

A FINER ASPECT OF EIGENVALUE DISTRIBUTION OF SELFADJOINT BAND TOEPLITZ MATRICES*

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Abstract. The asymptotics of eigenvalues of Toeplitz operators has received a lot of attention in the mathematical literature and has been applied in several disciplines. This paper describes two of such application disciplines and provides refinements of existing asymptotic results using new methods of proof. The following result is typical: Let $T(\varphi)$ be a selfadjoint band limited Toeplitz operator with a (real valued) symbol φ , which is a nonconstant trigonometric polynomial. Consider finite truncations $T_n(\varphi)$ of $T(\varphi)$, and a finite union of finite intervals of real numbers E . We prove a refinement of the Szegő asymptotic formula

$$\lim_{n \rightarrow \infty} \frac{N_n(E)}{n} = \frac{1}{2\pi} m(F).$$

Indeed, we show that

$$N_n(E) - \frac{1}{2\pi} m(F)n = O(1).$$

Here $m(F)$ denotes the measure of $F = \varphi^{-1}(E)$ on the unit circle, and $N_n(E)$ denotes the number of eigenvalues of $T_n(\varphi)$ inside E . We prove similar results for singular values of general Toeplitz operators involving a refinement of the Avram-Parter theorem.

Key words. Toeplitz matrix, Eigenvalue distribution, Szegő formula, Avram-Parter theorem.

AMS subject classifications. 15A18, 47A10, 47A58, 47B35.

1. Introduction. The eigenvalue distribution of Toeplitz matrices and operators has been a fascinating and abundant source of topics of mathematical inquiries. The prominent monographs [9] and [10] respectively provide extensive analysis of Toeplitz matrices and operators. Among key historical papers are [11] (on operators), [19] (on matrices) and [20] (on block matrices). A comprehensive account on the theory involved is provided in [12].

From the interdisciplinary point of view, the above field also possesses a considerable potential, especially in terms of a wide range of applications and connections to disciplines outside mathematics. In the first part of this section, two application areas (see (I) and (II) below) are addressed which have motivated the authors to study the asymptotics of Toeplitz eigenvalues.

In the second part of the introduction, the mathematical contribution of this paper to the asymptotics of eigenvalues and singular values shall be outlined. We conclude the introduction with some clarification on notation used in the paper.

(I) Vast uncharted regions lie between mathematics and chemistry on the map of science. Communication across the border of these disciplines is still generally

*The authors would like to acknowledge professor A. Böttcher for his extensive comments, which have resulted in the description of refined singular value asymptotics of general Toeplitz matrices.

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sporadic and uncoordinated, despite modern trends of cross-disciplinary investigations in each of these fields. In the present work, we have for the first time formed a linkage between:

- (i) The mathematical branch of Toeplitz matrices, and
- (ii) The "repeat space theory" (RST) in theoretical chemistry, which originates in the study of the zero-point vibrational energies of hydrocarbons having repeating identical moieties [1].

Namely, in dealing with Toeplitz matrices in the proof of our main theorem, Theorem 2.3, we have recalled, sharpened, and applied a mathematical technique developed in the RST (to estimate quantum boundary effects in polymeric molecules). It is also remarkable that the sharpened technique in the proof of Theorem 2.3 can be applied to molecular problems by embedding the technique into the RST. In our opinion, researchers investigating in areas of (i) and (ii) can mutually benefit. The reader who is interested in cross-disciplinary mathematical investigations in chemistry is referred to Refs. [1, 2, 3, 4, 5, 6] and references therein, where he can find the genesis of the RST (in conjunction with experimental chemistry) and a variety of applications of the RST to quantum, thermodynamic, and structural chemistry.

Sequences of band circulant matrices are called "Alpha sequences" and play a dominant role in the RST [1, 2, 3, 4, 5, 6]. The band circulant matrix associated with a band Toeplitz matrix has been used in the proof of the present paper based on the approach and technique originally developed in the RST, especially in [1] and [6]. Further, we remark that the study of asymptotic spectra of band Toeplitz matrices in [7] arises from the analysis of difference approximations of partial differential equations and that in [7] the asymptotic spectra of the band Toeplitz matrix and its associated circulant matrix were studied.

