

The Onsager Formula, the Fisher–Hartwig Conjecture, and Their Influence on Research into Toeplitz Operators

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This is not primarily a paper about applications of mathematics to statistical physics, but rather a report on how a particular problem of statistical physics has resulted in an extensive mathematical theory. The problem alluded to is the computation of the spontaneous magnetization $M_0(T)$ of the two-dimensional Ising model with nearest-neighbor interactions, whose solution for temperatures T below the Curie point T_C was given by the famous formula of Lars Onsager in 1948. The theory grown out of this formula is the edifice of Toeplitz determinants, matrices, and operators.

KEY WORDS: Ising model; correlation functions; spontaneous magnetization; Toeplitz determinants; Szegő limit theorems; Toeplitz operators.

1. THE STRONG SZEGŐ LIMIT THEOREM

In 1963, Montroll *et al.*⁽¹⁾ gave a crystal-clear derivation of the Onsager formula by first showing that the spin–spin correlation $\langle \sigma_{0,0}, \sigma_{0,N} \rangle$ between the spins at $0, 0$ and $0, N$ is a certain Toeplitz determinant $\det T_N(a)$ of dimension N and by subsequently computing the limit of these determinants as N goes to infinity. This in conjunction with the relation

$$[M_0(T)]^2 = \lim_{N \rightarrow \infty} \langle \sigma_{0,0}, \sigma_{0,N} \rangle \quad (1)$$

implied a rigorous verification of the Onsager formula for $T < T_C$ and the equality $M_0(T) = 0$ for $T > T_C$. The author knows of no published work by Onsager himself containing a proof of his formula via Toeplitz

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determinants, but John Nagle has kindly brought to the author’s attention a letter by Lars Onsager to Bruria Kaufman dated April 12, 1950, in which Onsager outlined some basic ideas for asymptotically computing Toeplitz determinants currently appearing in crystal statistics.

Let us first recall a few definitions and notations. Given a complex-valued Lebesgue-integrable function a on the complex unit circle $\mathbf{T} = \{z \in \mathbf{C} : |z| = 1\}$, $a \in L^1(\mathbf{T})$, we denote by $\{a_n\}_{n=-\infty}^{\infty}$ the sequence of its Fourier coefficients:

$$a_n = \frac{1}{2\pi} \int_0^{2\pi} a(e^{i\theta}) e^{-in\theta} d\theta \tag{2}$$

The infinite Toeplitz matrix $T(a)$ generated by a is the matrix

$$T(a) = (a_{j-k})_{j,k=0}^{\infty} = \begin{pmatrix} a_0 & a_{-1} & a_{-2} & \cdots \\ a_1 & a_0 & a_{-1} & \cdots \\ a_2 & a_1 & a_0 & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{pmatrix} \tag{3}$$

the principal $N \times N$ section of $T(a)$ is denoted by $T_N(a)$, i.e., $T_N(a) = (a_{j-k})_{j,k=0}^{N-1}$, and the determinant of $T_N(a)$ is usually designated by $D_N(a)$, i.e., $D_N(a) = \det T_N(a)$. In this context, the function a is frequently referred to as the symbol of the corresponding operator, matrices, and determinants.

What a proof of the Onsager formula required was results on the asymptotic behavior of $D_N(a)$ as N approaches infinity. A first result of this type was established by Gabor Szegő in 1915.⁽²⁾ He showed that if the symbol a is a real-valued and positive function [in which case the matrix $T(a)$ is Hermitian and positively definite], then

$$\lim_{N \rightarrow \infty} \frac{D_N(a)}{D_{N-1}(a)} = G(a) := \exp \left(\frac{1}{2\pi} \int_0^{2\pi} \log a(e^{i\theta}) d\theta \right) \tag{4}$$

