

Natural Boundary for a Sum Involving Toeplitz Determinants

Craig A. Tracy and Harold Widom

For Albrecht Böttcher on the occasion of his sixtieth birthday

Abstract. In the theory of the two-dimensional Ising model, the *diagonal susceptibility* is equal to a sum involving Toeplitz determinants. In terms of a parameter k the diagonal susceptibility is analytic for $|k| < 1$, and the authors proved the conjecture that this function has the unit circle as a natural boundary. The symbol of the Toeplitz determinants was a k -deformation of one with a single singularity on the unit circle. Here we extend the result, first, to deformations of a larger class of symbols with a single singularity on the unit circle, and then to deformations of (almost) general Fisher–Hartwig symbols.

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1. Introduction

In the theory of the two-dimensional Ising model there is a quantity, depending on a parameter k , called the *magnetic susceptibility*, which is analytic for $|k| < 1$. It is an infinite sum over $M, N \in \mathbb{Z}$ involving correlations between the spins at sites $(0, 0)$ and (M, N) . It was shown in [12] to be representable as a sum over $n \geq 1$ of n -dimensional integrals. In [8] B. Nickel found a set of singularities of these integrals which became dense on the unit circle as $n \rightarrow \infty$. This led to the (as yet unproved) *natural boundary conjecture* that the unit circle is a natural boundary for the susceptibility.

Subsequently [4] a simpler model was introduced, called the *diagonal susceptibility*, in which the sum of correlations was taken over the diagonal sites (N, N) . These correlations were equal to Toeplitz determinants, and the diagonal susceptibility was expressible in terms of a sum involving Toeplitz determinants.

The Toeplitz determinant $D_N(\varphi)$ is $\det(\varphi_{i-j})_{1 \leq i, j \leq N}$, where φ_j is the j th Fourier coefficient of the symbol φ defined on the unit circle. The sum in question is

$$\sum_{N=1}^{\infty} [D_N(\varphi) - \mathcal{M}^2], \quad \text{where } \varphi(\xi) = \sqrt{\frac{1 - k/\xi}{1 - k\xi}},$$

and \mathcal{M} , the spontaneous magnetization, is equal to $(1 - k^2)^{1/8}$. This also (as we explain below) is equal to a sum of n -dimensional integrals, the sum is analytic for $|k| < 1$, and the singularities of these summands also become dense on the unit circle as $n \rightarrow \infty$. This led to a natural boundary conjecture for the diagonal susceptibility, which we proved in [11].

The question arises whether the occurrence of the natural boundary is a statistical mechanics phenomenon and/or a Toeplitz determinant phenomenon. This note shows that at least the latter is true. We consider here the more general class of symbols

$$\varphi(\xi) = (1 - k\xi)^{\alpha_+} (1 - k/\xi)^{\alpha_-} \psi(\xi), \tag{1}$$

where ψ is a nonzero function analytic in a neighborhood of the unit circle with winding number zero and geometric mean one. We assume $\alpha_{\pm} \notin \mathbb{Z}$, $\text{Re } \alpha_{\pm} < 1$.¹ The parameter k satisfies $|k| < 1$. We define

$$\chi(k) = \sum_{N=1}^{\infty} [D_N(\varphi) - E(\varphi)], \tag{2}$$

where

$$E(\varphi) = \lim_{N \rightarrow \infty} D_N(\varphi). \tag{2}$$

Each summand in (2) is analytic in the unit disc $|k| < 1$, the only singularities on the boundary being at $k = \pm 1$, and the series converges uniformly on compact subsets. Therefore $\chi(k)$ is analytic in the unit disc.

Theorem 1. *The unit circle $|k| = 1$ is a natural boundary for $\chi(k)$.*

The result in [11] was established, and here will be established, by showing that the singularities of the n th summand of the series are not canceled by the infinitely many remaining terms of the series.³ We shall see that a certain derivative of the n th term is unbounded as k^2 tends to an n th root of unity while the same derivative of the sum of the later terms is bounded, and if it is a primitive n th root the same derivative of each earlier term is also bounded.

¹Observe that we never consider a limiting symbol with k on the unit circle, and so do not require that $\text{Re } \alpha_{\pm} > -1$. The condition stated is one that will be needed for the integrability on the unit circle of a function that arises in the proof of the theorem.

²When $\psi(\xi) = 1$ it equals $(1 - k^2)^{-\alpha_+ + \alpha_-}$. In general it equals this times a function that extends analytically beyond the unit disc.

³A nice example [9] where such a cancelation does occur is

$$\frac{z}{1 - z} = \frac{z}{1 - z^2} + \frac{z^2}{1 - z^4} + \frac{z^4}{1 - z^8} + \cdots + \frac{z^{2^n}}{1 - z^{2^{n+1}}} + \cdots$$

To put what we have done into some perspective, we start with a symbol

$$(1 - \xi)^{\alpha_+} (1 - 1/\xi)^{\alpha_-}.$$

Then we introduce its k -deformation, times a “nice” function $\psi(\xi)$, and consider their Toeplitz determinants as functions of the parameter k inside the unit circle. Is it important that we begin with a symbol with only one singularity on the boundary? It is not. We may begin instead with a general Fisher–Hartwig symbol [5]

$$\prod_{p=1}^P (1 - u_p \xi)^{\alpha_p^+} \prod_{q=1}^Q (1 - v_q/\xi)^{\alpha_q^-},$$

where $|u_p|, |v_q| = 1$ and $P, Q > 0$. With some conditions imposed on the α_p^+ and the α_q^- , we show that the conclusion of the theorem holds for the deformations of these symbols.

Here is an outline of the paper. In the next section we derive the expansion for $\chi(k)$ as a series of multiple integrals. In the following section the theorem is proved, and in the section after that we show how to extend the result to (almost) general Fisher–Hartwig symbols. In two appendices we give the proof of a proposition used in Section II and proved in [11], and discuss a minimum question that arises in Section IV.