(II) The asymptotics of eigenvalues of Toeplitz operators is an important issue in the study of time-frequency localization of signals. Essentially time- and band-limited functions can be studied by means of Toeplitz matrix eigenvalue asymptotics; see [15, 17]. Quite recently, these results have been used in the analysis of seismic records [16].

It is hoped that the present work provides researchers of the asymptotic eigenvalue distribution of Toeplitz matrices with a fresh insight into the theme, and that it contributes to dissolving the traditional boundary between the mathematical branch of Toeplitz matrices and other research areas such as quantum chemistry of molecules having repeating identical moieties, and time-frequency localization of (seismic) signals.

We shall now discuss the asymptotics of eigenvalues of Toeplitz matrices in further detail. Let φ be a real valued continuous function defined on the unit circle $\mathbf{T} = \{z \in \mathbf{C} : |z| = 1\}$. The Fourier coefficients of φ are given by $\varphi_k = (2\pi i)^{-1} \int_{\mathbf{T}} \varphi(z) z^{-k-1} dz$, $k \in \mathbf{Z}$. The corresponding Toeplitz operator $T(\varphi) = (\varphi_{i-j})_{i,j \in \mathbf{Z}^+}$ is selfadjoint and its finite truncations $T_n(\varphi) = (\varphi_{i-j})_{i,j=0}^{n-1}$ are Hermitian matrices. The spectrum of the operator $T(\varphi)$ coincides with the closed interval $\mathcal{I} = \{\varphi(z) : z \in \mathbf{T}\}$. In particular, the norm of $T(\varphi)$ is given by $\|T(\varphi)\| = \sup\{|\varphi(z)| : z \in \mathbf{T}\}$.

Moreover, the eigenvalues of the truncations $T_n(\varphi)$ are contained in the closed interval \mathcal{I} ; see for example Section 5.2b in [13] and Proposition 2.17 in [9]. However, much more can be said about the eigenvalue distribution of $T_n(\varphi)$. As a first step, we mention that the asymptotic behaviour of the eigenvalues is expressed by the well-known Szegő formula (cf. Theorem 5.2 in [13] and Theorem 5.10 in [9]): If f is a

continuous function on the closed interval \mathcal{I} , and if $\{\lambda_{i,n}\}_{i=1}^n$ are the eigenvalues of $T_n(\varphi)$, then

$$\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{i=1}^n f(\lambda_{i,n}) = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(\varphi(e^{i\theta})) d\theta.$$

Moreover, if φ is smooth, e.g., $C^{1+\varepsilon}$ with $\varepsilon > 0$ and f is analytic in an open neighborhood of \mathcal{I} , then one has a second order formula

$$\frac{1}{n} \sum_{i=1}^n f(\lambda_{i,n}) = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(\varphi(e^{i\theta})) d\theta + \frac{E_f(\varphi)}{n} + o\left(\frac{1}{n}\right)$$

with some completely identified constant $E_f(\varphi)$ (see [20] or Theorem 5.6 in [9]).

We shall now make the further assumption that φ is actually a nonconstant trigonometric polynomial of degree $r \geq 1$, i.e., $\varphi(z) = \sum_{k=-r}^r \varphi_k z^k$. In this manner, $T(\varphi)$ becomes a selfadjoint band limited Toeplitz operator. Let E denote a finite union of compact intervals on the real line and let χ_E be its characteristic function. Let m denote the Lebesgue measure on the unit circle. Since $m(\varphi^{-1}(\partial E)) = 0$, the Szegő formula can be extended to $f = \chi_E$ (see [22]) and we get:

$$(1.1) \quad \lim_{n \rightarrow \infty} \frac{N_n(E)}{n} = \frac{1}{2\pi} m(F),$$

where $N_n(E)$ denotes the number of eigenvalues of $T_n(\varphi)$ in the set E and $F = \varphi^{-1}(E)$. The purpose of this paper is to sharpen the formula for the case of band limited Toeplitz operators. Indeed, formula (1.1) states that $N_n(E) - \frac{1}{2\pi} m(F)n = o(n)$. The main result of this paper refines this asymptotic result to $N_n(E) - \frac{1}{2\pi} m(F)n = O(1)$. In addition to such results for eigenvalues of selfadjoint Toeplitz operators, we prove similar results for singular values of general Toeplitz operators.

