The Fisher-Hartwig Conjecture and Toeplitz Eigenvalues

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ABSTRACT

The conjecture of Fisher and Hartwig, published in 1968, describes the asymptotic expansion of Toeplitz determinants with singular generating functions. For more than twenty years progress was made in extending the validity of the conjecture, but recent computer experiments led to counterexamples that show the limits of the original conjecture and pointed the way to a revised conjecture. This paper describes the history of the problem, several numerical examples, and the revised conjecture.

1. INTRODUCTION

Given an $n \times n$ Toeplitz matrix, what can be said about its eigenvalues? For many types of Toeplitz matrices there is a surprisingly simple answer to this question. In order to describe the answer, suppose we start with a complex-valued function ϕ defined on the circle. The Fourier coefficients of ϕ are

$$\phi_n = \frac{1}{2\pi} \int_0^{2\pi} \phi(\theta) e^{-in\theta} d\theta.$$

The Toeplitz matrix $T_n[\phi]$ is said to be generated by ϕ if

$$T_n[\phi] = (\phi_{i-j}), \quad i, j = 0, \ldots, n-1.$$

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In this paper we will consider mainly piecewise smooth ϕ , and we will describe conditions that guarantee that the eigenvalues of $T_n[\phi]$, for n large, approximate the image of ϕ .

Of course, an eigenvalue λ of $T_n[\phi]$ is a solution of $\det T_n[\phi-\lambda]=0$. Hence, a key ingredient in finding information about eigenvalues for n large is asymptotic information about $\det T_n[\phi-\lambda]$. Such information has been known for many years, first from the theorems of Szegö, and later from generalizations of Szegö's results by many people. One of the most important conjectured generalizations involving nonsmooth ϕ was given by Fisher and Hartwig [9] in 1968. This conjecture has been verified in many cases, shown to be false in others, and recently reformulated. In the following sections of this paper we will describe how implications of the conjecture answer the questions about eigenvalues. Some of the results are theorems, but others are experimental numerical results shown in plots of eigenvalues.

The paper is organized as follows. In Section 2 we give a brief survey of the Fisher-Hartwig conjecture and subsequent applications to the eigenvalue problem. Section 3 contains the reformulated conjecture and discussion of its implications for the eigenvalue problems. In many ways this is the most interesting case, since it shows that even when the eigenvalues are not near the image of ϕ , something can still be said about their behavior.

The authors wish to emphasize that the results of this paper are not new, but rather illustrations and applications of the current state of knowledge in this area. We hope that such a collection of results and ideas will be useful to applied mathematicians, physicists, and engineers who otherwise might not notice such results in the literature.

Finally, we should point out that in some special cases the eigenvalues of a Toeplitz matrix are known explicitly. The results of Day [8] compute eigenvalues for generating functions that are rational with poles away from the unit circle. Similar results for general Laurent polynomials were found by Schmidt and Spitzer [15] and Hirschman [10]. These results concern the limiting measure of the eigenvalues, and the answers are unrelated to the image of ϕ . Results for the limiting measure of the eigenvalues were found by Widom [19] in the case where ϕ is smooth except for one discontinuity or is continuous and piecewise smooth but not smooth. These results show that the eigenvalues are distributed as the values of the generating function. More will be said about this in Section 2, and, in fact, Widom's results, which are also proved via determinants, constitute half of Theorem 1. It was conjectured by Widom [20] that the eigenvalues approximate the image of ϕ for a generic set of generating functions and that the results of Day, Hirschman, Schmidt, and Spitzer are nongeneric. Widom has conjectured that the canonical behavior for the limiting eigenvalue measure should hold unless ϕ extends analytically to an annulus. The example and numerical computations presented here support this conjecture.