2. Preliminaries

We invoke the formula of Geronimo–Case [6] and Borodin–Okounkov [2] to write the Toeplitz determinant in terms of the Fredholm determinant of a product of Hankel operators. The Hankel operator $H_N(\varphi)$ is the operator on $\ell^2(\mathbb{Z}^+)$ with kernel $(\varphi_{i+j+N+1})_{i,j \geq 0}$.

We have a factorization $\varphi(\xi) = \varphi_+(\xi) \varphi_-(\xi)$, where φ_+ extends analytically inside the unit circle and φ_- outside, and $\varphi_+(0) = \varphi_-(\infty) = 1$. More explicitly,

$$\varphi_+(x) = (1 - k\xi)^{\alpha_+} \psi_+(\xi) \quad \text{and} \quad \varphi_-(\xi) = (1 - k/\xi)^{\alpha_-} \psi_-(\xi).$$

If $\psi(\xi)$ is analytic and nonzero for $s < |\xi| < s^{-1}$ then $\psi_+(\xi)$ resp. $\psi_-(\xi)$ is analytic and nonzero for $|\xi| < s^{-1}$ resp. $|\xi| > s$.

The formula of G-C/B-O is

$$D_N(\varphi) = E(\varphi) \det \left(I - H_N \left(\frac{\varphi_-}{\varphi_+} \right) H_N \left(\frac{\tilde{\varphi}_+}{\tilde{\varphi}_-} \right) \right),$$

where for a function f we define $\tilde{f}(\xi) = f(\xi^{-1})$. Thus, if we write

$$\Lambda(\xi) = \frac{\varphi_-(\xi)}{\varphi_+(\xi)} = (1 - k\xi)^{-\alpha_+} (1 - k/\xi)^{\alpha_-} \frac{\psi_-(\xi)}{\psi_+(\xi)},$$

$$K_N = H_N(\Lambda) H_N(\tilde{\Lambda}^{-1}), \tag{3}$$

then $\chi(k)$ equals $E(\varphi)$ times

$$\mathcal{S}(k) = \sum_{N=1}^{\infty} [\det(I - K_N) - 1].$$

In [11] the following was proved. We give the proof in Appendix A.

Proposition. *Let $H_N(du)$ and $H_N(dv)$ be two Hankel matrices acting on $\ell^2(\mathbb{Z}^+)$ with i, j entries*

$$\int x^{N+i+j} du(x), \quad \int y^{N+i+j} dv(y), \tag{4}$$

respectively, where u and v are measures supported in the open unit disc. Set $K_N = H_N(du) H_N(dv)$. Then

$$\begin{aligned} & \sum_{N=1}^{\infty} [\det(I - K_N) - 1] \\ &= \sum_{n=1}^{\infty} \frac{(-1)^n}{(n!)^2} \int \dots \int \frac{\prod_i x_i y_i}{1 - \prod_i x_i y_i} \left(\det \left(\frac{1}{1 - x_i y_j} \right) \right)^2 \prod_i du(x_i) dv(y_i), \end{aligned}$$

where indices in the integrand run from 1 to n .

We apply this to the operator $K_N = H_N(\Lambda) H_N(\tilde{\Lambda}^{-1})$ given by (3). The matrix for $H_N(\Lambda)$ has i, j entry

$$\frac{1}{2\pi i} \int \Lambda(\xi) \xi^{-N-i-j-2} d\xi,$$

where the integration is over the unit circle. The integration may be taken over a circle with radius in $(1, |k|^{-1})$ as long as $|k| > s$. (Recall that $\psi_{\pm}(\xi)$ are analytic and nonzero for $s < |\xi| < s^{-1}$.) We assume this henceforth.

Setting $\xi = 1/x$ we see that the entries of $H_N(\Lambda)$ are given as in (4) with

$$du(x) = \frac{1}{2\pi i} \Lambda(x^{-1}) dx,$$

and integration is over a circle \mathcal{C} with radius in $(|k|, 1)$. Similarly, $H_N(\tilde{\Lambda}^{-1}) = H_N(dv)$ where in (4)

$$dv(y) = \frac{1}{2\pi i} \Lambda(y)^{-1} dy,$$

with integration over the same circle \mathcal{C} .

Hence the proposition gives

$$\mathcal{S}(k) = \sum_{n=1}^{\infty} \mathcal{S}_n(k), \tag{5}$$

where

$$\begin{aligned} \mathcal{S}_n(k) &= \frac{(-1)^n}{(n!)^2} \frac{1}{(2\pi i)^{2n}} \\ &\quad \times \int \dots \int \frac{\prod_i x_i y_i}{1 - \prod_i x_i y_i} \left(\det \left(\frac{1}{1 - x_i y_j} \right) \right)^2 \prod_i \frac{\Lambda(x_i^{-1})}{\Lambda(y_i)} \prod_i dx_i dy_i, \end{aligned}$$

with all integrations over \mathcal{C} .

We deform each \mathcal{C} to the circle with radius $|k|$ (after which there are integrable singularities on the contours). Then we make the substitutions $x_i \rightarrow kx_i$, $y_i \rightarrow ky_i$, and obtain

$$\mathcal{S}_n(k) = \frac{(-1)^n \kappa^{2n}}{(n!)^2 (2\pi i)^{2n}} \times \int \dots \int \frac{\prod_i x_i y_i}{1 - \kappa^n \prod_i x_i y_i} \left(\det \left(\frac{1}{1 - \kappa x_i y_j} \right) \right)^2 \prod_i \frac{\Lambda(k^{-1} x_i^{-1})}{\Lambda(k y_i)} \prod_i dx_i dy_i, \tag{6}$$

where integrations are on the unit circle. We record that

$$\frac{\Lambda(k^{-1} x^{-1})}{\Lambda(k y)} = \frac{(1 - \kappa x)^{\alpha_-} (1 - x^{-1})^{-\alpha_+} \rho(k^{-1} x^{-1})}{(1 - \kappa y)^{-\alpha_+} (1 - y^{-1})^{\alpha_-} \rho(k y)}, \tag{7}$$

where we have set

$$\kappa = k^2, \quad \rho(x) = \frac{\psi_-(x)}{\psi_+(x)}.$$

The complex planes are cut from κ^{-1} to ∞ for the first quotient in (7) and from 0 to 1 for the second quotient.