In the remaining part of this paper, $\text{tr } A$ denotes the trace of the square matrix A . The space $BV(\mathcal{I})$ consists of functions of bounded variation on the closed interval $\mathcal{I} = [a, b]$. For such a function f , there exists a constant $V > 0$, such that for each partition $a = x_0 < x_1 < \dots < x_m = b$, we get

$$\sum_{j=1}^m |f(x_j) - f(x_{j-1})| \leq V.$$

The minimum $V > 0$ which satisfies this condition is called the total variation of f on \mathcal{I} and is denoted by $V_{\mathcal{I}}(f)$. If the natural domain of f contains \mathcal{I} and $f|_{\mathcal{I}}$ is of bounded variation on \mathcal{I} , then $V_{\mathcal{I}}(f) = V_{\mathcal{I}}(f|_{\mathcal{I}})$. If $g : \mathbf{T} \rightarrow \mathbf{R}$, let $f(t) = g(e^{it})$, for $t \in \mathbf{R}$, and let $V_{\mathbf{T}}(g) = V_{[-\pi, \pi]}(f)$. Denote the eigenvalues of a Hermitian $n \times n$ matrix H by $\lambda_1(H) \leq \lambda_2(H) \leq \dots \leq \lambda_n(H)$. The singular values of an arbitrary complex $m \times n$ matrix M are equal to the eigenvalues of the Hermitian matrix $(M^*M)^{1/2}$ and labeled so that $\sigma_1(M) \leq \sigma_2(M) \leq \dots \leq \sigma_n(M)$. The spectral norm $\|M\|$ of M is equal to $\sigma_n(M)$.

2. Refined eigenvalue asymptotics. In this section, we prove a number of estimates which lead to the refined asymptotics result in Corollary 2.5. This corollary involves the characteristic function χ_E , while the preparatory results are stated for general functions of bounded variation. First, we state Theorem 2.1 from [6]. For convenience of the reader, and for reference later on, we include the proof.

THEOREM 2.1. *Consider the integers $1 \leq r < n$ and let $K = \{k_1, \dots, k_r\}$ be a subset of $\{1, 2, \dots, n\}$ consisting of r distinct elements. Define $L = \{1, 2, \dots, n\} \setminus K$. Let M and M' be $n \times n$ Hermitian matrices such that the ij^{th} entries of M and M' coincide for all $(i, j) \in L \times L$, i.e. such that*

$$(M - M')_{ij} = 0$$

for all $(i, j) \in L \times L$. Consider a closed interval $\mathcal{I} = [a, b]$ which contains all the eigenvalues of both M and M' . Then we have

$$|\text{tr } f(M) - \text{tr } f(M')| \leq rV_{\mathcal{I}}(f)$$

for all $f \in BV(\mathcal{I})$.

Proof Case 1: $r = 1$. We may and do assume that $K = \{n\}$, since this situation can be achieved by transforming $M - M'$ by means of a permutation similarity. Let M_0 denote the $(n-1) \times (n-1)$ matrix given by $(M_{ij})_{i,j=1}^{n-1}$. Observe that $M_0 = (M'_{ij})_{i,j=1}^{n-1}$. If we write $\lambda_0 = a$, $\lambda_j = \lambda_j(M_0)$ for $j = 1, \dots, n-1$, and $\lambda_n = b$, then by the Sturmian separation theorem [14], we get

$$\lambda_{j-1} \leq \lambda_j(M) \leq \lambda_j, \quad \lambda_{j-1} \leq \lambda_j(M') \leq \lambda_j, \quad j = 1, \dots, n.$$

