Physica A 177 (1991) 167–173
North-Holland

The Fisher–Hartwig conjecture and generalizations ☆

Estelle L. Basor [a] and Craig A. Tracy [b,1]

[a] *Department of Mathematics, California Polytechnic State University, San Luis Obispo, CA 93407, USA*

[b] *Department of Mathematics and Institute of Theoretical Dynamics, University of California, Davis, CA 95616, USA*

We discuss the status of the Fisher–Hartwig conjecture concerning the asymptotic expansion of a class of Toeplitz determinants with singular generating functions. A counterexample is given for a nonrational generating function; and we formulate a generalized Fisher–Hartwig conjecture.

There is a long history of interaction between statistical mechanics and the theory of determinants of Toeplitz matrices. It is well documented how Onsager's work on the spontaneous magnetization of the 2D Ising model led to the strong Szegö limit theorem. What was known to Onsager [25], and later made explicit by Montroll, Potts and Ward [24], is that the spin–spin correlation function $\langle \sigma_{00}\sigma_{0n} \rangle$ can be expressed as a Toeplitz determinant. To calculate the spontaneous magnetization through the formula

$$M(T)^2 = \lim_{n\to\infty} \langle \sigma_{00}\sigma_{0n} \rangle_{T<T_c},$$

one needs the limiting asymptotic behavior of large Toeplitz determinants which is given by the strong Szegö limit theorem. For fixed $T<T_c$ or fixed $T>T_c$ corrections to the limiting behavior for the 2D Ising model we studied by Wu [37] and Kadanoff [17] (see also refs. [23,38]). These results are the prototype for corrections to the Szegö formula.

As M.E. Fisher [13] was one of the first to understand, we expect different asymptotic behavior of the spin–spin correlation function at $T=T_c$. This suggests that critical systems are prototypes for qualitatively different Szegö type theorems. Indeed, in ref. [37] we find a detailed analysis of the 2D Ising critical correlations (see also refs. [1,23,32]). What is perhaps less known to physicists is that Fisher and Hartwig [14], using their insight gained from these special cases, formulated a conjecture for the asymptotic behavior of a class of Toeplitz determinants that correspond to the "crit-

☆ Dedicated to Professor Michael E. Fisher on the occasion of his sixtieth birthday.

[1] Supported in part by the National Science Foundation, Grant No. DMS-90-01794.

ical case". It is our goal here to discuss the status of the Fisher–Hartwig conjecture and to give some indication of its impact in mathematics. Finally, we would like to indicate some future directions that might prove profitable to mathematicians given certain results coming from mathematical physics.

For a function φ defined on the unit circle with Fourier coefficients φ_k one can define the finite $n\times n$ Toeplitz matrices $T_n[\varphi]=(\varphi_{j-k})$, $j, k=0, ..., n-1$. The Fisher–Hartwig conjecture [14] concerns the asymptotic behavior of determinants of these matrices. Fisher and Hartwig considered functions of the form

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

where $b(\theta)$ is smooth, nonzero and has winding number equal to zero, $t_\beta(\theta)=\exp[-\mathrm{i}\beta(\pi-\theta)]$, $0<\theta<2\pi$, and $u_\alpha(\theta)=(2-2\cos\theta)^\alpha$, $\mathrm{Re}(\alpha)>-\frac{1}{2}$. They conjectured that the corresponding Toeplitz determinants $D_n[\varphi]=\det T_n[\varphi]$ would have the asymptotic expansion as $n\to\infty$

$$D_n[\varphi]\sim G[b]^n n^{\sum_r(\alpha_r^2-\beta_r^2)}E\,, \tag{2}$$

where $G[b]=\exp[(1/2\pi)\int_0^{2\pi}\log b(\theta)\,\mathrm{d}\theta]$ and E is some constant depending on b, θ_r, α_r and β_r.

It is interesting here to note that the function $\varphi(\theta)$ can possess singularities, jump discontinuities or zeros. Previous results, for example the already mentioned strong Szegö limit theorem, had almost exclusively been concerned with functions that were much better behaved. It is no surprise then that the statement of the conjecture caught the eye of many mathematicians. This interest spurred the discovery of new techniques required to handle the delicate questions of convergence that arise from such generating functions. Eventually, new results were obtained about classical Toeplitz operators defined on $\ell_2(\mathbb{Z}^+)$ and many of these were extended to more general convolution type operators.

