hopf operator has the form

$$(K_\tau f)(t) := f(t) + \int_0^\tau k(t-s)f(s)\,ds, \qquad t\in(0,\tau). \tag{5.1}$$

We assume here that k is a function in $L^2(\mathbb{R})$, so the integral operator in (5.1) is a compact Hilbert-Schmidt operator on $L^2(0,\tau)$ for every $\tau > 0$. Let $\operatorname{sp} K_\tau$ denote the spectrum of K_τ. As $K_\tau - I$ is compact, all points in $\operatorname{sp} K_\tau \setminus \{1\}$ are eigenvalues.

Here we make the two basic assumptions. First, k is a symmetric complex function, that is $k(t) = k(-t)$ for $t \in \mathbb{R}$. Second,

$$a(x) := 1 + \int_{-\infty}^{\infty} k(t) e^{ixt}\, dt, \qquad x \in \mathbb{R},$$

the so-called symbol of the operator, is rational. These two assumptions are equivalent to a representation of the form

$$k(t) = \begin{cases} \displaystyle\sum_{\ell=1}^{m} p_\ell(t) e^{-\lambda_\ell t} & \text{for } t > 0, \\ \displaystyle\sum_{\ell=1}^{m} p_\ell(-t) e^{-\lambda_\ell t} & \text{for } t < 0, \end{cases}$$

where the λ_ℓ are complex numbers with $\operatorname{Re}\lambda > 0$ and the $p_\ell(t)$ are polynomials with complex coefficients. Since $k(t) = k(-t)$ for all $t \in \mathbb{R}$ if and only if $a(x) = a(-x)$ for all $x \in \mathbb{R}$, the symbol is an even rational function, and we can write

$$a(x) = \prod_{j=1}^{r} \frac{x^2 - \zeta_j^2}{x^2 - \mu_j^2}, \qquad x \in \mathbb{R},$$

where $\zeta_j \in \mathbb{C}$, $\mu_j \in \mathbb{C}$, $\operatorname{Re}\mu_j > 0$ and $\zeta_j^2 \neq \mu_j^2$ for all j and k. To stress the dependence of K_τ on the symbol a, following [54] we denote K_τ by $W_\tau(a)$.

Putting $\overline{\mathbb{R}} := \mathbb{R} \cup \{\pm\infty\}$ we extend the symbol by setting $a(\pm\infty) = 1$. As before, let $\mathscr{R}(a)$ be the essential image of a, that is, $\mathscr{R}(a) := a(\overline{\mathbb{R}})$. By our assumptions $\mathscr{R}(a)$ is an analytic curve in the plane such that as x varies from $-\infty$ to 0 the value $a(x)$ of the symbol ranges from 1 to $a(0)$ on this curve, and when x varies further from 0 to $+\infty$, the value of the symbol traverses $\mathscr{R}(a)$ from $a(0)$ to 1 in the reverse direction.

It was shown in [54] that in our case the limit of $\operatorname{sp} W_\tau(a)$ coincides with $\mathscr{R}(a)$. So we will look for eigenvalues in a neighbourhood of $\mathscr{R}(a)$. We assume in addition that $\mathscr{R}(a)$ is a curve without self-intersections.

With each positive number τ we associate the half-strip

$$S_\tau := \left\{ z \in \mathbb{C} \colon\ \operatorname{Re} z > 0,\ |\operatorname{Im} z| \leqslant \frac{\beta}{\tau} \right\},$$

where $\beta > 0$ is fixed and sufficiently large. Consider a finite covering of the half axis by open intervals $I_1 \cup \cdots \cup I_N = (0,\infty)$. For each interval $I \in \{I_n\}_{n=1}^N$ we consider either the closed subintervals of I of the form

$$I_{k,t} := \left[\left(k - \frac{1}{2}\right)\frac{\pi}{\tau}, \left(k + \frac{1}{2}\right)\frac{\pi}{\tau} \right]$$

or the closed intervals of the form

$$I_{k,t} := \left[k\frac{\pi}{\tau}, (k+1)\frac{\pi}{\tau} \right]$$

lying in I (depending on the position of $b(I)$[1] in $\mathbb{C}$); see (3.6) and (3.7) in [51]. In this way we obtain N families of rectangles

$$S_{k,\tau} := \{z \in S_\tau\colon \operatorname{Re} z \in I_{k,\tau}\}.$$

The proofs of the main results in this section are based on an explicit formula (see [55]) for the Fredholm determinants

$$\det\left(\frac{1}{1-\lambda}(W_\tau(a) - \lambda I)\right). \tag{5.2}$$

Note that for each $\lambda \in \mathscr{R}(a) \setminus \{1\}$ the equation $a(z) = \lambda$ has precisely $2r$ complex roots

$$\omega_1(\lambda),\ \omega_2(\lambda),\ \ldots,\ \omega_r(\lambda),\ -\omega_1(\lambda),\ -\omega_2(\lambda),\ \ldots,\ -\omega_r(\lambda). \tag{5.3}$$

We can number them so that $\omega_1(\lambda) \in \mathbb{R}$ and $\operatorname{Im} \omega_j(\lambda) > 0$ for $j \geqslant 2$.

Fix an open neighbourhood U of $\mathscr{R}(a)$. Then $\operatorname{sp} W_\tau \subset U$ if τ is sufficiently large. Set $\Pi = \{z \in \mathbb{C}\colon |\operatorname{Im} z| < \delta,\ a(z) \in U\}$. For $z \in \Pi$ consider the two functions

$$Q(z) := \prod_{\ell=1}^{r} (z - i\mu_\ell) \quad \text{and} \quad P(z) := \prod_{\ell=2}^{r} [z - \omega_\ell(a(z))]$$

and set

$$b(z) := \frac{Q(-z)^2}{Q(z)^2} \cdot \frac{P(z)^2}{P(-z)^2}.$$

The main result of this section is the following.