The relevance of Toeplitz determinants in the derivation of the Onsager formula was communicated to Szegő by S. Kakutani, and in 1952 Szegő⁽³⁾ sharpened his “first” theorem to what is now called the “strong” Szegő limit theorem: if a is a smooth, real-valued, and positive function, then

$$\lim_{N \rightarrow \infty} \frac{D_N(a)}{G(a)^N} = E(a) := \exp \sum_{k=1}^{\infty} k(\log a)_k (\log a)_{-k} \tag{5}$$

where $(\log a)_k$ stands for the k th Fourier coefficient of $\log a$. This was almost what was needed to prove the Onsager formula, but it was

nevertheless not yet sufficient. The point is that the symbol a occurring in the expression $D_N(a)$ for the correlation is not real-valued. Many mathematicians, including M. Kac, G. Baxter, I. I. Hirschman, M. Krein, and A. Devinatz, then realized that in the complex-valued case Szegő's "positivity hypothesis" must be replaced by an "index zero condition," and they showed that Szegő's strong limit formula remains valid if a is smooth, has no zeros on \mathbb{T} , and has vanishing index (= winding number) about the origin. This extension of the original version of the strong Szegő limit theorem was just the result needed to prove the Onsager formula for $T < T_c$.

Subsequent work on Szegő's strong limit theorem has been mainly devoted to relaxing the smoothness one has to impose upon the symbol, to higher-order correction terms in the formula, or to extending the theorem to so-called block Toeplitz matrices. In the latter case, the entries a_{j-k} are themselves matrices, and block Toeplitz determinants arise, for example, in the study of the Ising model with next-nearest-neighbor interactions.

However, despite the beauty of Szegő's final formula and its extensions, the proofs one had "were indirect, and worst of all gave no natural indication why the terms in the expansions, especially the $E(a)$, occurred."⁽⁴⁾ Only in 1976 was Harold Widom⁽⁵⁾ able to present a very short, direct, and elegant proof. Nowadays, we have proofs that occupy less than one page (excluding the prerequisites!). The basic idea of such proofs is as follows. It is easy to compute the determinants of the $N \times N$ section $P_N T^{-1}(a) P_N$ of the inverse of an infinite Toeplitz matrix: a simple trick shows that

$$\det P_N T^{-1}(a) P_N = 1/G(a)^N \quad \text{for all } N \geq 1 \tag{6}$$

Now think of P_N as the infinite diagonal matrix whose first N diagonal entries are 1 and whose remaining entries are zero. Under appropriate conditions, the difference $T(a) - T^{-1}(a^{-1}) =: K$ is a trace class operator, and we have

$$\begin{aligned} \det T_N(a) &= \det P_N T(a) P_N = \det(P_N T^{-1}(a^{-1}) P_N + P_N K P_N) \\ &= \det P_N T^{-1}(a^{-1}) P_N \\ &\quad \times \det(I + (P_N T^{-1}(a^{-1}) P_N)^{-1} P_N K P_N) \end{aligned} \tag{7}$$

By what was said above,

$$\det P_N T^{-1}(a^{-1}) P_N = 1/G(a^{-1})^N = G(a)^N \tag{8}$$

Invoking results on the so-called finite section method, one can show that $(P_N T^{-1}(a^{-1}) P_N)^{-1} P_N$ converges strongly (i.e., pointwise on an

appropriately chosen space) to $(T^{-1}(a^{-1}))^{-1} = T(a^{-1})$, and since K is a trace class operator, it follows that

$$\begin{aligned} \det(I + (P_N T^{-1}(a^{-1}) P_N)^{-1} P_N K P_N) \\ \rightarrow \det(I + T(a^{-1}) K) = \det T(a^{-1}) T(a) \end{aligned} \quad (9)$$

Here the latter two determinants refer to the determinant defined for operators of the form identity plus trace class operator. Hence, we have

$$\lim_{N \rightarrow \infty} \frac{D_N(a)}{G(a)^N} = \det T(a) T(a^{-1}) \quad (10)$$

That $\det T(a) T(a^{-1})$ equals the expression given by Szegö follows from the remarkable identity

$$\det e^A e^B e^{-A} e^{-B} = \exp \operatorname{tr}(AB - BA) \quad (11)$$

which was shown by Helton, Howe, and Pincus to be valid whenever A and B are bounded operators for which $AB - BA$ is of trace class. For details see refs. 5 and 6. In any case, the reader should notice that Szegö's strong limit theorem is perhaps most easily understood from the viewpoint of operator theory.