2. THE CONJECTURE

The Fisher-Hartwig conjecture [9] concerns the asymptotic behavior of the determinants of Toeplitz matrices for a certain class of singular symbols. (Note: *symbol* is a synonym for generating function.) These symbols are of the form

$$\phi(\theta) = b(\theta) \prod_{r=1}^{R} t_{\beta_r} (\theta - \theta_r) u_{\alpha_r} (\theta - \theta_r), \qquad (1)$$

where

$$t_{\beta}(\theta) = \exp[-i\beta(\pi - \theta)], \quad 0 < \theta < 2\pi,$$
 (2)

and

$$u_{\alpha}(\theta) = (2 - 2\cos\theta)^{\alpha}$$
, Re $\alpha > -\frac{1}{2}$, (3)

and $b:S^1\to \mathbf{C}$ is a smooth nonvanishing function with winding number 0. The type of function allowed by these definitions is quite general: a piecewise smooth function with jump discontinuities, zeros, or singularities. What is important is the special form that the factors have in order to account for the jumps and singularities. Define the determinant

$$D_n[\phi] = \det T_n[\phi], \quad i, j = 0, ..., n - 1.$$
 (4)

Fisher and Hartwig conjectured that

$$D_n[\phi] \sim G[b]^n n^{\sum_r (\alpha_r^2 - \beta_r^2)} E \quad \text{as} \quad n \to \infty,$$
 (5)

where

$$G[b] = \exp\left(\frac{1}{2\pi} \int_0^{2\pi} \log b(\theta) d\theta\right)$$
 (6)

is the geometric mean of b, and E is of constant. (They did not give a complete description of the constant.) In the past twenty years much progress has been made determining the range of the α and β parameters for which the Fisher-Hartwig conjecture is true and determining the constant E. We sketch the history of the conjecture here; the reader is referred to [7] for a complete discussion of the conjecture and Toeplitz operators.

The foundation for such a conjecture consists of several earlier results. The first ingredient is Szegö's strong limit theorem [16], which handles the case of a smooth function with winding number zero so that R=0 and $\phi(\theta)=b(\theta)$. The next ingredient is the explicit calculation for the case $\phi(\theta)=t_{\beta}(\theta)$, in which there is one discontinuity. In that case the Fourier coefficients are

$$\phi_n = \frac{\sin \pi \beta}{\pi (n + \beta)},\tag{7}$$

and the corresponding determinant $D_n[\phi]$ is of Cauchy type and can be evaluated explicitly. Lenard [11, 12] had treated the case where $b \equiv 1$, R = 2, $\theta_2 = \theta_1 + \pi$, $\beta_1 = \beta_2 = 0$, α_1 , α_2 real and positive. Szegö had also found the answer for $\alpha_1 = \alpha_2$; $\beta_i = 0$, $b \equiv 1$. From these earlier results and using some heuristic arguments, Fisher and Hartwig extrapolated to find a common generalization.

The first general results on the conjecture were obtained by Widom [19] for Re $\alpha_r > -\frac{1}{2}$ and $\beta_r = 0$ for all r. This gave a complete result for functions without jumps, because the condition on the real part of α merely insures that ϕ is integrable, so that it has Fourier coefficients. Next Basor [1] extended the validity of the conjecture for Re $\alpha_r > -\frac{1}{2}$ and Re $\beta_r = 0$, thus allowing the β_r to be purely imaginary. She was also able to determine the constant E, which we now describe.

Let $b(\theta) = b_+(e^{i\theta})b_-(e^{-i\theta})$, where b_+ (respectively, b_-) extends to be analytic and nonzero inside (respectively, outside) the unit circle. Normalize b so that $b_+(0) = b_-(\infty) = 1$. Then

$$E = \exp\left(\sum_{k=1}^{\infty} k s_k s_{-k}\right)$$

$$\times \prod_{r=1}^{R} b_{-} \left(e^{i\theta_r}\right)^{-\alpha_r - \beta_r} b_{+} \left(e^{-i\theta_r}\right)^{-\alpha_r + \beta_r}$$

$$\times \prod_{1 \leqslant r \neq s \leqslant R} \left\{1 - \exp\left[i\left(\theta_s - \theta_r\right)\right]\right\}^{-(\alpha_r + \beta_r)(\alpha_s - \beta_s)}$$

$$\times \prod_{r=1}^{R} \frac{G(1 + \alpha_r + \beta_r)G(1 + \alpha_r - \beta_r)}{G(1 + 2\alpha_r)}, \tag{8}$$

where $(\log b(\theta))_k = s_k$ and G is the Barnes G-function.\(^1\) A year later Basor [2] proved the conjecture for the case that $\alpha_r = 0$ and $|\text{Re }\beta_r| < \frac{1}{2}$, which is a more general case of jump discontinuities without zeros. Böttcher and Silbermann [5] extended the conjecture to $|\text{Re }\alpha_r| < \frac{1}{2}$ and $|\text{Re }\beta_r| < \frac{1}{2}$. Also in the case R = 1, Böttcher and Silbermann [6] verified the conjecture for $\text{Re }\alpha \geqslant 0$, $\text{Re }\alpha + \text{Re }\beta > -1$, and $\text{Re }\alpha - \text{Re }\beta > -1$. Then for R = 1 Libby [13] proved it for $\alpha = 0$ and $|\text{Re }\beta| < \frac{5}{2}$, and later for $\alpha = 0$ and $|\text{Re }\beta|$ arbitrary [14].