Using the fact that the determinant in the integrand is a Cauchy determinant we obtain the alternative expression

$$\mathcal{S}_n(k) = \frac{(-1)^n \kappa^{n(n+1)}}{(n!)^2 (2\pi i)^{2n}} \times \int \dots \int \frac{\prod_i x_i y_i}{1 - \kappa^n \prod_i x_i y_i} \frac{\Delta(x)^2 \Delta(y)^2}{\prod_{i,j} (1 - \kappa x_i y_j)^2} \prod_i \frac{\Lambda(k^{-1} x_i^{-1})}{\Lambda(k y_i)} \prod_i dx_i dy_i, \tag{8}$$

where $\Delta(x)$ and $\Delta(y)$ are Vandermonde determinants

3. Proof of Theorem 1

For any $\delta < 1 - s$ we can deform each contour of integration to one that goes back and forth along the segment $[1 - \delta, 1]$ and then around the circle with center zero and radius $1 - \delta$.⁴ This is the contour we use from now on.

There will be three lemmas. In these, $\epsilon \neq 1$ will be an n th root of unity and we consider the behavior of $\mathcal{S}(k)$ as $\kappa \rightarrow \epsilon$ radially. Because the argument that follows involves only the local behavior of $\mathcal{S}(k)$, we may consider κ as the underlying variable and in (7) replace k by the appropriate $\sqrt{\kappa}$. We define

$$\mu = \kappa^{-n} - 1, \quad \beta = \alpha_+ + \alpha_-, \quad b = \text{Re } \beta,$$

so that $\mu > 0$ and $\mu \rightarrow 0$ as $\kappa \rightarrow \epsilon$.

⁴To expand on this, it goes from $1 - \delta$ to 1 just below the interval $[1 - \delta, 1]$, then from 1 to $1 - \delta$ just above the interval $[1, 1 - \delta]$, then counterclockwise around the circle with radius $1 - \delta$ back to $1 - \delta$.

Lemma 1. *We have*⁵

$$\left(\frac{d}{d\kappa}\right)^{2n^2-[bn]} \mathcal{S}_n(k) \approx \mu^{[bn]-\beta n-1}.$$

Proof. We set

$$\ell = 2n^2 - [bn]$$

and first consider

$$\int \cdots \int \frac{\prod_i x_i y_i}{(1 - \kappa^n \prod_i x_i y_i)^{\ell+1}} \frac{\Delta(x)^2 \Delta(y)^2}{\prod_{i,j} (1 - \kappa x_i y_j)^2} \prod_i \frac{\Lambda(k^{-1} x_i^{-1})}{\Lambda(k y_i)} \prod_i dx_i dy_i, \quad (9)$$

where all indices run from 1 to n . This will be the main contribution to $d^\ell \mathcal{S}_n(k)/d\kappa^\ell$.

For the i, j factor in the denominator in the second factor, if x_i or y_j is on the circular part of the contour then $|x_i y_j| \leq 1 - \delta$ and the factor is bounded away from zero; otherwise $x_i y_j$ is real and positive and this factor is bounded away from zero as $\kappa \rightarrow \epsilon$ since $\epsilon \neq 1$. So we consider the rest of the integrand.

If $\prod_i |x_i y_i| < 1 - \delta$ then the rest of the integrand is bounded except for the last quotient, and the integral of that is $O(1)$ since $\operatorname{Re} \alpha_\pm < 1$.

When $\prod_i |x_i y_i| > 1 - \delta$ then each $|x_i|, |y_i| > 1 - \delta$, so each x_i, y_i is integrated below and above the interval $[1 - \delta, 1]$. If all the integrals are taken over the interval itself we must multiply the result by the nonzero constant $(4 \sin \pi \alpha_+ \sin \pi \alpha_-)^n$. The factors $1 - \kappa x_i y_j$ in the second denominator equal $1 - \kappa(1 + O(\delta)) = (1 - \kappa)(1 + O(\delta))$ since κ is bounded away from 1. From this we see that if we factor out $\kappa^{(\ell+1)n}$ from the first denominator, $(1 - \kappa)^{n^2}$ from the second denominator, and $(1 - \kappa)^{\beta n} (\rho(k^{-1})/\rho(k))^n$ from the last factor (all of these having nonzero limits as $\kappa \rightarrow \epsilon$), the integrand becomes

$$\frac{\Delta(x)^2 \Delta(y)^2}{(\kappa^{-n} - \prod_i x_i y_i)^{\ell+1}} \prod_i (1 - x_i)^{-\alpha_+} (1 - y_i)^{-\alpha_-} (1 + O(\delta)). \quad (10)$$

We make the substitutions $x_i = 1 - \xi_i, y_i = 1 - \eta_i$ and set $r = \sum_i (\xi_i + \eta_i)$. Then since $\prod_i (1 - \xi_i)(1 - \eta_i) = 1 - r + O(r^2)$ this becomes

$$\frac{\Delta(\xi)^2 \Delta(\eta)^2}{(\mu + r + O(r^2))^{\ell+1}} \prod_i \xi_i^{-\alpha_+} \eta_i^{-\alpha_-} (1 + O(\delta)).$$

The integration domain becomes $r < \delta + O(\delta^2)$. Consider first the integral without the $O(\delta)$ term. By homogeneity of the Vandermondes and the product, the integral

⁵We use the usual notation $[bn]$ for the greatest integer in bn . The symbol \approx here indicates that the ratio tends to a nonzero constant as $\mu \rightarrow 0$.

equals a nonzero constant⁶ times

$$\int_0^{\delta+O(\delta^2)} \frac{r^{2n^2-\beta n-1}}{(\mu+r+O(r^2))^{\ell+1}} dr. \tag{11}$$

Making the substitution $r \rightarrow \mu r$ results in

$$\begin{aligned} &\mu^{2n^2-\beta n-\ell-1} \int_0^{(\delta+O(\delta^2))/\mu} \frac{r^{2n^2-\beta n-1}}{(1+r+O(\mu^2 r^2))^{\ell+1}} dr \\ &= \mu^{[bn]-\beta n-1} \int_0^{(\delta+O(\delta^2))/\mu} \frac{r^{2n^2-\beta n-1}}{(1+r+O(\mu^2 r^2))^{2n^2-[bn]+1}} dr, \end{aligned} \tag{12}$$

where we have put in our value of ℓ . The integral has the $\mu \rightarrow 0$ limit the convergent integral

$$\int_0^\infty \left(\frac{r}{1+r}\right)^{2n^2-[bn]+1} r^{[bn]-\beta n-2} dr,$$

and (11) is asymptotically this times $\mu^{[bn]-\beta n-1}$.