2. THE FISHER-HARTWIG CONJECTURE

An entirely different direction of extending Szegö's limit theorem was born in 1968 with Fisher and Hartwig's paper.⁽⁷⁾ They reminded us of the fact that the correlation functions of the Ising model for temperatures $T \geq T_c$ lead to Toeplitz determinants whose symbols are smooth functions with a nonvanishing index for $T > T_c$ and a function with a jump discontinuity for $T = T_c$. They also realized that many other problems of statistical physics result in Toeplitz determinants with "singular" symbols. Here singular symbols mean symbols with zeros, poles, jumps, discontinuities of oscillating type, or nonvanishing index.

Szegö's theorem as extended by Kac, Baxter, Hirschman, and others is not applicable to such situations. Taking advantage of the concrete structure of the symbols arising in several physical applications, Montroll *et al.*⁽¹⁾ and McCoy and Wu,⁽⁸⁾ to cite only two works, were nevertheless able to describe the asymptotic behavior of Toeplitz determinants with some singular symbols. Fisher and Hartwig, however, used their insight into many special situations in order to formulate a general conjecture on the behavior of Toeplitz determinants for an astonishingly large class of

singular symbols. This conjecture was so fascinating that it has attracted many mathematicians (the author himself knows at least a dozen of them) since the late sixties.

Fisher and Hartwig considered symbols a with a finite number of singularities and wrote these symbols as a product

$$a(e^{i\theta}) = \left(\prod_{j=1}^R \omega_{\alpha_j, \beta_j, \theta_j}(e^{i\theta}) \right) b(e^{i\theta}) \tag{12}$$

where b is a “nice” function (smooth, nonzero, vanishing index) and each of the factors $\omega_{\alpha, \beta, \theta_0}$ carries a single singularity:

$$\omega_{\alpha, \beta, \theta_0}(e^{i\theta}) = \varphi_{\beta, \theta_0}(e^{i\theta}) |e^{i\theta} - e^{i\theta_0}|^{2\alpha} \tag{13}$$

Clearly, $|e^{i\theta} - e^{i\theta_0}|^{2\alpha}$ has a zero at $e^{i\theta} = e^{i\theta_0}$ if $\Re\alpha > 0$, a pole at $e^{i\theta} = e^{i\theta_0}$ if $\Re\alpha < 0$, and a discontinuity of oscillating type at $e^{i\theta} = e^{i\theta_0}$ if $\Re\alpha = 0$ but $\Im\alpha \neq 0$. The factor $\varphi_{\beta, \theta_0}$ is defined by

$$\varphi_{\beta, \theta_0}(e^{i\theta}) = e^{-i\beta(\pi - \theta + \theta_0)} \quad (0 \leq \theta - \theta_0 < 2\pi) \tag{14}$$

and a little thought shows that $\varphi_{\beta, \theta_0}$ is a function [the restriction to the unit circle of a certain branch of $(-z)^\beta$] with a jump at $e^{i\theta} = e^{i\theta_0}$ satisfying

$$\varphi_{\beta, \theta_0}(e^{i(\theta_0 - 0)}) = e^{-i\pi\beta}, \quad \varphi_{\beta, \theta_0}(e^{i(\theta_0 + 0)}) = e^{i\pi\beta} \tag{15}$$

Note that α and β are allowed to be arbitrary complex numbers; the only restriction is that $\Re\alpha > -1/2$, which ensures that $\omega_{\alpha, \beta, \theta_0}$ is in $L^1(\mathbf{T})$ and so has well-defined Fourier coefficients.