To illustrate the consequences of the verified conjecture, first consider the piecewise continuous function $\phi(\theta) = b(\theta)t_{\beta}(\theta)$. Notice that $\beta = (1/2\pi i)\log[\phi(0^{-})/\phi(0^{+})]$ for the proper choice of logarithm. By Fisher and Hartwig,

$$D_n[\phi] \sim G^{n+1} n^{-\beta^2} E \tag{9}$$

where from (8) we note that E does not vanish. Let A_n be the set of eigenvalues for $T_n[\phi]$, and let B be image of ϕ . The set B is a nonclosed curve in the plane.

THEOREM 1. Let $\varepsilon > 0$ be arbitrary, and suppose $\phi(\theta) = b(\theta)t_{\beta}(\theta)$. Then there exists an N such that if $n \ge N$ then $h(A_n, B) < \varepsilon$, where h is the Hausdorff metric on sets. Equivalently, A_n converges to B in the Hausdorff metric.

Proof. Recall $h(A, B) = \max\{d(A, B), d(B, A)\}$, where $d(A, B) = \min\{d(a, B) \mid a \in A\}$. Suppose that $\varepsilon > 0$ and that $\lambda \in A_n$. We need to show that $\min\{d(\lambda, B) \mid \lambda \in A_n\} < \varepsilon$ for n sufficiently large. Consider the function $\phi(\theta) - \lambda = b(\theta)t_{\beta}(\theta) - \lambda$. If λ does not lie in the image of ϕ , then we can put $\phi(\theta) - \lambda = b_{\lambda}(\theta)t_{\beta(\lambda}(\theta))$, where

$$\beta(\lambda) = \frac{1}{2\pi i} \log \left(\frac{\phi(0^-) - \lambda}{\phi(0^+) - \lambda} \right)$$
 (10)

and the log is chosen so that $b_{\lambda}(\theta)$ has winding number zero. Thus, by Fisher and Hartwig, $D_n[\phi - \lambda] \neq 0$ for n sufficiently large. Now by considering the proofs of Fisher and Hartwig this same argument can be applied uniformly

¹ The Barnes G-function is an entire function defined by $G(z+1)=(2\pi)^{z/2}\exp\{-[z+(\gamma+1)z^2]/2\}\prod_{k=1}^{\infty}(1+z/k)^k\exp(-z+z^2/2k)$, where γ is Euler's constant.

for λ in any open ball lying in the complement of any neighborhood of the set B. In addition, it is easy to verify that the eigenvalues of $T_n[\phi]$ must be confined to a bounded set. Thus, reducing the argument to one about compact sets, we see that in any neighborhood of the complement of B, we can find N such that for $n \geq N$, no eigenvalues of $T_n[\phi]$ will occur. By considering the neighborhood $\bigcup_{x \in B} \{y \mid |y - x| < \varepsilon\}$, we have shown that $\min\{d(\lambda, B) \mid \lambda \in A_n\} < \varepsilon$. This proves half of the theorem. The second half, the fact that $d(B, A_n)$ is sufficiently small for n large, follows from the results of Widom in [20]. For details the reader should refer to that paper.

As an intuitive aid to understanding the asymptotic eigenvalue distribution of Toeplitz matrices, we would like to point out that the multiplication operator

$$M[\phi]: L^2(S^1) \to L^2(S^1): g \mapsto \phi g$$

is represented by the doubly infinite matrix (ϕ_{i-j}) for $i, j \in \mathbf{Z}$ by using the Fourier basis $e^{in\theta}$ for $n \in \mathbf{Z}$. If we restrict the multiplication operator to the span of $e^{-in\theta}, \ldots, e^{in\theta}$ the matrix is a Toeplitz matrix of size 2n + 1. Now as $n \to \infty$ one might naively suppose that the eigenvalues of the Toeplitz matrices approach the spectrum of the multiplication operator, which, as is well known, consists of the essential range of ϕ .