For the integral with the $O(\delta)$ we take the absolute values inside the integrals and find that it is $O(\delta)$ times what we had before, except that the β in the exponents are replaced by b , and in footnote 6 the exponents α_\pm are replaced by their real parts. Since δ is arbitrarily small, it follows that the integral of (10) is asymptotically a nonzero constant times $\mu^{[bn]-\beta n-1}$.

To compute the derivative of order $2n^2 - [bn]$ of the integral in (8) one integral we get is what we just computed. The other integrals are similar but in each the ℓ in the first denominator is at most $2n^2 - [bn] - 1$, while we get extra factors obtained by differentiating the rest of the integrand for $\mathcal{S}_n(k)$. These factors are of the form $(1 - \kappa x_i y_i)^{-1}$, $(1 - \kappa x_i)^{-1}$, $(1 - \kappa y_i)^{-1}$, or derivatives of $\rho(k^{-1} x_i^{-1})$ or of $\rho(k y_i)^{-1}$. These are all bounded. Because $\ell \leq 2n^2 - [bn] - 1$ the integral (11) is $O(\mu^{-1+\gamma})$ for some $\gamma > 0$. The lemma follows. \square

Lemma 2. *If $\epsilon^m \neq 1$ then*

$$\left(\frac{d}{d\kappa}\right)^{2n^2-[bn]} \mathcal{S}_m(k) = O(1).$$

Proof. If $\epsilon^m \neq 1$ all terms, aside from those coming from the last factors, obtained by differentiating the integrand in (8) with n replaced by m are bounded as $\kappa \rightarrow \epsilon$. Differentiating the last factor in the integrand any number of times results in an integrable function. \square

⁶This is the integral of $\Delta(\xi)^2 \Delta(\eta)^2 \prod \xi_i^{-\alpha_+} \eta_i^{-\alpha_-}$ over $r = 1$. It can be evaluated using a Selberg integral [7, (17.6.5)], with the result

$$\frac{1}{\Gamma(2n^2 - \beta n)} \prod_{j=0}^{n-1} \Gamma(j+2)^2 \Gamma(j - \alpha_+ + 1) \Gamma(j - \alpha_- + 1).$$

Lemma 3. We have $\sum_{m>n} (d/d\kappa)^{2n^2-[bn]} S_m(k) = O(1)$.

Proof. We shall show that for κ sufficiently close to ϵ all integrals we get by differentiating the integral for $S_m(k)$ are at most $A^m m^m$, where A is some constant.⁷ Because of the $1/(m!)^2$ appearing in front of the integrals this will show that the sum is bounded.

As before, we first use (8) with n replaced by m , and consider the integral we get when the first factor in the integrand is differentiated $2n^2 - [bn]$ times. All indices in the integrands now run from 1 to m .

First,

$$|1 - \kappa^m \prod_i x_i y_i| \geq 1 - \prod_i |x_i y_i|.$$

Next we use that either $|x_i| = 1 - \delta$ or $x_i \in [0, 1]$, and $\kappa \in [0, \epsilon]$, to see that $|1 - \kappa x_i| \geq \min(\delta, d)$, where $d = \text{dist}(1, [0, \epsilon])$. We may assume $\delta < d$. Then $|1 - \kappa x_i| \geq \delta$, and similarly, $|1 - \kappa y_i| \geq \delta$. It follows that the integrand in (8) after differentiating the first factor has absolute value at most A^m times

$$\frac{1}{(1 - \prod_i |x_i y_i|)^{2n^2-[bn]+1}} \frac{\Delta(x)^2 \Delta(y)^2}{\prod_{i,j} |1 - \kappa x_i y_j|^2} \prod_i |1 - x_i|^{-a_+} |1 - y_i|^{-a_-}, \quad (13)$$

where $a_{\pm} = \text{Re } \alpha_{\pm}$.

If $\prod_i |x_i y_i| < 1 - \delta$ then the first factor is at most $\delta^{-2n^2+[bn]-1}$. When $\prod_i |x_i y_i| > 1 - \delta$ we set, as before, $x_i = 1 - \xi_i$, $y_i = 1 - \eta_i$ with $\xi_i, \eta_i \in [0, \delta]$. Since we are to integrate back and forth over these intervals we must multiply the estimate below by the irrelevant factor 2^{2m} .

We have $\prod_i (1 - \xi_i)(1 - \eta_i) \leq (1 - \xi_i)(1 - \eta_i)$ for each i , and so averaging gives

$$\prod_i (1 - \xi_i)(1 - \eta_i) \leq \frac{1}{2m} \sum_i (1 - \xi_i)(1 - \eta_i),$$

and therefore

$$\begin{aligned} 1 - \prod_i (1 - \xi_i)(1 - \eta_i) &\geq \frac{1}{2m} \sum_i (1 - (1 - \xi_i)(1 - \eta_i)) \\ &= \frac{1}{2m} \sum_i (\xi_i + \eta_i - \xi_i \eta_i) \geq \frac{1}{2m} \sum_i (\xi_i + \eta_i)/2 \end{aligned} \quad (14)$$

if $\delta < 1/2$, since each $\xi_i, \eta_i < \delta$. From this we see that in the region where $\sum_i (\xi_i + \eta_i) > \delta$ the first factor in (13) is at most $(4m/\delta)^{2n^2-[bn]+1}$.