The conjecture of Fisher and Hartwig says that if a is as in the preceding paragraph, then

$$\lim_{N \rightarrow \infty} D_N(a)/(G(b)^N N^{\sum_{j=1}^R (\alpha_j^2 - \beta_j^2)}) = \tilde{E}(a) \tag{16}$$

where $\tilde{E}(a)$ is some nonzero constant. The most remarkable ingredient in this formula is the exponent $\sum (\alpha_j^2 - \beta_j^2)$, which precisely describes the asymptotics of $D_N(a)$ in terms of the orders α_j of the zeros and the numbers β_j measuring the jumps. Also notice that the above formula is equivalent to the relation

$$\log D_N(a) = N \log G(b) + q \log N + \log \tilde{E}(a) + o(1) \tag{17}$$

with $q = \sum (\alpha_j^2 - \beta_j^2)$. Thus, whereas the strong Szegő limit theorem says that $\log D_N(a)$ is asymptotically equal to $AN + B$ with certain constants A and B , Fisher and Hartwig predict an asymptotic behavior of the form

$AN + q \log N + B$ in the singular case. Let us also mention that the Ising model at $T = T_c$ leads to

$$\langle \sigma_{0,0}, \sigma_{0,N} \rangle = D_N(\omega_{0,1/2,0} b) \tag{18}$$

with $G(b) = 1$; hence, a confirmation of the conjecture for $R = 1$, $\alpha_1 = 0$, $\beta_1 = 1/2$ would give the physically expected result

$$[M_0(T)]^2 = \lim_{N \rightarrow \infty} \langle \sigma_{0,0}, \sigma_{0,N} \rangle = \lim_{N \rightarrow \infty} \tilde{E}(a) N^{-1/4} = 0 \tag{19}$$

The Fisher–Hartwig conjecture was proved to be true by Widom⁽⁹⁾ in 1973 if $\beta_j = 0$ for all j , by Basor⁽¹⁰⁾ in 1978 if $\Re \beta_j = 0$ for all j , and also by Basor⁽¹¹⁾ in 1979 if $\alpha_j = 0$ and $|\Re \beta_j| < 1/2$ for all j . In 1985, Bernd Silbermann and the author⁽¹²⁾ confirmed the conjecture in case $|\Re \alpha_j| < 1/2$ and $|\Re \beta_j| < 1/2$ for all j . The latter result is, in a sense, the best thing one can show: it is now known that the conjecture is in general no longer true if the symbol has at least two singularities of a “size” greater than $1/2$ (see, e.g., ref. 13).

Much more can be said if the symbol has only one singularity, that is, if

$$a(e^{i\theta}) = \omega_{x,\beta,\theta_0}(e^{i\theta}) b(e^{i\theta}) \tag{20}$$

In ref. 14 we showed that then the conjecture is valid whenever $\Re \alpha \geq 0$, $\Re(\alpha + \beta) > -1$, $\Re(\alpha - \beta) > -1$. This result includes in particular the case $\alpha = 0$ and $\beta = 1/2$ and thus gives (19). Richard Libby has recently informed the author that he is able to prove the conjecture in case $\alpha = 0$ and β is an arbitrary complex number (see ref. 14 for $|\Re \beta| < 1$ and ref. 15 for $|\Re \beta| < 5/2$). Moreover, everything is clear if $b(e^{i\theta}) \equiv 1$; in ref. 12 we showed that for all $N \geq 1$,

$$D_N(\omega_{x,\beta,\theta_0}) = \frac{G(1 + \alpha + \beta) G(1 + \alpha - \beta)}{G(1 + 2\alpha)} \times \frac{G(N + 2) G(N + 2 + 2\alpha)}{G(N + 2 + \alpha + \beta) G(N + 2 + \alpha - \beta)} \tag{21}$$

where $G(z)$ is the so-called Barnes function, which is an entire function satisfying $G(z + 1) = \Gamma(z) G(z)$ and is thus some kind of a double gamma function (see, e.g., ref. 6). This result implies that as $N \rightarrow \infty$,