At the same time the finite Toeplitz matrices are finite-dimensional approximations for the infinite Toeplitz matrix (ϕ_{i-j}) , $i,j \ge 0$, that represents the Toeplitz operator on the space $H^2(S^1)$, which is the span of $1, e^{i\theta}, e^{2i\theta}, \ldots$ The spectrum of the Toeplitz operator is known for continuous functions to be the union of the range of ϕ and its interior [17]. One might also expect the eigenvalues of the Toeplitz matrices to approach this spectrum in some way.

Obviously, these are conflicting pictures and the truth is a mixture of the two, with the eigenvalues approaching the range but staying in the interior, as can be seen in the plots of actual examples. This behavior is typical, but it has not been rigorously proved for a large class of symbols. Overall it aids one's understanding to keep in mind that the important results on eigenvalue distribution can be understood as describing how the actual asymptotic distribution deviates from the range of ϕ .

We now consider some examples that illustrate the theorem. In some cases we computed the exact Fourier coefficients and then used commercial software to approximate the eigenvalues for matrices up to about size 200. In other cases we first approximated the Fourier coefficients by using the discrete Fourier transform on the sampled function. In order to get reasonable accuracy for the Fourier coefficients to be put into the Toeplitz matrix

we used 2^{10} sample points in $[0,2\pi]$. In a matrix of size 200, about 400 of the coefficients are used of the 1024 that are approximated. We did some partial checks on the coefficients by comparing them with the results of numerical integration done much more accurately, but we know that we do not have rigorous justification and error bounds on the resulting eigenvalues.

EXAMPLE 1. Define $\phi(\theta) = -i\pi e^{i\theta/2}$. The image of ϕ is a semicircle which is the solid curve in Figure 1. The function has only one point of discontinuity, namely 0, and fits the standard form of (1) and (2) with R=1 and $\beta=\frac{1}{2}$. The eigenvalues of $T_{51}[\phi]$ are also shown, and they lie close to the image of ϕ .

EXAMPLE 2. Let $\phi(\theta) = \theta(\cos \theta + i \sin \theta)$, whose image is a spiral. There is a single discontinuity at $\theta = 0$. Figure 2 shows both the image (solid curve) and the eigenvalues for n = 51.

EXAMPLE 3. Another spiral example is given by

$$\phi(\theta) = \theta(\cos\frac{3}{2}\theta + i\sin\frac{3}{2}\theta). \tag{11}$$

The image is the arc of a spiral passing through an angular change of 3π . Figure 3 shows the eigenvalues of $T_{51}[\phi]$ and the image of ϕ . Until quite recently [14] this example was not covered by any theorem, but now we know that the eigenvalues converge nicely to the arc of the spiral.

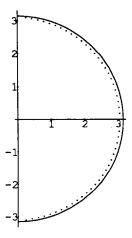


FIG. I. Eigenvalues of $T_{51}[\phi]$ and the image of ϕ .

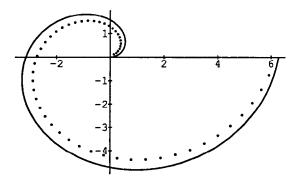


Fig. 2. Eigenvalues of $T_{51}[\phi]$ and the image of ϕ .

3. THE NEW CONJECTURE

The proof given in Section 2 can be extended to any case where the Fisher-Hartwig conjecture is known to be verified and the constant E is not zero. Two years ago we began to look numerically at the eigenvalues of some Toeplitz matrices not covered by theorems. The following examples show that the case of two singularities is more complicated. The pictures of the eigenvalue distributions proved to be illuminating and suggestive of theoretical results to reach for. They provided the experimental evidence that the Fisher-Hartwig conjecture was false for some functions with two discontinuities and pointed the way to a simple counterexample that could be rigorously verified by hand.

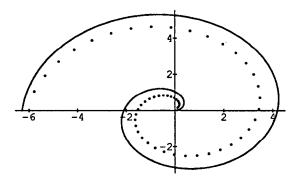


Fig. 3. Eigenvalues of $T_{51}[\phi]$ and the image of ϕ .