So in either of these two regions the first factor is at most A^m . We then use (13) with the second factor replaced by the absolute value of

$$(\det(1/(1 - \kappa x_i y_j)))^2.$$

Each denominator has absolute value at least δ , so by the Hadamard inequality the square of the determinant has absolute value at most $\delta^{-2m} m^m$. Therefore the

⁷The value of A will change with each of its appearances. It may depend on n and δ , which are fixed, but not on m .

integral over this region has absolute value at most

$$A^m m^m \int \dots \int \prod_i |1 - x_i|^{-a_+} |1 - y_i|^{-a_-} \prod_i dx_i dy_i.$$

The integral here is A^m , and so we have shown that the integral in the described region is at most $A^m m^m$.

It remains to bound the integral over the region where $x_i = 1 - \xi_i$, $y_i = 1 - \eta_i$ with $\xi_i, \eta_i \in [0, \delta]$, and $r = \sum_i (\xi_i + \eta_i) < \delta$. Using (14) again, we see that the integrand has absolute value at most A^m times

$$d^{-m^2} \frac{\Delta(\xi)^2 \Delta(\eta)^2}{(\sum_i (\xi_i + \eta_i))^{2n^2 - [bn] + 1}} \prod_i \xi_i^{-a_+} \eta_i^{-a_-}.$$

(Recall that $d = \text{dist}(1, [0, \epsilon])$, and $\kappa x_i y_j \in [0, \epsilon]$. The factor $(4m^2)^{2n^2 - [\gamma n] + 1}$ coming from using (14) were absorbed into A^m .) Integrating this with respect to r over $r < \delta$, using homogeneity, gives

$$\int_{r=1} \Delta(\xi)^2 \Delta(\eta)^2 \prod_i \xi_i^{-a_+} \eta_i^{-a_-} d(\xi, \eta)$$

(where $d(\xi, \eta)$ denotes the $(2n - 1)$ -dimensional measure on $r = 1$) times

$$d^{-m^2} \int_0^\delta r^{2m^2 - 2n^2 + [bn] - bn - 1} dr.$$

The first integral is given in footnote 6 with n replaced by m and α_\pm replaced by a_\pm , and is exponentially small in m . The last integral is $O(\delta^{2m^2})$ since $m > n$ and n is fixed. Since $\delta^2 < d$, the product is exponentially small in m .

So we have obtained a bound for one term we get when we differentiate $2n^2 - [\gamma n]$ times the integrand for $\mathcal{S}_m(k)$. The number of factors in the integrand involving κ is $O(m^2)$ so if we differentiate $2n^2 - 1$ times we get a sum of $O(m^{4n^2})$ terms. In each of the other terms the denominator in the first factor has a power even less than $2n^2 - [\gamma n]$ and at most $2n^2$ extra factors appear which are of the form $(1 - \kappa x_i y_i)^{-1}$, $(1 - \kappa x_i)^{-1}$, or $(1 - \kappa y_i)^{-1}$. Also, $\rho(k^{-1} x_i^{-1})$ or $\rho(k y_i)^{-1}$ may be replaced by some of its derivatives. Each has absolute value at most δ^{-1} , so their product is $O(\delta^{-4n^2})$. It follows that we have the bound $A^m m^m$ for the sum of these integrals. Lemma 3 is established. \square

Proof of the theorem. Let ϵ be a primitive n th root of unity. Then $\epsilon^m \neq 1$ when $m < n$ so Lemma 2 applies for these m . Combining this with Lemmas 1 and 3 we obtain

$$(d/d\kappa)^{2n^2 - [bn]} \mathcal{S}(k) \approx \mu^{[bn] - \beta n - 1}$$

as $\kappa \rightarrow \epsilon$. This is unbounded, so $\mathcal{S}(k)$ cannot be analytically continued beyond any such ϵ , and these are dense on the unit circle.

Thus the unit circle is a natural boundary for $\mathcal{S}(k)$, and this implies that the same is true of $\chi(k)$. This completes the proof of the theorem. \square

4. Fisher–Hartwig symbols

In this section we show how to extend the proof of the theorem to deformations of Fisher–Hartwig symbols. We start with a Fisher–Hartwig symbol⁸

$$\prod_{p=1}^P (1 - u_p \xi)^{\alpha_p^+} \prod_{q=1}^Q (1 - v_q/\xi)^{\alpha_q^-},$$

where $|u_p|, |v_q| = 1$ and $P, Q > 0$, and then its k -deformation

$$\varphi(\xi) = \prod_{p=1}^P (1 - k u_p \xi)^{\alpha_p^+} \prod_{q=1}^Q (1 - k v_q/\xi)^{\alpha_q^-}.$$

We assume that $\text{Re } \alpha_p^+, \text{Re } \alpha_q^- < 1$ and $\alpha_p^+, \alpha_q^- \notin \mathbb{Z}$. (Plus a simplifying assumption that comes later.) Now the singularities of $D_N(\varphi)$ on the unit circle are at the $(u_p v_q)^{-1/2}$, and

$$E(\varphi) = \prod_{p,q} (1 - k^2 u_p v_q)^{-\alpha_p^+ \alpha_q^-}.$$

Theorem 2. *With the given assumptions, the unit circle $|k| = 1$ is a natural boundary for $\chi(k)$.*

Proof. Using previous notation, we have now

$$\Lambda(\xi) = \prod_{p,q} (1 - k u_p \xi)^{-\alpha_p^+} (1 - k v_q/\xi)^{\alpha_q^-},$$

$$\frac{\Lambda(k^{-1}x^{-1})}{\Lambda(ky)} = \prod_{p,q} \frac{(1 - u_p/x)^{-\alpha_p^+} (1 - \kappa v_q x)^{\alpha_q^-}}{(1 - \kappa u_p y)^{-\alpha_p^+} (1 - v_q/y)^{\alpha_q^-}}.$$

Again we begin by considering the integral

$$\int \dots \int \frac{\prod_i x_i y_i}{(1 - \kappa^n \prod_i x_i y_i)^{\ell+1}} \frac{\Delta(x)^2 \Delta(y)^2}{\prod_{i,j} (1 - \kappa x_i y_j)^2} \prod_i \frac{\Lambda(k^{-1}x_i^{-1})}{\Lambda(ky_i)} \prod_i dx_i dy_i. \quad (15)$$

For $\delta \in (0, 1)$, our integrations are for the x_i around the cuts $[1 - \delta, 1] u_p$ and for the y_i around the cuts $[1 - \delta, 1] v_q$ and then both around the circle with radius $1 - \delta$. If we replace integrals around the cuts by integrals on the cuts, then for a cut $[1 - \delta, 1] u_p$ we must multiply by $2 \sin \pi \alpha_p^+$ and for a cut $[1 - \delta, 1] v_q$ we multiply by $2 \sin \pi \alpha_q^-$. These are both nonzero. We assume that this has been done.