Therefore, we arrive at

$$|\text{tr } f(M) - \text{tr } f(M')| = \left| \sum_{j=1}^n \{f(\lambda_j(M)) - f(\lambda_j(M'))\} \right| \leq \sum_{j=1}^n |f(\lambda_j(M)) - f(\lambda_j(M'))| \leq V_{\mathcal{I}}(f).$$

Case 2: $r > 1$. As in the first part of the proof, we may and do assume that K has a specific form, say $K = \{n-r+1, \dots, n\}$. Define $n \times n$ Hermitian matrices $M^{(0)}, M^{(1)}, \dots, M^{(r)}$ such that $M^{(0)} = M$, $M^{(r)} = M'$, and such that the pairs $M^{(\nu-1)}, M^{(\nu)}$ for $\nu = 1, \dots, r$ each satisfy the conditions of Case 1. This can be achieved by setting ($0 \leq \nu \leq r$)

$$M_{ij}^{(\nu)} = \begin{cases} M_{ij}, & 1 \leq i, j \leq n - \nu \\ M'_{ij}, & n - \nu < i \leq n \text{ or } n - \nu < j \leq n \end{cases}.$$

Let $[\tilde{a}, \tilde{b}] = \tilde{\mathcal{I}} \supseteq \mathcal{I} = [a, b]$ be an interval which contains all eigenvalues of $M^{(\nu)}$ for $\nu = 1, \dots, r-1$, and let \tilde{f} be the extension of f to $\tilde{\mathcal{I}}$ given by

$$\tilde{f}(t) = \begin{cases} f(a), & \tilde{a} \leq t \leq a \\ f(t), & a \leq t \leq b \\ f(b), & b \leq t \leq \tilde{b} \end{cases}.$$

We have obtained

$$|\text{tr } f(M) - \text{tr } f(M')| \leq \sum_{\nu=1}^r \left| \sum_{j=1}^n \{ \tilde{f}(\lambda_j(M^{(\nu-1)})) - \tilde{f}(\lambda_j(M^{(\nu)})) \} \right| \leq rV_{\tilde{\mathcal{I}}}(\tilde{f}) = rV_{\mathcal{I}}(f).$$

□

We now state and prove two new results for functions of bounded variation f and apply them to the characteristic function χ_E in the corollaries. If n is a positive integer, let P_n denote the cyclic shift $n \times n$ matrix with $(P_n)_{ij} = 1$ if $i - j \equiv 1 \pmod n$ and 0 otherwise. Let $A_n = A_n(\varphi) = \sum_{k=-r}^r \varphi_k P_n^k$.

THEOREM 2.2. *For any $f \in BV(\mathcal{I})$ and any positive integer n , we have*

- (i) $|\operatorname{tr}(f(T_n)) - \operatorname{tr}(f(A_n))| \leq rV_{\mathcal{I}}(f)$,
- (ii) $\left| \operatorname{tr}(f(A_n)) - \frac{n}{2\pi} \int_{-\pi}^{\pi} f(\varphi(e^{i\theta})) d\theta \right| \leq 2rV_{\mathcal{I}}(f)$,
- (iii) $\left| \operatorname{tr}(f(T_n)) - \frac{n}{2\pi} \int_{-\pi}^{\pi} f(\varphi(e^{i\theta})) d\theta \right| \leq 3rV_{\mathcal{I}}(f)$.

Proof (i) If $n \leq r$, then $\operatorname{tr}(f(T_n)) - \operatorname{tr}(f(A_n))$ is just the sum of the differences of the values of f at n pairs of points from \mathcal{I} . Thus,

$$|\operatorname{tr}(f(T_n)) - \operatorname{tr}(f(A_n))| \leq nV_{\mathcal{I}}(f) \leq rV_{\mathcal{I}}(f).$$