Example 4. Define

$$\phi(\theta) = \begin{cases} \theta + i & \text{if } 0 < \theta < \pi, \\ \theta + 2i & \text{if } \pi < \theta < 2\pi. \end{cases}$$
 (12)

This function has two discontinuities, and the range is two disjoint line segments (Figures 4a and 4b). When ϕ is put into standard form, we see R=2 with discontinuities at $\theta_1=0$ and $\theta_2=\pi$. Pay particular attention to the difference between odd and even n and to the slight bending in the "curves" of eigenvalues where the real part is $\frac{1}{2}$.

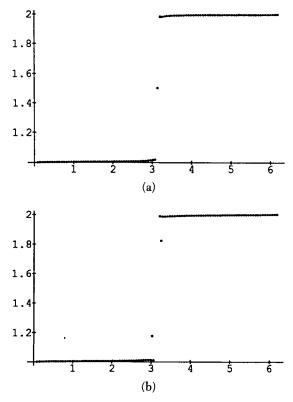


Fig. 4. (a) Eigenvalues of $T_{101}[\phi]$. (b) Eigenvalues of $T_{102}[\phi]$.

EXAMPLE 5. Similar to the previous example is that of the function

$$\phi(\theta) = \begin{cases} (1+i)\theta/\pi & \text{if } 0 < \theta < \pi, \\ 1+2i+(\theta/\pi-1)(1-i) & \text{if } \pi < \theta < 2\pi. \end{cases}$$
(13)

The function is piecewise linear in θ with two jump discontinuities. The image of the top half of the circle is the line segment from the origin to 1+i and the image of the bottom half of the circle is the line segment from 1+2i to 2+i. Figures 5a and 5b show the image of the function and the eigenvalues of $T_n[\phi]$ for n=32 and 51.

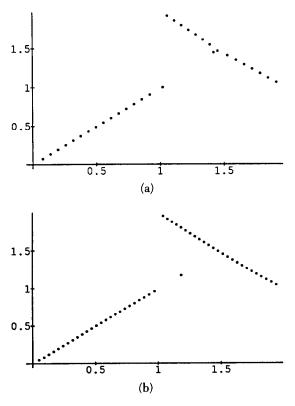


Fig. 5. (a) Eigenvalues of $T_{32}[\phi]$. (b) Eigenvalues of $T_{51}[\phi]$.

In trying to discover the essential features of this example we looked at an even simpler function, namely the piecewise constant function

$$\phi(\theta) = \begin{cases} \pi/2 & \text{if } 0 < \theta < \pi, \\ -\pi/2 & \text{if } -\pi < \theta < 0. \end{cases}$$
 (14)

The Fourier coefficients are given by

$$\phi_n = \begin{cases} 0 & \text{if} \quad n \text{ is seven,} \\ -i/n & \text{if} \quad n \text{ is odd.} \end{cases}$$
 (15)

The Toeplitz matrix $T_n[\phi]$ is skew-symmetric, and so for n odd there is always a zero eigenvalue. It is impossible for the eigenvalues to converge to the image! Immediately we see that the Fisher-Hartwig conjecture must be false for this function, since the asymptotic expansion for the determinant is not zero. Now for n even one may, by rearranging the rows and columns, put the matrix into block form in which each block is a Toeplitz matrix with a generating function for which the Fisher-Hartwig conjecture is known to be true. This allows the computation of the determinant, for which we get

$$D_n[\phi] \sim (i\pi/2)^n n^{-1/2} 2^{1/2} G(\frac{1}{2})^2 G(\frac{3}{2})^2,$$
 (16)

where $G(\frac{1}{2}) = \exp[\frac{3}{2}\zeta'(-1) - \frac{1}{4}\log \pi + \frac{1}{24}\log 2] \approx 0.603...$ and $G(\frac{3}{2}) = \Gamma(\frac{1}{2})G(\frac{1}{2})$ coming from the recurrence formula $G(z+1) = \Gamma(z)G(z)$. It was already known that the eigenvalues in this case do not converge to the image, which in this case is a set with two points. Since the generating function is real, it is known, again using results of Widom [18], that the eigenvalues are dense in the interval $[-\pi/2, \pi/2]$.

However, it was not pointed out until [3] that this generating function fits the form of the Fisher-Hartwig conjecture. It is easy to verify that $\phi(\theta) = it_{1/2}(\theta)t_{-1/2}(\theta+\pi)$. This representation is not unique, since it is also the case that $\phi(\theta) = -it_{-1/2}(\theta)t_{1/2}(\theta+\pi)$. It was also known that for integer $\alpha_r \pm \beta_r$ the conjecture was not true. Fisher and Hartwig excluded this case from the original conjecture about the asymptotics, and the correct answer was given by Böttcher and Silbermann [4]. (See also Day [8].)