We now let $\kappa \rightarrow \epsilon$ radially, where ϵ is an n th root of $\prod (u_{p_i} v_{q_i})^{-1}$, but not equal to any $(u_p v_q)^{-1}$. We also choose it so that it is not an m th root of any product of the form $\prod (u_{p_i} v_{q_i})^{-1}$ with $m < n$. These ϵ become dense on the unit circle as $n \rightarrow \infty$. The last condition assures that the integrals with $m < n$ are bounded, which will give the analogue of Lemma 2. We now consider the analogue of Lemma 1.

⁸We could easily add a factor $\psi(\xi)$ to give the general Fisher–Hartwig symbol. Then the δ chosen below would depend on the region of analyticity of ψ .

The integral over $\prod |x_i y_i| < 1 - \delta$ is bounded, as before. In the region where $\prod |x_i y_i| > 1 - \delta$ each x_i and y_i is integrated on the union of its associated cuts. This is the sum of integrals in each of which each x_i is integrated over one of the cuts and each y_i is integrated over one of the cuts. Suppose that x_i is integrated over $[1 - \delta, 1] u_{p_i}$ and y_i is integrated over $[1 - \delta, 1] v_{q_i}$. (We consider this one possibility at first. Then we will have to sum over all possibilities.)

If we factor out $\prod u_{p_i} v_{q_i}$ from the first numerator, $\prod (1 - \kappa u_{p_i} v_{q_i})^2$ from the second denominator, and $\prod (1 - \kappa u_{p_i} v_{q_i})^{\alpha_{p_i} + \alpha_{q_i}}$ from the last product the integrand becomes $1 + O(\delta)$ times

$$\frac{\Delta(x)^2 \Delta(y)^2}{(1 - \kappa^n \prod_i x_i y_i)^{\ell+1}} \prod_i (1 - u_{p_i}/x_i)^{-\alpha_{p_i}^+} (1 - v_{q_i}/y_i)^{-\alpha_{q_i}^-}. \tag{16}$$

We make the substitutions $x_i = (1 - \xi_i) u_{p_i}$, $y_i = (1 - \eta_i) v_{q_i}$, and define

$$I_p = \{i : p_i = p\}, \quad I_q = \{i : q_i = q\}.$$

Then

$$\prod_i (1 - u_{p_i}/x_i)^{-\alpha_{p_i}^+} (1 - v_{q_i}/y_i)^{-\alpha_{q_i}^-} = \prod_{p, i \in I_p} \xi_i^{-\alpha_p^+} \cdot \prod_{q, i \in I_q} \eta_i^{-\alpha_q^-} \times (1 + O(\delta)).$$

As for the Vandermondes, we have

$$\Delta(x) = \pm \prod_p \Delta(x_i : i \in I_p) \cdot \prod_{p \neq p'} \prod_{j \in I_p, j' \in I_{p'}, j < j'} (x_j - x_{j'}), \tag{17}$$

and similarly for $\Delta(y)$. If we define $n_p = |I_p|$, $n_q = |I_q|$, then the last double product is to within a factor $1 + O(\delta)$ equal to

$$\pm \prod_{p < p'} (u_p - u_{p'})^{n_p n_{p'}},$$

while the first product is to within a factor $1 + O(\delta)$ equal to

$$\prod_p u_p^{n_p(n_p+1)/2} \prod_p \Delta(\xi_i : i \in I_p).$$

Thus, if we factor out $(\kappa^n \prod u_{p_i} v_{q_i})^{\ell+1}$ from the denominator in (16), and set $\mu = \kappa^{-n} \prod (u_{p_i} v_{q_i})^{-1} - 1$, then (16) may get replaced by a constant times $1 + O(\delta)$ times

$$\frac{1}{(\mu + \sum_i (\xi_i + \eta_i))^{\ell+1}} \prod_{p, i \in I_p} \Delta(\xi_i : i \in I_p)^2 \xi_i^{-\alpha_p^+} \cdot \prod_{q, i \in I_q} \Delta(\eta_i : i \in I_q)^2 \eta_i^{-\alpha_q^-}. \tag{18}$$

If we use homogeneity the integral of (18) becomes a nonzero constant⁹ times

$$\int_0^\delta \frac{1}{(\mu + r)^{\ell+1}} r^{-1 + \sum_p n_p(n_p - \alpha_p^+) + \sum_q n_q(n_q - \alpha_q^-)} dr. \tag{19}$$

⁹Also computable using the Selberg integral, it is [see next page]

This is largest when the power of r is smallest. So we minimize

$$\sum_p n_p(n_p - a_p^+), \quad (a_p^+ = \operatorname{Re} \alpha_p^+)$$

over all $\{n_p\}$ with $n_p \geq 0$, $\sum_p n_p = n$. The solution is not necessarily unique.¹⁰ But in any case

$$M_n^+ := \min \sum_p n_p(n_p - a_p^+) = \frac{n^2}{P} + O(n), \quad (20)$$

and $M_{n+1}^+ > M_n^+$ for large enough n .¹¹ Similarly, with $a_q^- = \operatorname{Re} \alpha_q^-$ and

$$M_n^- := \min \sum_q n_q(n_q - a_q^-) = \frac{n^2}{Q} + O(n). \quad (21)$$

Then we choose

$$\ell = \sum_p n_p^2 + \sum_q n_q^2 - \left[\sum_p n_p a_p^+ + \sum_q n_q a_q^- \right] \quad (22)$$

with the minimal n_p and n_q . The integral (19) is equal to

$$\mu^{-1 + [\sum_p n_p a_p^+ + \sum_q n_q a_q^-] - (\sum_p n_p \alpha_p^+ + \sum_q n_q \alpha_q^-)}$$

times

$$\int_0^{\delta/\mu} \frac{1}{(1+r)^{\ell+1}} r^{-1 + \sum_p n_p(n_p - \alpha_p^+) + \sum_q n_q(n_q - \alpha_q^-)} dr.$$

The exponent of μ has real part in $(-2, -1]$ and the integral has a nonzero limit (a Beta function) as $\mu \rightarrow 0$.

