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Asymptotics of determinants of discrete Schrödinger operators

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Abstract. We consider the asymptotics of the determinants of large discrete Schrödinger operators, i.e. "discrete Laplacian + diagonal":

$$T_n(f) = -[\delta_{j,j+1} + \delta_{j+1,j}] + \mathrm{diag}(f(1/n), f(2/n), \dots, f(n/n))$$

We extend a result of M. Kac [3] who found a formula for

$$\lim_{n\to\infty} \frac{\det(T_n(f))}{G(f)^n}$$

in terms of the values of f, where $G(f)$ is a constant. We extend this result in two ways: First, we consider shifting the index: Let

$$T_n(f;\varepsilon) = -[\delta_{j,j+1} + \delta_{j+1,j}] + \mathrm{diag}\Big(f\Big(\frac{\varepsilon}{n}\Big), f\Big(\frac{1+\varepsilon}{n}\Big), \dots, f\Big(\frac{n-1+\varepsilon}{n}\Big)\Big).$$

We calculate $\lim \det T_n(f;\varepsilon)/G(f)^n$ and show that this limit can be adjusted to any positive number by shifting ε, even though the asymptotic eigenvalue distribution of $T_n(f;\varepsilon)$ does not depend on ε. Secondly, we derive a formula for the asymptotics of $\det T_n(f)/G(f)^n$ when f has jump discontinuities. In this case the asymptotics depend on the fractional part of cn, where c is a point of discontinuity.

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1. Introduction and main results

This paper is concerned with a remarkable and little known result of M. Kac on the asymptotics of the determinant of the discrete Schrödinger operator

$$T_n(f) = \begin{bmatrix} f\left(\frac{1}{n}\right) & -1 & 0 & \cdots & 0 \\ -1 & f\left(\frac{2}{n}\right) & -1 & \cdots & 0 \\ 0 & -1 & f\left(\frac{3}{n}\right) & \cdots & 0 \\ & & & \ddots & \\ 0 & 0 & 0 & \cdots & f\left(\frac{n}{n}\right) \end{bmatrix}. \tag{1}$$

By a result of Kac, Murdock, and Szegő [2], the following holds for the trace. As long as f is real valued and Riemann integrable, we have

$$\lim_{n\to\infty} \frac{\mathrm{Tr}[\varphi(T_n(f))]}{n} = \frac{1}{2\pi}\int_0^1\int_0^{2\pi} \varphi(f(x) - 2\cos t)\, dt\, dx \tag{2}$$

for any continuous $\varphi(s)$. This result says, roughly, that as $n \to \infty$, the eigenvalues of $T_n(f)$ distribute like the values of $f(x) - 2\cos t$ sampled at regularly spaced points in the rectangle $0 \le x \le 1,\ 0 \le t \le 2\pi$.

The formula (2) gives us some information about the determinant. Let

$$D_n(f) = \det T_n(f)$$

Then, with $\varphi = \log$, as long as $f > 2$, (2) can be written

$$\lim_{n\to\infty} D_n(f)^{1/n} = G(f)$$

where

$$G(f) = \exp\left\{\int_0^1 \log\left(\frac{f(x) + \sqrt{f^2(x) - 4}}{2}\right) dx\right\}$$

is the geometric mean of $f(x) - 2\cos t$.

In the early 1960's, Mejlbo and Schmidt [4] considered determinants of a broader class of matrices, of which (1) is a special case. Their result implies that, as long as $f > 2$ and $f \in C^{2+\alpha}([0,1])$ for some $\alpha > 0$, then we have the more precise statement

$$\lim_{n\to\infty} \frac{D_n(f)}{G(f)^n} = E(f)$$

where $E(f)$ is a constant defined in the following way. Let

$$V_k(f;x) = \frac{1}{2\pi}\int_0^{2\pi} \log(f(x) - 2\cos t) e^{-ikt}\, dt$$

be the kth Fourier coefficient of $\log(f(x) - 2\cos t)$. Then

$$E(f) = \exp \frac{1}{2}\Big\{V_0(f;0) + V_0(f;1) + \sum_{k=1}^{\infty} kV_k(f;0)V_{-k}(f;0) + \sum_{k=1}^{\infty} kV_k(f;1)V_{-k}(f;1)\Big\}.$$

Remarkably, $E(f)$ depends on the value of f only at $x = 0$ and $x = 1$.

In 1969 Kac [3] derived a beautiful and simple formula for $E(f)$ for this case.

Theorem 1 (Kac, 1969). *Let f be twice differentiable on* $[0, 1]$*, with a bounded second derivative, and satsify $f > 2$. Then,*

$$\lim_{n\to\infty} \frac{D_n(f)}{G(f)^n} = \frac{1}{2} \frac{f(1) + \sqrt{f^2(1) - 4}}{\sqrt[4]{(f^2(0) - 4)(f^2(1) - 4)}}. \tag{3}$$

In §2 we will repeat Kac's proof of this theorem, with a few details that Kac omitted. We will then show how his proof can be modified for the two theorems below.