$$D_N(\omega_{x,\beta,\theta_0}) \sim \frac{G(1 + \alpha + \beta) G(1 + \alpha - \beta)}{G(1 + 2\alpha)} N^{x^2 - \beta^2} \tag{22}$$

whenever $\Re\alpha > -1/2$ and neither $\alpha + \beta$ nor $\alpha - \beta$ is a negative integer, while $D_N(\omega_{\alpha, \beta, \theta_0}) = 0$ for all $N \geq 1$ in case $\alpha + \beta$ or $\alpha - \beta$ is a negative integer.

Overall, the Fisher–Hartwig conjecture is now proved under the assumption that either all singularities are of an “order” less than $1/2$ or that we have only one singularity (or arbitrary order). Complications arise as soon as at least two of the numbers $\alpha_j \pm \beta_j$ are integers. The rather exotic behavior of the determinants $D_N(a)$ was completely described by Silbermann and the author in ref. 16 if all the numbers $\alpha_j \pm \beta_j$ are integers. Combining all these results, one arrives at the conjecture⁽¹³⁾ that in the general case $D_N(a)$ is asymptotically a finite sum of the form

$$\sum_k A_k^N N^{q_k} B_k \quad (23)$$

where A_k are complex numbers of equal modulus and q_k are complex numbers with the same real part. The confirmation of this extended Fisher–Hartwig conjecture is part of present-day research and is, for example, of great importance in the theory of so-called τ -functions (see ref. 13 for a survey of this topic).

3. RESEARCH INTO TOEPLITZ OPERATORS

Szegő’s limit theorem and the Fisher–Hartwig conjecture have left a strong imprint on the whole theory of Toeplitz operators.

When sketching the “modern” proof of the Szegő formula in Section 1, we entered operator theory and were thus led to questions concerning the action of infinite Toeplitz matrices on certain spaces. In this context one prefers to speak of *Toeplitz operators* rather than Toeplitz matrices.

If the symbol a is continuous, has no zeros on the unit circle, and has index zero, then $T(a)$ is known to be invertible on the Hilbert space l^2 of all square-summable sequences. Moreover, in that case the finite section method is applicable to $T(a)$ on l^2 , i.e., the matrices $T_N(a)$ are invertible for all sufficiently large N and the operators $T_N^{-1}(a)P_N$ converge strongly (= pointwise) to $T^{-1}(a)$ on l^2 . These two observations along with the fact that $T(a) - T^{-1}(a^{-1})$ is of trace class whenever a is sufficiently smooth form the foundation of the proof of the Szegő formula presented in Section 1.

Things are more complicated if a is merely piecewise continuous. Then for $T(a)$ to be invertible on l^2 [and also for the finite section method to be applicable to $T(a)$ on l^2] it is necessary and sufficient that the curve $a^\#$ obtained from the range of a by filling in line segments between the

endpoints of the jumps does not contain the origin and has vanishing index. On the basis of this criterion and with the help of a certain separation technique one can prove the Fisher–Hartwig conjecture in the case where $\alpha_j = 0$ and $|\Re\beta_j| < \frac{1}{2}$ for all j .⁽¹¹⁾ However, the Ising model at $T = T_c$ confronts us with a piecewise continuous symbol a for which $a^\#$ passes through the origin...

Toeplitz operators with piecewise continuous symbols a such that $a^\#$ meets the origin or with continuous symbols having zeros admit no nice theory on l^2 , but may be favorably considered on the sequence spaces l^p with weights or on the Hardy spaces H^p with weights, where $1 < p < \infty$. The theory of Toeplitz operators on such spaces had been worked out to some extent up to the end of the seventies by many mathematicians. In the eighties, we realized the significance of this theory in connection with Toeplitz determinants, extended it by a series of additional results, and were hence able to find the right spaces in order to save the main ideas of the proof-sketch in Section 1 for operators with singular symbols.⁽¹⁴⁾ Thus, part of recent developments in the *Banach space theory* of Toeplitz operators are in fact motivated by the Ising model, and it was this Banach space theory that eventually proved the validity of the Ising model at the Curie point!