If $r < n$, then we make use of some auxiliary matrices. We have already introduced P_n in order to define the circulant matrix A_n . Further, for $|k| < n$, let $S_n(k)$ denote the $n \times n$ matrix with $(S_n(k))_{ij} = 1$ if $i - j = k$ and 0 otherwise. Let $S_n(k) = 0$ if $|k| \geq n$. Clearly $((P_n)^k)_{ij} = (S_n(k))_{ij}$ for $1 \leq i, j \leq n - |k|$. Since $T_n = T_n(\varphi) = \sum_{k=-r}^r \varphi_k S_n(k)$, we get

$$T_n - A_n = \sum_{k=-r}^r \varphi_k (S_n(k) - P_n^k).$$

Since $(T_n)_{ij} = (A_n)_{ij}$ for $1 \leq i, j \leq n - r$, we get by Theorem 2.1,

$$|\operatorname{tr}(f(T_n)) - \operatorname{tr}(f(A_n))| \leq rV_{\mathcal{I}}(f).$$

(ii) Let $h(\theta) = f(\varphi(e^{i\theta}))$, for $\theta \in \mathbf{R}$. Then

$$\operatorname{tr}(f(A_n)) = \sum_{j=1}^n h\left(\frac{2\pi j}{n}\right).$$

This implies

$$\begin{aligned} & \left| \operatorname{tr}(f(A_n)) - \frac{n}{2\pi} \int_{-\pi}^{\pi} f(\varphi(e^{i\theta})) d\theta \right| = \left| \sum_{j=1}^n h\left(\frac{2\pi j}{n}\right) - \frac{n}{2\pi} \int_{-\pi}^{\pi} h(\theta) d\theta \right| \\ & \leq \frac{n}{2\pi} \sum_{j=1}^n \int_{\frac{2\pi(j-1)}{n}}^{\frac{2\pi j}{n}} \left| h\left(\frac{2\pi j}{n}\right) - h(\theta) \right| d\theta \leq \frac{n}{2\pi} \sum_{j=1}^n \int_{\frac{2\pi(j-1)}{n}}^{\frac{2\pi j}{n}} V_{[\frac{2\pi(j-1)}{n}, \frac{2\pi j}{n}]}(h) d\theta = V_{[0, 2\pi]}(h). \end{aligned}$$

Now, let $u(\theta) = \varphi(e^{i\theta})$. Since φ is a nonconstant trigonometric polynomial of degree r , u' has at least 2 and at most $2r$ distinct roots in $[0, 2\pi)$. Let $\theta_1 < \theta_2 < \dots < \theta_l$ be the roots of u' in $[0, 2\pi)$. Then

$$V_{[0, 2\pi]}(h) = V_{[\theta_1, \theta_1 + 2\pi]}(f \circ u) =$$

$$V_{[\theta_1, \theta_2]}(f \circ u) + V_{[\theta_2, \theta_3]}(f \circ u) + \cdots + V_{[\theta_l, \theta_1 + 2\pi]}(f \circ u) \leq lV_{\mathcal{I}}(f).$$

It follows that

$$\left| \operatorname{tr}(f(A_n)) - \frac{n}{2\pi} \int_{-\pi}^{\pi} f(\varphi(e^{i\theta})) d\theta \right| \leq 2rV_{\mathcal{I}}(f).$$

Now (iii) follows immediately from (i) and (ii). \square

THEOREM 2.3. *If $f \in BV(\mathcal{I})$ and if n is any positive integer, then*

$$\left| \sum_{i=1}^n f(\lambda_{i,n}) - \frac{n}{2\pi} \int_{-\pi}^{\pi} f(\varphi(e^{i\theta})) d\theta \right| \leq rV_{\mathcal{I}}(f) + V_{\mathbf{T}}(f \circ \varphi) \leq 3rV_{\mathcal{I}}(f).$$

Proof If we apply Theorem 2.2 (i) to the setting of this theorem, we get

$$|\operatorname{tr}(f(T_n)) - \operatorname{tr}(f(A_n))| \leq rV_{\mathcal{I}}(f),$$

and the proof of Theorem 2.2 (ii) yields

$$\left| \operatorname{tr}(f(A_n)) - \frac{n}{2\pi} \int_{-\pi}^{\pi} f(\varphi(e^{i\theta})) d\theta \right| \leq V_{\mathbf{T}}(f \circ \varphi) \leq 2rV_{\mathcal{I}}(f).$$