Remark 1. Kac's paper [3] contains a typo in the formula for $\lim_{n\to\infty} \frac{D_n(f)}{G(f)^n}$. His formula (eqn (3.15) in [3]) is missing the factor $1/2$.

Remark 2. Kac's result can be viewed as a Szegö Strong Limit Theorem (SSLT) for the matrices in (1). In the past few decades, the SSLT has been extensively used to study the spectral theory of discrete Schrödinger operators. See, for example, the recent book of Simon [5] and the references therein.

Remark 3. Theorem 1 holds under the slightly weaker condition that $f \in C^{1+\alpha}([0, 1])$ for some $\alpha > 0$. Kac's proof can easily be modified in this case, but it involves some tedious technicalities, which we omit. However, see Remark 8 after the proof of Theorem 1 for the outline of how to modify the proof for this case.

Our first extension of Theorem 1 has to do with shifting the indexing. Kac [3] noted that if one shifts the indexing by 1, one obtains a different formula for $\lim D_n(f)/G(f)^n$. We extend this to any shift.

Theorem 2. *Let f be twice differentiable on some open interval I containing* $[0, 1]$. *Suppose f has a bounded second derivative and satisfies $f > 2$. Let $\varepsilon \in \mathbb{R}$ and define the matrices*

$$T_n(f;\varepsilon) = \begin{bmatrix} f\left(\frac{\varepsilon}{n}\right) & -1 & 0 & \cdots & 0 \\ -1 & f\left(\frac{1+\varepsilon}{n}\right) & -1 & \cdots & 0 \\ 0 & -1 & f\left(\frac{2+\varepsilon}{n}\right) & \cdots & 0 \\ & & & \ddots & \\ 0 & 0 & 0 & \cdots & f\left(\frac{n-1+\varepsilon}{n}\right) \end{bmatrix}.$$

Then

$$\lim_{n\to\infty} \frac{\det T_n(f;\varepsilon)}{G(f)^n} = \frac{\left(f(0) + \sqrt{f^2(0)-4}\right)^{1-\varepsilon}\left(f(1) + \sqrt{f^2(1)-4}\right)^{\varepsilon}}{2\sqrt[4]{(f^2(0)-4)(f^2(1)-4)}}. \tag{4}$$

Remark 4. When $\varepsilon = 1$, (4) reduces to (3). As long as $f(0) \neq f(1)$, the above limit can be adjusted to any positive number just by choosing the correct shift ε. Notice that the limiting statistical distribution of the eigenvalues of $T_n(f;\varepsilon)$ does not depend on ε. The result (2) holds for $T_n(f;\varepsilon)$ for any ε:

$$\lim_{n\to\infty} \frac{\mathrm{Tr}[\varphi(T_n(f;\varepsilon))]}{n} = \frac{1}{2\pi}\int_0^1\int_0^{2\pi} \varphi(f(x) - 2\cos t)\,dt\,dx.$$

Thus, if one scales $T_n(f;\varepsilon)$ by $G(f)$, one has a family of matrices whose asymptotic eigenvalue distribution is invariant, but the determinant can be made to converge to any positive number.

Remark 5. The formulas (3) and (4) remain unchanged if we take the super-and sub-diagonals to be $+1$, instead of -1.

Given how sensitive the limits (3) and (4) are to the slightest change, it might seem that we have no hope of deriving a limit for the determinant when the symbol is discontinuous. However, there is one important case when we can do it. When the function f has a finite number of jump discontinuities, we can obtain a formula for $D_n(f)/G(f)^n$ that depends on n (modulo $o(1)$ terms). This demonstrates the impossibility of the limit of $D_n(f)/G(f)^n$ existing when f is discontinuous.

Theorem 3. (i) *Let f be twice differentiable on* $[0, 1]$, *with a bounded second derivative, except for $r < \infty$ jump discontinuities at $c_1, \ldots, c_r \in (0, 1)$, where both sided limits exist and are finite, and f is left-continuous at c_j: $f(c_j) = f(c_j-)$. Suppose, also, that $f > 2 + \epsilon$ for some $\epsilon > 0$. Then*

$$\frac{D_n(f)}{G(f)^n} = \alpha \prod_{j=1}^{r} \beta_j \gamma_j^{\{nc_j\}} + o(1) \tag{5}$$

where $\{x\} = x - \lfloor x \rfloor$ *is the fractional part of* x*,*

$$\alpha = \frac{1}{2} \frac{f(1) + \sqrt{f^2(1) - 4}}{\sqrt[4]{(f^2(0) - 4)(f^2(1) - 4)}}$$

as in (3)*,*

$$\beta_j = \frac{f(c_j-) - f(c_j+) + \sqrt{f^2(c_j+) - 4} + \sqrt{f^2(c_j-) - 4}}{2\sqrt[4]{(f^2(c_j+) - 4)(f^2(c_j-) - 4)}},$$

and

$$\gamma_j = \frac{f(c_j+) + \sqrt{f^2(c_j+) - 4}}{f(c_j-) + \sqrt{f^2(c_j-) - 4}}.$$