The proof of the Fisher–Hartwig conjecture for $|\Re\alpha_j| < 1/2$ and $|\Re\beta_j| < 1/2$ given in ref. 12 consists of two parts: a “computational” part, in which we established the equality (21), and a “functional analytic” part, in which we reduced the problem of describing the asymptotics of $D_N(a)$ for general a to the special case covered by (21). The key result for the second part of the proof was to show that the finite section method is applicable to an operator of the form $T^{-1}(f)T(g)T^{-1}(h)$, where f, g, h are certain piecewise continuous functions. We were so led to *algebras generated by Toeplitz operators* with discontinuous symbols, could again profit from the many results already known about such algebras, but were also forced to gain deeper insight into the structure of these algebras. The investigations on Toeplitz algebras initiated in this connection have meanwhile led to profound results far away from the original problem of computing Toeplitz determinants (see, e.g., ref. 17).

Furthermore, it has been the study of Toeplitz determinants that has continuously required new criteria for the applicability of the *finite section method* to Toeplitz operators in various situations. In 1981, Silberman⁽¹⁸⁾ discovered in ingenious technique of applying local principles (which may be considered as extensions of the Gelfand theory to noncommutative algebras) to the investigation of the finite section method. This technique is now one of the most powerful tools for proving the convergence of a variety of approximation methods (including, for example, spline

collocation) for singular integral and convolution type integral equations (see ref. 19 for an encyclopedic treatment of this large field). The author is not sure whether every numerical analyst who now uses local principles in convergence analysis is aware of the fact that such techniques have their origin in the theory of Toeplitz determinants!

Another topic of present-day research into Toeplitz operators is *index formulas*. Recall that an operator A on a Hilbert space H is said to be Fredholm if its range $\text{Im } A := \{Ah : h \in H\}$ is closed and its kernel $\text{Ker } A := \{h \in H : Ah = 0\}$ and cokernel $\text{Coker } A := H/\text{Im } A$ are of finite dimension; in that case its index is the difference of the kernel and cokernel dimensions (see, e.g., ref. 6). A Toeplitz operator $T(a)$ with continuous symbol a is Fredholm if and only if a has no zeros, and the index of $T(a)$ is then minus the index (=winding number) of a about the origin. If a is discontinuous, one tries to "smoothen" a , i.e., to approximate a by a sequence $\{a_\lambda\}_{\lambda \in (1, \infty)}$ of continuous functions such that the index of $T(a)$ equals the limit of the indices of $T(a_\lambda)$ as λ goes to infinity. It turned out that Silbermann's local techniques for studying the finite section method [i.e., for the approximation of $T(a)$ by the "truncated" operators $T_N(a)$] can also be employed for investigating the relation between the indices of $T(a)$ and $T(a_\lambda)$. In this way index formulas were recently found for Toeplitz operators with symbols from extremely large classes of discontinuous functions.⁽⁶⁾

Finally, once Szegő published his theorem on Toeplitz determinants, M. Kac⁽²⁰⁾ and N. Achiezer established a continuous analog of it, i.e., a formula for the asymptotic behavior (as $\tau \rightarrow \infty$) of the Fredholm determinants of finite Wiener–Hopf integral operators of the form

$$\varphi(x) \mapsto \varphi(x) + \int_0^\tau k(x-y) \varphi(y) dy \quad (0 < x < \tau) \quad (24)$$

The hypotheses of Kac and Achiezer included the supposition that the symbol of the Wiener–Hopf operator is sufficiently smooth, nonvanishing, and of index zero. So a natural question is to state and prove a *continuous analog of the Fisher–Hartwig conjecture*, that is, to describe the asymptotic behavior of truncated Wiener–Hopf operators with singular symbols. For more about this topic see ref. 21.

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