Once we take care of the integrals with the $O(\delta)$ as in the proof of Lemma 1 we deduce that this is the asymptotic result for the integral when we choose this set of cuts.

*We now assume the minimal solutions are unique.*¹²

Then for the other choices of cuts the integral (19) is $O(\mu^{-1+\gamma})$ for some $\gamma > 0$, and so the integral over the chosen set of cuts dominates. We still have to allocate the x_i and y_i to the various cuts, once the numbers of each have been

$$\frac{1}{\Gamma(\sum_p n_p(n_p - \alpha_p^+) + \sum_q n_q(n_q - \alpha_q^-))} \\ \times \prod_p \prod_{j=0}^{n_p-1} \Gamma(j+2) \Gamma(j - \alpha_p^+ + 1) \cdot \prod_q \prod_{j=0}^{n_q-1} \Gamma(j+2) \Gamma(j - \alpha_q^- + 1).$$

¹⁰A similar minimum problem was encountered in [3], where an asymptotic formula was a sum over all solutions. We shall eventually assume a unique solution to avoid the possibility of cancellation of terms of the same order.

¹¹See Appendix B.

¹²We shall see in Appendix B that for large n uniqueness is a condition on the a_p^+ and a_q^- that depends only on the residue classes of n modulo P and Q . It suffices for our purposes that we have uniqueness for some sequence $n \rightarrow \infty$.

chosen. The number of ways of doing this is $n!/\prod n_p!$ for the x_i and $n!/\prod n_q!$ for the y_i . (The total number of ways is at most $P^n Q^n$.)

This takes care of the integral (15), the main contributions to $(d/d\kappa)^\ell S_n(\kappa)$. We complete the proof of the analogue of Lemma 1 as we did at the end of the proof of that lemma. Thus, with ℓ given by (22),

$$\left(\frac{d}{d\kappa}\right)^\ell S_n(k) \approx \mu^{-1+[\sum_p n_p a_p^+ + \sum_q n_q a_q^-] - (\sum_p n_p \alpha_p^+ + \sum_q n_q \alpha_q^-)}.$$

For the analogue of Lemma 3 we first consider the integral (15) with n replaced by $m > n$, and ℓ given by (22). As before it remains to bound the integrals over the regions where each $x_i = (1 - \xi_i)u_{p_i}$ and each $y_i = (1 - \eta_i)v_{q_i}$, with $\xi_i, \eta_i \in [0, \delta]$, and $r = \sum_i (\xi_i + \eta_i) < \delta$.

Replacing the first denominator in (15) by $(\sum(\xi_i + \eta_i))^{\ell+1}$ introduces a factor $(4m^2/\delta)^{\ell+1}$ as before, a factor that can be ignored. The reciprocal of the second denominator is at most d^{-m^2} where $d = \min_{p,q} \text{dist}([0, \epsilon], (u_p v_q)^{-1})$. The product of the terms involving κ in the last product is $d^{-O(m)}$, and so may also be ignored. The square of the product over $p < p'$ in (17), times the square of the analogous product over $q < q'$, is at most $2^{(P^2+Q^2)m^2}$. There remains an integrand whose absolute value is bounded by

$$\frac{1}{(\sum_i (\xi_i + \eta_i))^{\ell+1}} \prod_{p, i \in I_p} \Delta(\xi_i : i \in I_p)^2 \xi_i^{-a_p^+} \cdot \prod_{q, i \in I_q} \Delta(\eta_i : i \in I_q)^2 \eta_i^{-a_q^-}.$$

The integral of the products over $r = 1$ (given exactly in footnote 9) is trivially at most its maximum (at most $A^m 4^{m^2}$) times the $(2m - 1)$ -dimensional measure of $r = 1$, which is $1/\Gamma(2m)$. We use the crude bound 4^{m^2} . This is to multiply

$$\int_0^\delta r^{-\ell-2+\sum_p m_p(m_p-a_p^+)+\sum_q m_q(m_q-a_q^-)} dr.$$

Now

$$\sum_p m_p(m_p - a_p^+) + \sum_q m_q(m_q - a_q^-)$$

is at least $M_m^+ + M_m^-$, and it follows from (20) and (21), and the strict monotonicity of the sequences $\{M_n^\pm\}$, that for large enough n and some R this greater than $\ell + 1 + m^2/R$ for all $m > n$. Then the integral is at most $\delta^{m^2/R}$.

This integral is one of at most $P^m Q^m$ integrals, and this factor also can be ignored. The factors we had before that could not be ignored combine to $(4 \cdot 2^{P^2+Q^2}/d)^{m^2}$. It follows that if we choose $\delta < (4 \cdot 2^{P^2+Q^2}/d)^{-R}$ the integral over $r < \delta$ of (15) with m replacing n is exponentially small.