Connections were made between the various terms in the asymptotic expansion and commutators of trace-class operators. Much work was done in investigating the properties of $T_n^{-1}[\varphi]$ and Toeplitz operators were investigated on more general weighted spaces. For a complete account of such work the reader is referred to ref. [7]. The Fisher–Hartwig conjecture was extended (and proved in certain cases) to certain kinds of integral operators including pseudo-differential operators with discontinuous symbol. The most general results in this area are to be found in ref. [35].

The simplest case of the conjecture was verified by Fisher and Hartwig themselves. They noticed that if $\varphi(\theta)=t_\beta(\theta)$, then the corresponding Toeplitz matrix has entries $a_{ij}=\sin(\pi\beta)/\pi(i-j+\beta)$. The matrix then is of Cauchy form and can be evaluated explicitly. Moreover, they showed that in this case $E=\exp[-\beta^2(\gamma+1)]\prod_{n=1}^{\infty}(1-\beta^2/n^2)^n\exp(\beta^2/n)$ where γ is Euler's constant.

Interestingly, the conjecture for n even, $b=1$, $R=2$, $\theta_2=\theta_1+\pi$, $\beta_1=\beta_2=0$, and α_1,

α_2 real and positive had already been confirmed by Lenard in a preliminary version of ref. [19]. Lenard's interest in this problem dated back to 1963 when he was concerned with the physical problem of the one-particle reduced density matrix of a system of impenetrable bosons [18]. In a series of letters between Szegö and Lenard, Szegö had computed the determinant in the above case for $\alpha_1=\alpha_2=\frac{1}{2}$ and had also given bounds for $\alpha_1=\alpha_2=\frac{1}{2}$ and θ_1, θ_2 arbitrary. These results were reported in ref. [18], and gave rise to the work done in ref. [19]. There, Lenard gave a conjecture for the general form of the constant for $\beta_r=0$, extended the above mentioned result for both n even and odd and expressed the answer for E in terms of the Barnes G-function [#1]. Lenard pointed out that his computation leading to the verification of the conjecture required "nine very rapidly growing factors" to cancel and that the " 'little left over' yields the asymptotic formula".

Lenard's work was then greatly extended by Widom, who was the first to prove a general case of the conjecture. In ref. [36], Widom proved that the conjecture was true in the case of $\mathrm{Re}(\alpha_r)>-\frac{1}{2}$ and $\beta_r=0$ for all r. Since $\mathrm{Re}(\alpha_r)>-\frac{1}{2}$ is a necessary requirement for φ to be an integrable function this was a complete result for functions without jump discontinuities. In the same paper Widom verified the conjecture in the case $R=1$, $|\alpha|<\frac{1}{2}$, $|\beta|<\frac{1}{2}$ but did not determine the constant.

In 1978, Basor [3], using the same techniques, extended Widom's result to the case $\mathrm{Re}(\alpha_r)>-\frac{1}{2}$ and $\mathrm{Re}(\beta_r)=0$; and in addition, the constant E was determined. Let $b(\theta)=b_+(\exp(\mathrm{i}\theta))\,b_-(\exp(-\mathrm{i}\theta))$ where b_+ (respectively b_-) extends to be analytic and nonzero inside (respectively outside) the unit circle. Normalize b so that $G[b]=b_+(0)=b_-(\infty)=1$, then

$$E=E[b]\prod_{r=1}^{R} b_-(\exp(\mathrm{i}\theta_r))^{-\alpha_r-\beta_r}b_+(\exp(-\mathrm{i}\theta_r))^{-\alpha_r+\beta_r}$$
$$\times\prod_{1\leqslant s\neq r\leqslant R}\{1-\exp[\mathrm{i}(\theta_s-\theta_r)]\}^{-(\alpha_r+\beta_r)(\alpha_s-\beta_s)}$$
$$\times\prod_{r=1}^{R}\mathrm{G}(1+\alpha_r+\beta_r)\,\mathrm{G}(1+\alpha_r-\beta_r)/\mathrm{G}(1+2\alpha_r)\,, \tag{3}$$

where G is the Barnes G-function, $E[b]=\exp(\sum_{k=1}^{\infty}kS_kS_{-k})$, and $[\log b(\theta)]_k=S_k$.