This, together with $\operatorname{tr}(f(T_n)) = \sum_{i=1}^n f(\lambda_{i,n})$, provides

$$\left| \sum_{i=1}^n f(\lambda_{i,n}) - \frac{n}{2\pi} \int_{-\pi}^{\pi} f(\varphi(e^{i\theta})) d\theta \right| \leq rV_{\mathcal{I}}(f) + V_{\mathbf{T}}(f \circ \varphi) \leq 3rV_{\mathcal{I}}(f).$$

\square

The following two corollaries are easy consequences of Theorem 2.3. We leave it to the reader to check the necessary minor details. Let E be a subset of \mathbf{R} that is a finite union of compact intervals and let $F = \varphi^{-1}(E)$ be the corresponding subset of \mathbf{T} . Note that if E is a union of N compact intervals and \mathcal{I} is an interval in \mathbf{R} , then $V_{\mathcal{I}}(\chi_E) \leq 2N$.

COROLLARY 2.4. *Let T be a band limited selfadjoint Toeplitz operator with the symbol φ , a real-valued trigonometric polynomial of degree $r \geq 1$. Then*

$$\left| N_n(E) - \frac{1}{2\pi} m(F)n \right| \leq rV_{\mathcal{I}}(\chi_E) + V_{\mathbf{T}}(\chi_F) \leq 3rV_{\mathcal{I}}(\chi_E)$$

for every $n \geq 1$.

COROLLARY 2.5. *Let T be a band limited selfadjoint Toeplitz operator with the symbol φ , a real-valued trigonometric polynomial of degree $r \geq 1$. Then*

$$N_n(E) - \frac{n}{2\pi} m(F) = O(1).$$

3. Singular Values. The results proved in the previous section for the eigenvalues of selfadjoint band Toeplitz matrices can easily be generalized to results concerning the singular values of arbitrary band Toeplitz matrices, although the constants in the new estimates are slightly worse. In this section, the main steps of the proofs are outlined. The analogue of Theorem 2.1 reads as follows:

THEOREM 3.1. *For $1 \leq r < n$, let $K = \{k_1, \dots, k_r\}$ be a subset of $\{1, 2, \dots, n\}$ having exactly r elements, and put $L = \{1, 2, \dots, n\} \setminus K$. Let M and M' be two complex $n \times n$ matrices such that $(M - M')_{ij} = 0$ for all $(i, j) \in L \times L$. If $\mathcal{I} = [a, b]$ is a closed interval which contains the singular values of both M and M' and if $f \in BV(\mathcal{I})$, then*

$$\sum_{j=1}^n |f(\sigma_j(M)) - f(\sigma_j(M'))| \leq 2rV_{\mathcal{I}}(f).$$

Proof We can proceed as in the proof of Theorem 2.1. The only difference is that we need to replace the Sturmian separation theorem by the following interlacing result (see e.g. [8], pp. 81-82). Let $A = (a_{ij})_{i,j=1}^n$ be a complex $n \times n$ matrix and let $B = (a_{ij})_{i,j=1}^{n-1}$ be the $(n-1) \times (n-1)$ principal sub-matrix. Then

$$0 \leq \sigma_1(A) \leq \sigma_2(B),$$

$$\sigma_{j-1}(B) \leq \sigma_j(A) \leq \sigma_{j+1}(B), \quad j = 2, \dots, n-2,$$

and $\|B\| \leq \|A\|$. If we abbreviate $\sigma_j = \sigma_j(M_0)$ for $j = 1, \dots, n-1$ (notation as in Theorem 2.1), then in the case of $r = 1$, we get

$$\sum_{j=1}^n |f(\sigma_j(M)) - f(\sigma_j(M'))| \leq$$

$$V_{[a, \sigma_2]}(f) + \sum_{j=2}^{n-2} V_{[\sigma_{j-1}, \sigma_{j+1}]}(f) + V_{[\sigma_{n-2}, b]}(f) \leq V_{[a, \sigma_{n-1}]}(f) + V_{[\sigma_1, b]}(f) \leq 2V_{[a, b]}(f).$$