The existence of more than one representation and the form of the answer in [4] led to the following reformulated conjecture in [3].

Conjecture 1. Suppose

$$\phi(\theta) = b^{i}(\theta) \prod_{r=1}^{R} t_{\beta_{r}^{i}}(\theta - \theta_{r}) u_{\alpha_{r}^{i}}(\theta - \theta_{r})$$
(17)

for values $\beta_1^i, \ldots, \beta_R^i, \alpha_1^i, \ldots, \alpha_R^i$ and smooth nonzero functions $b^i(\theta)$ each with winding number zero for $i = 1, 2, \ldots$ (When R > 1 there are a countable number of different representations.) Define

$$\Omega(i) = \sum_{r=1}^{R} \left[\left(\alpha_r^i \right)^2 - \left(\beta_r^i \right)^2 \right], \tag{18}$$

$$\Omega = \max_{i} \operatorname{Re} \Omega(i), \tag{19}$$

$$\mathcal{S} = \{i | \text{Re } \Omega(i) = \Omega\}. \tag{20}$$

Then as $n \to \infty$,

$$D_n[\phi] \sim \sum_{i \in \mathscr{S}} G[b^i]^n n^{\Omega(i)} E[b^i, \alpha_r^i, \beta_r^i, \theta_r].$$
 (21)

This conjecture fits all the known cases.

4. STRAY EIGENVALUES

Let us now suppose the new conjecture is true and see what it says about the stray eigenvalues in Examples 4 and 5. Suppose we have $\phi(\theta) = b(\theta)t_{\beta_1}(\theta)t_{\beta_2}(\theta + \pi)$. The values of Re β_i can only differ by an integer, and the requirement that $b(\theta)$ have winding number zero means that if we begin with some choice of β_1 and β_2 , then any new choice β'_1 , β'_2 must satisfy

$$\beta_1' = \beta_1 + j, \tag{22}$$

$$\beta_2' = \beta_2 + k,\tag{23}$$

where j=-k. A simple calculation shows that there is more than one contributing representation (i.e., $|\mathcal{S}| > 1$) in (20) only when $-\text{Re } \beta_1 + \text{Re } \beta_2$ equals some odd integer.

Turn now to Example 4. Let us look at all possible λ such that $-\operatorname{Re} \beta_1(\lambda) + \operatorname{Re} \beta_2(\lambda) = l$ where l is odd. If $\lambda = x + iy$, then an elementary computation shows that x and y must lie on the cubic curve defined by

$$2y^{3} + 2yx^{2} - 4\pi xy - 9y^{2} - 3x^{2} + 5\pi x + (13 + 2\pi^{2})y - 2\pi^{2} - 6$$

$$= 0.$$
(24)

We leave this as an exercise for the reader. Notice that the three stray eigenvalues in Figures 4a and 4b are nearly on this curve, which is shown in Figure 6.

We can make a similar analysis for any function ϕ with two jump discontinuities to obtain a cubic curve which is now the conjectured location for the possible stray eigenvalues. The coefficients of the cubic will vary with the left and right limits of the discontinuities of the generating functions.

So many unanswered questions remain. Are all the stray eigenvalues (asymptotically) on this curve? Are they dense on part of this curve? A reasonable guess would be that they are dense on the part of the cubic that lies in the convex hull of the image of ϕ . What happens for more than two discontinuities? And finally, the examples we have described all have discontinuities at 0 and π . In the example of the piecewise constant function, it is easy to see that the location of the discontinuities yields the difference in behavior between odd and even n. In general, the reformulated conjecture would imply that discontinuities at other locations would yield more complicated asymptotic behavior.

We would like to thank Harold Widom for his time discussing the Toeplitz eigenvalue problem over many years. His influence in this subject has been great. And we would like to thank Chris Dalton, whose senior project contained computation of stray eigenvalues that increased our understanding of the problem.

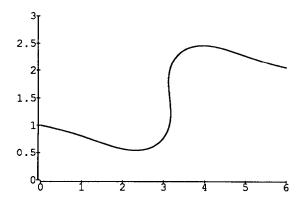


Fig. 6. The cubic curve containing stray eigenvalues.

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