Theorem 5.1. *Let* $\operatorname{clos} I$ *be the closure of* I *in* $[0,\infty]$ *and assume that for* λ *in* $a(\operatorname{clos} I)$ *all the roots* $\omega_2(\lambda), \ldots, \omega_r(\lambda)$ *are distinct. Then there exists* τ_0 *such that the following results hold for all* $\tau > \tau_0$.

(i) *If* $\lambda = a(z) \in U$ *is an eigenvalue of* $W_\tau(a)$ *such that* $\operatorname{Re} z \in I_{k,\tau}$ *for some* $I_{k,\tau} \subset I$, *then* $z \in S_{k,\tau}$.

(ii) *For each* $I_{k,\tau} \subset I$ *the set* $a(S_{k,\tau})$ *contains a unique eigenvalue* $\lambda_{k,\tau}$ *of* $W_\tau(a)$, *which has algebraic multiplicity* 1.

(iii) *The function*

$$\Phi_{k,\tau}(z) := \frac{k\pi}{\tau} + \frac{1}{2i\tau} \log b(z)$$

is a contraction mapping of $S_{k,\tau}$ *into itself; for*

$$z_{k,\tau}^{(0)} := \frac{k\pi}{\tau} \quad \text{and} \quad z_{k,\tau}^{(n)} := \Phi_{k,\tau}\big(z_{k,\tau}^{(n-1)}\big), \quad n \geqslant 1,$$

the relation

$$\lambda_{k,\tau} = a(z_{k,\tau}^{(n)}) + O\left(\frac{1}{\tau^{n+1}}\right) \quad \text{as } \tau \to \infty$$

holds uniformly in k: *there exist constants* $C_n < \infty$ *independent of* k *and* τ *such that*

$$|\lambda_{k,\tau} - a\big(z_{k,\tau}^{(n)}\big)| \leqslant \frac{C_n}{\tau^{n+1}}.$$

[1] See the definition of the function $b(z)$ below.

(iv) *The following asymptotic expression holds for the points* ${z_{k,\tau}}$[2]*:*

$$z_{k,\tau} = z_{k,\tau}^{(0)} + \frac{c_1(z_{k,\tau}^{(0)})}{2i\tau} + \frac{c_2(z_{k,\tau}^{(0)})}{(2i\tau)^2} + \frac{c_3(z_{k,\tau}^{(0)})}{(2i\tau)^3} + O\biggl(\frac{1}{\tau^4}\biggr),$$

where

$$c_1(z) = \log b(z), \qquad c_2(z) = \frac{b'(z)}{b(z)} \log b(z)$$

and

$$c_3(z) = \frac{b'(z)^2}{b(z)^2} \log b(z) + \frac{b''(z)b(z) - b'(z)^2}{2b(z)^2} (\log b(z))^2.$$

(v) *The following asymptotic expression holds for* $\lambda_{k,\tau}$*:*

$$\lambda_{k,\tau} = a(z_{k,\tau}^{(0)}) + \frac{d_1(z_{k,\tau}^{(0)})}{2i\tau} + \frac{d_2(z_{k,\tau}^{(0)})}{(2i\tau)^2} + \frac{d_3(z_{k,\tau}^{(0)})}{(2i\tau)^3} + O\biggl(\frac{1}{\tau^4}\biggr), \tag{5.4}$$

where

$$d_1(z) = a'(z)c_1(z), \qquad d_2(z) = a'(z)c_2(z) + \frac{a''(z)}{2} c_1(z)^2$$

and

$$d_3(z) = a'(z)c_3(z) + a''(z)c_1(z)c_2(z) + \frac{a'''(z)}{6} c_1(z)^3.$$

Remark 5.1. We have presented formula (5.4) as an example of an explicit calculation of a few of the first terms in the asymptotic expansion. Using our method we can find an arbitrary number of these terms.

In conclusion we present a result concerning eigenfunctions.

Theorem 5.2. *Assume that all the numbers* $\mu_1, \dots, \mu_r$ *are distinct. Let* λ *be an eigenvalue of the operator* $W_\tau(a)$ *such that all the roots* $\omega_2(\lambda), \dots, \omega_\tau(\tau)$ *are distinct. Then each eigenfunction* $\varphi_\tau \in L^2(0,\tau)$ *of* $W_\tau(a)$ *corresponding to* λ *has the following form*:

$$\varphi_\tau(t) = \sum_{j=1}^{r} [c_j e^{i\omega_j(\lambda)t} + c_{r+j} e^{-i\omega_j(\lambda)t}] \tag{5.5}$$

and satisfies the relation $\varphi_\tau(\tau - t) = \theta\varphi_\tau(t)$ *with* $\theta \in \{\pm 1\}$ *for all* $t \in (0,\tau)$*; it can also be expressed by*

$$\varphi_\tau(t) = \begin{cases} \displaystyle\sum_{j=1}^{r} 2c_j e^{-i\omega_j(\lambda)\tau/2} \cos\biggl(\omega_j(\lambda)\Bigl(t - \frac{\tau}{2}\Bigr)\biggr) & \text{if } \theta = 1, \\ \displaystyle\sum_{j=1}^{r} 2ic_j e^{-i\omega_j(\lambda)\tau/2} \sin\biggl(\omega_j(\lambda)\Bigl(t - \frac{\tau}{2}\Bigr)\biggr) & \text{if } \theta = -1. \end{cases}$$

[2]This appears as z in (i).

Note that the coefficients $c_1, \dots, c_r$ in the last formulae can be calculated using a system of r linear equations with known coefficients.

The numerical aspects of the above formulae have been discussed in [51].

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