The general jump discontinuity case ($\alpha_r=0$) with $|\mathrm{Re}(\beta_r)|<\frac{1}{2}$ was done in ref. [4]. There, techniques were also developed to reduce many discontinuities to the case of one and describe the answers in terms of commutators of operators (see also refs. [5–7]). Since that time various other cases of the conjecture have been proved; and

[#1] The Barnes G-function [2] is an entire function defined by

$$G(z+1)=(2\pi)^{z/2}\exp[-z/2-\tfrac{1}{2}(\gamma+1)z^2]\prod_{k=1}^{\infty}\left(1+\frac{z}{k}\right)^k\exp(-z+z^2/2k)\,,$$

where γ is Euler's constant. It satisfies the functional equation $G(z+1)=\Gamma(z)\,G(z)$. Some special values are $G(1)=1$ and $G(\frac{1}{2})=\pi^{-1/4}\,2^{1/24}\exp[3\zeta'(-1)/2]=0.603244281209446$.

much of the credit here goes to Böttcher and Silbermann. It is now known [9] to be true when $|\mathrm{Re}(\alpha_r)| < \frac{1}{2}$ and $|\mathrm{Re}(\beta_r)| < \frac{1}{2}$. In the special case of $R=1$, Böttcher and Silbermann [10] were also able to verify the conjecture for $\mathrm{Re}(\alpha) \geqslant 0$, $\mathrm{Re}(\alpha) + \mathrm{Re}(\beta) > -1$, $\mathrm{Re}(\alpha) - \mathrm{Re}(\beta) > -1$. Recently, for $\alpha = 0$ and $|\mathrm{Re}(\beta)| < \frac{5}{2}$, Libby [20] also showed that the conjecture was true. In all these cases, the constant E is given by (3).

By now, the reader will certainly notice that while the conjecture has been proved in many cases, the results are surely not complete. The reason for this is because it is simply not always true. In fact, Fisher and Hartwig excluded the case when $\alpha_r \pm \beta_r$ was equal to an integer in their original statement. Then, the generating function is rational if $b(\theta) = 1$ and the asymptotics, more complicated than the original conjecture describes, were computed by Böttcher and Silbermann [8] (see also Day [11]). It was probably suspected by many that this is the only case when the conjecture failed. Surprisingly there is a simple example that shows otherwise. Let

$$\varphi(\theta) = \begin{cases} 1, & -\pi < \theta < 0, \\ -1, & 0 < \theta < \pi. \end{cases}$$

Then $\varphi(\theta) = \mathrm{i} t_{1/2}(\theta)\, t_{-1/2}(\theta + \pi)$ and

$$\varphi_k = \begin{cases} 0, & \text{if } k \text{ is even}, \\ -\dfrac{2\mathrm{i}}{\pi k}, & \text{if } k \text{ is odd}. \end{cases}$$

The Toeplitz matrix $T_n[\varphi]$ is antisymmetric if n is odd and hence $D_n[\varphi] = 0$. If n is even, by interchanging some rows and columns one can show that as $n \to \infty$

$$D_n[\varphi] \sim (\mathrm{i})^n n^{-1/2}\, 2^{1/2} G(\tfrac{1}{2})^2 G(\tfrac{3}{2})^2 . \tag{4}$$

An interesting feature of this function φ is that it has another representation in the standard product form which would yield the same order of asymptotics ($\varphi(\theta) = -\mathrm{i} t_{-1/2}(\theta)\, t_{1/2}(\theta + \pi)$). It was pointed out by Widom that whenever this happens, Fisher–Hartwig does not even have a clear interpretation. So the question remains, can anything be said in this case? The authors' guess is that probably the following modified conjecture is true. Suppose

$$\varphi(\theta) = b^i(\theta) \prod_{r=1}^{R} t_{\beta_r^i}(\theta - \theta_r)\, u_{\alpha_r^i}(\theta - \theta_r) \tag{5}$$

for values $\beta_1^i, \ldots, \beta_R^i$, $\alpha_1^i, \ldots, \alpha_R^i$ and a smooth nonzero function $b^i(\theta)$ with winding number zero ($i = 1, 2, \ldots$). Let

$$\Omega(i) = \sum_{r=1}^{R} (\alpha_r^i)^2 - (\beta_r^i)^2, \quad \Omega = \max_i \mathrm{Re}[\Omega(i)] \quad \text{and} \quad \mathscr{S} = \{i \mid \mathrm{Re}[\Omega(i)] = \Omega\}, \tag{6}$$

then as $n \to \infty$

$$D_n[\varphi] \sim \sum_{i\in\mathscr{S}} G[b^i]^n n^{\Omega(i)} E[b^i, \alpha_r^i, \beta_r^i, \theta_r] \,. \tag{7}$$

There is good reason to believe this to be true. In the already mentioned cases where the original conjecture is known to be true there is only one product representation that yields a maximum and so the answers agree. In the piecewise constant case we have $i=1,2$, $\Omega(1)=\Omega(2)=-\frac{1}{2}$, $E[b^i, \alpha_r^i, \beta_r^i, \theta_r]=2^{-1/2}G(\frac{3}{2})^2G(\frac{1}{2})^2$, $G[b^1]=-\mathrm{i}$, and $G[b^2]=\mathrm{i}$. When n is odd these terms cancel and when n is even they yield the correct answer. Finally, this also agrees with the rational function case in ref. [8].