The case of $r > 1$ is dealt with in the same fashion as in Theorem 2.1. \square

THEOREM 3.2. *Let ψ be a nonconstant trigonometric polynomial of degree $r \geq 1$, let $\mathcal{I} = [0, \|\psi\|_{\infty}]$, and let $g \in BV(\mathcal{I})$. Then for all $n \geq 1$,*

$$\left| \sum_{j=1}^n g(\sigma_j(T_n(\psi))) - \frac{n}{2\pi} \int_{-\pi}^{\pi} g(|\psi(e^{i\theta})|) d\theta \right| \leq 2rV_{\mathcal{I}}(g) + V_{\mathcal{I}}(g \circ |\psi|) \leq 6rV_{\mathcal{I}}(g).$$

Proof The singular values of the circulant matrix A_n introduced in the proof of Theorem 2.2(ii) are given by $|\psi(2\pi ij/n)|$ ($j = 1, \dots, n$). Consequently, the reasoning of the proof of Theorem 2.2(i), in conjunction with Theorem 3.1, gives

$$\left| \sum_{j=1}^n g(\sigma_j(T_n(\psi))) - \frac{n}{2\pi} \int_{-\pi}^{\pi} g(|\psi(e^{i\theta})|) d\theta \right| \leq 2rV_{\mathcal{I}}(g) + V_{[0, 2\pi]}(g \circ |\psi|).$$

Since $|\psi(e^{i\theta})|^2$ is a trigonometric polynomial of degree $2r$, we obtain as in the proof of Theorem 2.2(ii) that $|\psi(e^{i\theta})|$ has at most $4r$ local extrema in $[0, 2\pi)$, whence $V_{[0, 2\pi]}(g \circ |\psi|) \leq 4rV_{\mathcal{I}}(g)$. This implies the assertion. \square

While Theorem 2.3 is a refined version of Szegő's formula, Theorem 3.2 may be regarded as a refinement of the Avram-Parter theorem, which states that

$$\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{i=1}^n g(\sigma_i(T_n(\psi))) = \frac{1}{2\pi} \int_{-\pi}^{\pi} g(|\psi(e^{i\theta})|) d\theta$$

if, for example, ψ is continuous on \mathbf{T} and g is continuous on the range of $|\psi|$ (see [9] and [18] and the references therein). The counterpart of Corollaries 2.4 and 2.5 for singular values is as follows.

COROLLARY 3.3. *Let ψ be a trigonometric polynomial of degree $r \geq 1$, let $E \subset \mathbf{R}$ be a finite union of compact intervals, and let $F = \{t \in \mathbf{T} : |\psi(t)| \in E\}$. If $N_n(E)$ denotes the number of singular values of $T_n(\psi)$ in E , then*

$$\left| N_n(E) - \frac{n}{2\pi} m(F) \right| \leq 2rV_{\mathbf{I}}(\chi_E) + V_{\mathbf{T}}(\chi_F) \leq 6rV_{\mathbf{I}}(\chi_E)$$

for every $n \geq 1$. In particular,

$$N_n(E) - \frac{n}{2\pi} m(F) = O(1).$$

Acknowledgement The authors are indebted to professor A. Böttcher for pointing out the extension of the main results from eigenvalues to singular values for arbitrary band Toeplitz matrices, which has resulted in Section 3.