This takes care of the integral (15) with m replacing n , the main contributions to $(d/d\kappa)^\ell S_m(\kappa)$. We complete the proof of the analogue of Lemma 3 as we did at the end of the proof of that lemma. This completes the proof of the theorem. \square

Appendix A. Proof of the proposition

The Fredholm expansion is

$$\det(I - K_N) = 1 + \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \sum_{p_1, \dots, p_n \geq 0} \det(K_N(p_i, p_j)).$$

Therefore it suffices to show that

$$\begin{aligned} & \sum_{N=1}^{\infty} \sum_{p_1, \dots, p_n \geq 0} \det(K_N(p_i, p_j)) \\ &= \frac{1}{n!} \int \cdots \int \frac{\prod_i x_i y_i}{1 - \prod_i x_i y_i} \left(\det \left(\frac{1}{1 - x_i y_j} \right) \right)^2 du(x_1) \cdots du(x_n) dv(y_1) \cdots dv(y_n). \end{aligned}$$

We have

$$K_N(p_i, p_j) = \int \int \frac{x^{N+p_i} y^{N+p_j}}{1 - xy} du(x) dv(y).$$

It follows by a general identity [1] (eqn. (1.3) in [10]) that

$$\begin{aligned} & \det(K_N(p_i, p_j)) \\ &= \frac{1}{n!} \int \cdots \int \det(x_i^{N+p_j}) \det(y_i^{N+p_j}) \prod_i \frac{1}{1 - x_i y_i} \prod_i du(x_i) dv(y_i) \\ &= \frac{1}{n!} \int \cdots \int \left(\prod_i x_i y_i \right)^N \det(x_i^{p_j}) \det(y_i^{p_j}) \prod_i \frac{1}{1 - x_i y_i} \prod_i du(x_i) dv(y_i). \end{aligned}$$

Summing over N gives

$$\begin{aligned} & \sum_{N=1}^{\infty} \det(K_N(p_i, p_j)) \\ &= \frac{1}{n!} \int \cdots \int \frac{\prod_i x_i y_i}{1 - \prod_i x_i y_i} \det(x_i^{p_j}) \det(y_i^{p_j}) \prod_i \frac{1}{1 - x_i y_i} \prod_i du(x_i) dv(y_i). \end{aligned}$$

(Interchanging the sum with the integral is justified since the supports of u and v are in the open unit disc.)

Now we sum over $p_1, \dots, p_n \geq 0$. Using the general identity again (but in the other direction) gives

$$\sum_{p_1, \dots, p_n \geq 0} \det(x_i^{p_j}) \det(y_i^{p_j}) = n! \det \left(\sum_{p \geq 0} x_i^p y_j^p \right) = n! \det \left(\frac{1}{1 - x_i y_j} \right).$$

We almost obtained the desired result. It remains to show that

$$\det \left(\frac{1}{1 - x_i y_j} \right) \prod_i \frac{1}{1 - x_i y_i}, \tag{23}$$

which we obtain in the integrand, may be replaced by

$$\frac{1}{n!} \left(\det \left(\frac{1}{1 - x_i y_j} \right) \right)^2. \tag{24}$$

This follows by symmetrization over the x_i . (The rest of the integrand is symmetric.) For a permutation π , replacing the x_i by $x_{\pi(i)}$ multiplies the determinant in (23) by $\text{sgn } \pi$, so to symmetrize we replace the other factor by

$$\frac{1}{n!} \sum_{\pi} \text{sgn } \pi \prod_i \frac{1}{1 - x_{\pi(i)} y_i} = \frac{1}{n!} \det \left(\frac{1}{1 - x_i y_j} \right).$$

Thus, symmetrizing (23) gives (24). □

Appendix B. The minimum problem

Changing notation, we consider

$$M_n = \min \left\{ \sum_{i=1}^k n_i (n_i - a_i) : n_i \in \mathbb{Z}^+, \sum_{i=1}^k n_i = n \right\},$$

and ask when this is uniquely attained. Set

$$s = k^{-1} \sum_{i=1}^k a_i, \quad \bar{a}_i = (a_i - s)/2, \quad \bar{n}_i = n_i - n/k,$$

and define

$$\mathbb{N}^k = \left\{ (x_i) \in \mathbb{R}^k : \sum_{i=1}^k x_i = 0 \right\}.$$

Then $\bar{a} = (\bar{a}_i) \in \mathbb{N}^k$ and $\bar{n} = (\bar{n}_i) \in \mathbb{N}^k$. If $n \equiv \nu \pmod{k}$ the other conditions on the \bar{n}_i become

$$\bar{n}_i \geq -n/k, \quad \bar{n}_i \in \mathbb{Z} - \nu/k.$$

(Think of ν as fixed and n as large and variable.) A little algebra gives

$$\sum_{i=1}^k n_i (n_i - a_i) = \sum_{i=1}^k (\bar{n}_i - \bar{a}_i)^2 + k (n/k - s/2)^2 - \sum_{i=1}^k a_i^2/4.$$

Minimizing the sum on the left is the same as minimizing the first sum on the right, with the stated conditions on the \bar{n}_i . Several things follow from this. First, since the minimum of the first sum on the right is clearly $O(1)$, the condition $\bar{n}_i \geq -n/k$ may be dropped when n is sufficiently large; second, $M_n = n^2/k - sn + O(1)$; third (from this), $M_{n+1} - M_n = 2n/k + O(1) > 0$ for sufficiently large n ; and fourth, for uniqueness we may replace our minimum problem by

$$\min \left\{ \sum_{i=1}^k (\bar{n}_i - \bar{a}_i)^2 : \bar{n} \in \mathbb{N}^k, \bar{n}_i \in \mathbb{Z} - \nu/k \right\}.$$

This minimum is uniquely attained if and only if there is a unique point closest to \bar{a} in the set of lattice points $(\mathbb{Z} - \nu/k)^k$ in \mathbb{N}^k . This condition depends only on the residue class of n modulo k .

When $k = 2$ the subspace \mathbb{N}^2 is the line $x_1 + x_2 = 0$ in \mathbb{R}^2 . When n is even the lattice consists of the points on the line with coordinates in \mathbb{Z} and \bar{a} is equidistant

from two adjacent ones when $a_1 - a_2 \in 4\mathbb{Z} + 2$; when n is odd the lattice consists of the points of the line with coordinates in $\mathbb{Z} + 1/2$ and \bar{a} is equidistant from two adjacent ones when $a_1 - a_2 \in 4\mathbb{Z}$. Non-uniqueness occurs in these cases.

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Craig A. Tracy
 Department of Mathematics
 University of California
 Davis, CA 95616, USA
 e-mail: tracy@math.ucdavis.edu

Harold Widom
 Department of Mathematics
 University of California
 Santa Cruz, CA 95064, USA
 e-mail: widom@ucsc.edu