We now give some examples of correlation functions that suggest there are some important generalizations of Fisher–Hartwig awaiting discovery. Lenard [18] proved that the one-particle reduced density matrix, $\rho(\xi)$, of a system of impenetrable bosons in one dimension at zero temperature is given by

$$\rho(\xi)=\lim_{n\to\infty}\frac{1}{n}D_n\left[u_{1/2}\left(\theta-\frac{\pi\xi}{n}\right)u_{1/2}\left(\theta+\frac{\pi\xi}{n}\right)\right]. \tag{8}$$

Observe that now the zeros θ_r depend upon n. Proceeding heuristically we apply (2) and (3) to predict

$$\rho(\xi)\sim\frac{1}{\sqrt{\xi}}\frac{G^4(\frac{3}{2})}{\sqrt{2\pi}}\,. \tag{9}$$

Since this is derived by scaling the "critical correlations", we expect this formula to be valid for $\xi\to\infty$. Indeed, Jimbo, Miwa, Môri and Sato [15] have proved that $\rho(\xi)$, also expressible as a Fredholm minor, is a τ-function associated to a particular Painlevé transcendent of fifth kind. Furthermore, the leading large ξ expansion is given exactly by (9) (in the notation of ref. [15] $x=\pi\xi$). Thus $\rho(\xi)$ "connects" onto a "Fisher–Hartwig" expression as $\xi\to\infty$.

The critical (diagonal) 2D Ising correlation is [23,32]

$$\langle\sigma_{00}\sigma_{nn}\rangle_{T=T_c}=D_n[t_{1/2}(\theta)]\sim n^{-1/4}G(\tfrac{1}{2})\,G(\tfrac{3}{2})\,. \tag{10}$$

If we take the scaling limit of the spin–spin correlation function [22,38], then the scaling functions are τ-functions [16,26,31] associated to a particular Painlevé transcendent of third kind. To show that the scaling functions "connect" to the critical correlation result (10), one must derive an asymptotic formula for this τ-function as the scaling variable tends to zero [33]. It proved useful to consider a more general problem to solve this connection problem [33]. Namely, the underlying Painlevé equation has a one-parameter family of bounded solutions; and it is only for a particular choice of the integration constant, $\lambda=1/\pi$ in the notation of refs. [22,33], that corresponds to the Ising model. The connection problem was solved for $0<\lambda\leqslant 1/\pi$. Similarly, the τ-function appearing in the impenetrable boson problem [15] is also evaluated at a particular value of an integration constant ($\lambda=2/\pi$). For a different value for the integration constant ($\lambda = 1/\pi$), a closely related τ-function (the Fredholm determinant rather than the Fredholm minor above) corresponds to the level spacing probability distribution function in random matrices (see ref. [15] and references therein). The general connection problem at the level of τ-functions is not solved for this problem, however there is a great deal known about the connection problem at the level of Painlevé equations.

A third example can be found in the work of McCoy, Perk and Shrock [21] on the correlation function $\langle \sigma_0^x(t)\ \sigma_n^x(0) \rangle$ for the transverse Ising chain at the critical field. This correlation function is again a τ-function associated with Painlevé V; and the $t = 0$ result is of Fisher–Hartwig form. The close connection of their work with inverse scattering is made explicit by the introduction of Toda's equations.

Finally, Sarnak [30], Voros [34], and Fay [12] in their study of determinants of Laplacians on compact Riemann surfaces, have shown the occurrence of the Barnes G-function in ways similar to the above examples. This final example is perhaps not so far away from the other examples as the reader might first think. This is because Palmer [27–29] has shown that τ-functions associated to Painlevé equations [16,26] are determinants of (singular) Cauchy–Riemann operators. Here the "determinant" is defined by a trivialization of a holomorphic line bundle, det*, over an infinite-dimensional Grassmannian.

What these examples suggest is that the Fisher–Hartwig results are a limiting case for a wide class of results in the theory of τ-functions. To demonstrate this will require even more extensive and perhaps more clever mathematical techniques than already developed and used in the proof in the original Fisher–Hartwig conjecture.