REFERENCES

- [1] S. Arimoto, Preliminary Considerations towards a Theoretical Foundation of the Zero Point Energy Additivity Rules, *Phys. Lett.* **113A** (1985), 126-132.
- [2] S. Arimoto, K. Fukui, *Fundamental Mathematical Chemistry, Interdisciplinary Research in Fundamental Mathematical Chemistry and Generalized Repeat Space*, IFC Bulletin 1998, pp. 7-13. (PDF Full Text downloadable at: <http://duke.usask.ca/~arimoto/>)
- [3] S. Arimoto, K. Fukui, P. Zizler, K.F. Taylor, and P.G. Mezey, Structural Analysis of Certain Linear Operators Representing Chemical Network Systems via the Existence and Uniqueness Theorems of Spectral Resolution. V, *Int. J. Quantum Chem.* **74** (1999), 633-644.
- [4] S. Arimoto, M. Spivakovsky, H. Ohno, P. Zizler, K.F. Taylor, T. Yamabe, and P.G. Mezey, Structural Analysis of Certain Linear Operators Representing Chemical Network Systems via the Existence and Uniqueness Theorems of Spectral Resolution. VI, *Int. J. Quantum Chem.* **84** (2001), 389-400.
- [5] S. Arimoto, M. Spivakovsky, P. Zizler, R.A. Zuidwijk, K.F. Taylor, T. Yamabe, and P.G. Mezey, Structural Analysis of Certain Linear Operators Representing Chemical Network Systems via the Existence and Uniqueness Theorems of Spectral Resolution. VII. (to appear in: *Int. J. Quantum Chem.*)
- [6] Arimoto, S., Spivakovsky, M., *The Asymptotic Linearity Theorem for the study of additivity problems of the zero-point vibrational energy of hydrocarbons and the total pi-electron energy of alternant hydrocarbons*, *Journal of Mathematical Chemistry* **13** (1993) 217-247.
- [7] Beam, R.M., Warming, R.F., The asymptotic spectra of banded Toeplitz and quasi-Toeplitz matrices, *Siam J. Sci. Comput.* **14** (1993), 971-1006.
- [8] Bhatia, R., *Matrix Analysis*, Springer-Verlag, New York, 1996.
- [9] Böttcher, A., Silbermann, B., *Introduction to Large Truncated Toeplitz Matrices*, Springer-Verlag, New York, 1998.
- [10] Böttcher, A., Silbermann, B., *Analysis of Toeplitz Operators*, Akademie-Verlag, Berlin, 1989 and Springer-Verlag, Berlin, Heidelberg, New York, 1990.
- [11] Gohberg, I., Feldman, I.A., *Convolution Equations and Projection Methods for their Solution*, Amer. Math. Soc. Transl. of Math. Monographs, Vol. 41, Providence, R.I., 1974.
- [12] Gohberg, I., Goldberg, S., Kaashoek, M.A., *Classes of Linear Operators II*, Birkhauser Verlag, Basel, 1993.

- [13] Grenander, U., Szegő, G., *Toeplitz Forms and Their Applications*, University of California Press, Berkely, 1958.
- [14] Horn, R.A., Johnson, C.R., *Topics in matrix analysis*, Cambridge University Press, Cambridge (1991).
- [15] Landau, H.J., Widom, H., *Eigenvalue distribution of time and frequency limiting*, J. math. Anal. and Appl. **77** (1980), 469-481.
- [16] Lilly, J.M., Park, J., *Multiwavelet spectral and polarization analysis of seismic records*, Geophys. J. Int. **122** (1995), 1001-1021.
- [17] Slepian, D., On bandwidth, Proc. IEEE **64** (1976), 292-300.
- [18] Tyrtyshnikov, E.E., A unifying approach to some old and new theorems on distribution and clustering, *Lin. Alg. Appl.* **232** (1996), 1-43.
- [19] Widom, H., Toeplitz Matrices, in: *Studies in Real and Complex Analysis*, Hirshman I.I. Jr. (ed.), M.A.A. Studies in Mathematics, Vol. **3** (1965), 179-209.
- [20] Widom, H., Asymptotic Behaviour of block Toeplitz matrices and determinants II, *Advances in Math.* **21** (1976), 1-29.
- [21] Widom, H., On the singular values of Toeplitz matrices, *Z. Analysis Anw.* **8** (1989), 221-229.
- [22] Widom, H., *Eigenvalue distribution for nonselfadjoint Toeplitz matrices*, Operator Theory: Advances and Applications, Vol. **71**, Birkhauser Verlag, Basel (1994).