The authors wish to thank A. Lenard and H. Widom for their help in reporting the history of the Fisher–Hartwig conjecture. The authors are especially grateful to Professor Lenard for providing us with the Lenard–Szegö letters. Although not previously mentioned, Professor Lenard also sent copies of a series of letters written by Widom and himself concerning the form of the constant E. The Lenard–Szegö letters dated from April 10, 1963, to September 7, 1963; and the Lenard–Widom letters dated from November 12, 1971, to January 27, 1972. All of these letters contain delightful glances of the outstanding intuition and graciousness of their authors. The authors also wish to thank Professor J. Perk and Professor H. Widom for reading a preliminary version of this manuscript and for their helpful comments.

References

[1] H. Au-Yang and J.H.H. Perk, Phys. Lett. A 104 (1984) 131.
[2] E.W. Barnes, Quart. J. Pure Appl. Math. 31 (1900) 264.
[3] E. Basor, Trans. Am. Math. Soc. 239 (1978) 33.
[4] E. Basor, Indiana Univ. Math. J. 28 (1979) 975.

[5] E. Basor and J.W. Helton, J. Operator Theor. 3 (1980) 23.
[6] A. Böttcher, Z. Anal. Anw. 1 (1982) 23.
[7] A. Böttcher and B. Silbermann, Analysis of Toeplitz Operators (Akademie-Verlag, Berlin, 1989).
[8] A. Böttcher and B. Silbermann, Math. Nachr. 102 (1981) 79.
[9] A. Böttcher and B. Silbermann, J. Funct. Anal. 62 (1985) 178.
[10] A. Böttcher and B. Silbermann, Math. Nachr. 127 (1986) 95.
[11] K.M. Day, Trans. Am. Math. Soc. 209 (1975) 224.
[12] J. Fay, Perturbation of analytic torsion on Riemann surfaces, preprint.
[13] M.E. Fisher, J. Math. Phys. 5 (1964) 944.
[14] M.E. Fisher and R.E. Hartwig, Adv. Chem. Phys. 15 (1968) 333.
[15] M. Jimbo, T. Miwa, Y. Môri and M. Sato, Physica D 1 (1980) 80.
[16] M. Jimbo, T. Miwa and K. Ueno, Physica D 2 (1981) 306; M. Jimbo and T. Miwa, Physica D 2 (1981) 407; 4 (1981) 26.
[17] L.P. Kadanoff, Nuovo Cimento 44 (1966) 276.
[18] A. Lenard, J. Math. Phys. 5 (1964) 930.
[19] A. Lenard, Pacific J. Math. 42 (1972) 137.
[20] R. Libby, thesis, Univ. of California, Santa Cruz (1990).
[21] B.M. McCoy, J.H.H. Perk and R.E. Shrock, Nucl. Phys. B 220 (1983) 269.
[22] B.M. McCoy, C.A. Tracy and T.T. Wu, J. Math. Phys. 18 (1977) 1058.
[23] B.M. McCoy and T.T. Wu, The Two-Dimensional Ising Model (Harvard Univ. Press, Cambridge, MA, 1973).
[24] E.W. Montroll, R.B. Potts and J.C. Ward, J. Math. Phys. 4 (1963) 308.
[25] L. Onsager, in: Critical Phenomena in Alloys, Magnets, and Superconductors, R.E. Mills, E. Ascher and R.I. Jaffee, eds. (McGraw-Hill, New York, 1971) pp. 3–12.
[26] K. Okamoto, Physica D 2 (1981) 525.
[27] J. Palmer, Acta Appli. Math. 18 (1990) 199.
[28] J. Palmer, Tau functions for the Dirac operator in the Euclidean plane, preprint.
[29] J. Palmer, private communication.
[30] P. Sarnak, Commun. Math. Phys. 110 (1987) 113.
[31] M. Sato, T. Miwa and M. Jimbo, Publ. Res. Inst. Math. Sci., Kyoto Univ. 14 (1978) 223; 15 (1979) 201, 577, 871; 16 (1980) 531.
[32] J. Stephenson, J. Math. Phys. 5 (1964) 1009.
[33] C.A. Tracy, Commun. Math. Phys., to appear.
[34] A. Voros, Commun. Math. Phys. 110 (1987) 439.
[35] H. Widom, Lecture Notes in Mathematics, vol. 152 (Springer, Berlin, 1985).
[36] H. Widom, Am. J. Math. 95 (1973) 333.
[37] T.T. Wu, Phys. Rev. 149 (1966) 380.
[38] T.T. Wu, B.M. McCoy, C.A. Tracy and E. Barouch, Phys. Rev. B 13 (1976) 316.