(ii) *If* f *is right-continuous at* c_j*, then the formula* (5) *holds with* $\{c_j n\}$ *replaced by* $\{c_j n\}'$*, where*

$$\{x\}' = 1 + x - \lceil x \rceil$$

is the fractional part of x*, but equal to* 1 *if* x *is an integer.*

Remark 6. Note that β_j and γ_j are 1 if f is continuous at c_j, so (5) reduces to (3) when f is smooth. Since $\{c_j n\} = \{c_j n\}'$ if c_j is irrational, the difference between cases (i) and (ii) of the above theorem only occurs when c_j is rational. In that case the difference arises when f is evaluated at the point c_j.

Remark 7. Obviously, if there is a discontinuity in f, the limit

$$\lim_{n\to\infty} \frac{D_n(f)}{G(f)^n}$$

does not exist. However, we can calculate the lim sup and lim inf. For example, if there is one jump discontinuity at $c = p/q$,

$$\limsup_{n\to\infty} \frac{D_n(f)}{G(f)^n} = \alpha \cdot \beta \cdot \max\{\gamma^{1/q}, \gamma\},$$

$$\liminf_{n\to\infty} \frac{D_n(f)}{G(f)^n} = \alpha \cdot \beta \cdot \min\{\gamma^{1/q}, \gamma\}.$$

If c is irrational, the same is true with $\gamma^{1/q}$ replaced by 1. Analogous statements hold when there are r jump discontinuities.

To illustrate the asymptotic behavior of $D_n(f)/G(f)^n$, we consider the case of a single jump discontinuity at $c \in (0, 1)$. If $c = p/q$ is rational, $\{D_n(f)/G(f)^n\}$ (modulo an $o(1)$ term) is cyclic of order q. When c is irrational, $\{D_n(f)/G(f)^n\}$

is dense on the interval between $\alpha\beta$ and $\alpha\beta\gamma$. This is another indication of how exquisitely sensitive $D_n(f)/G(f)^n$ is. The slightest irrational perturbation of the point of discontinuity from $c = 1/2$, causes the values of $D_n(f)/G(f)^n$ (modulo the $o(1)$ term) to go from alternating between two values to taking on infinitely many values. This behavior is illustrated in figure 1. There we calculate $D_n(f)/G(f)^n$ for the piecewise function

$$f(x) = \begin{cases} 3.3 + x^2/2 + \sin(3x), & x < c, \\ 3.5 - x, & x \geq c. \end{cases} \tag{6}$$

We compare the values of $D_n(f)/G(f)^n$ with $\alpha\beta\gamma^{\{cn\}'}$. Agreement is quite good for moderately large n.

As another example, to illustrate the behavior of the $o(1)$ error in (5), we take the function

$$f(x) = \begin{cases} 3.3 + x^2/2 + \sqrt{x}\sin(13x) & x \leq 0.9 - 1/\pi \\ 3.5 - \cos(20x) & x > 0.9 - 1/\pi \end{cases} \tag{7}$$

In figure 2 we plot the values of $D_n(f)/G(f)^n$ and $\alpha\beta\gamma^{\{cn\}}$ for n to 200 (left panel) and the difference between these values for n to 3000 (right panel). Among power laws and exponential functions of the form AB^n and An^b, we found the best least square fit to the data $\left\{\left(n, D_n(f)/G(f)^n - \alpha\beta\gamma^{\{cn\}}\right)\right\}$ in figure 2 to be $2.82506\, n^{-0.965199}$. In other words, the error approaches zero like $1/n$.

2. Proofs of main results

Proof of Theorem 1. Kac's proof begins with the formula for the determinant of a positive definite matrix A. Let $\lambda_1, \ldots, \lambda_n$ be the eigenvalues of A. From

$$\int_{-\infty}^{\infty} e^{-\lambda_k t^2}\, dt = \frac{\sqrt{\pi}}{\sqrt{\lambda_k}},$$

and the spectral theorem, we see

$$\begin{aligned} \frac{1}{\sqrt{\det A}} &= \frac{1}{(\sqrt{\pi})^n} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} e^{-(\lambda_1 y_1^2 + \cdots + \lambda_n y_n^2)}\, dy_1 dy_2 \cdots dy_n \\ &= \frac{1}{(\sqrt{\pi})^n} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \exp\left[-x^T A x\right]\, dx_1 dx_2 \cdots dx_n. \end{aligned} \tag{8}$$

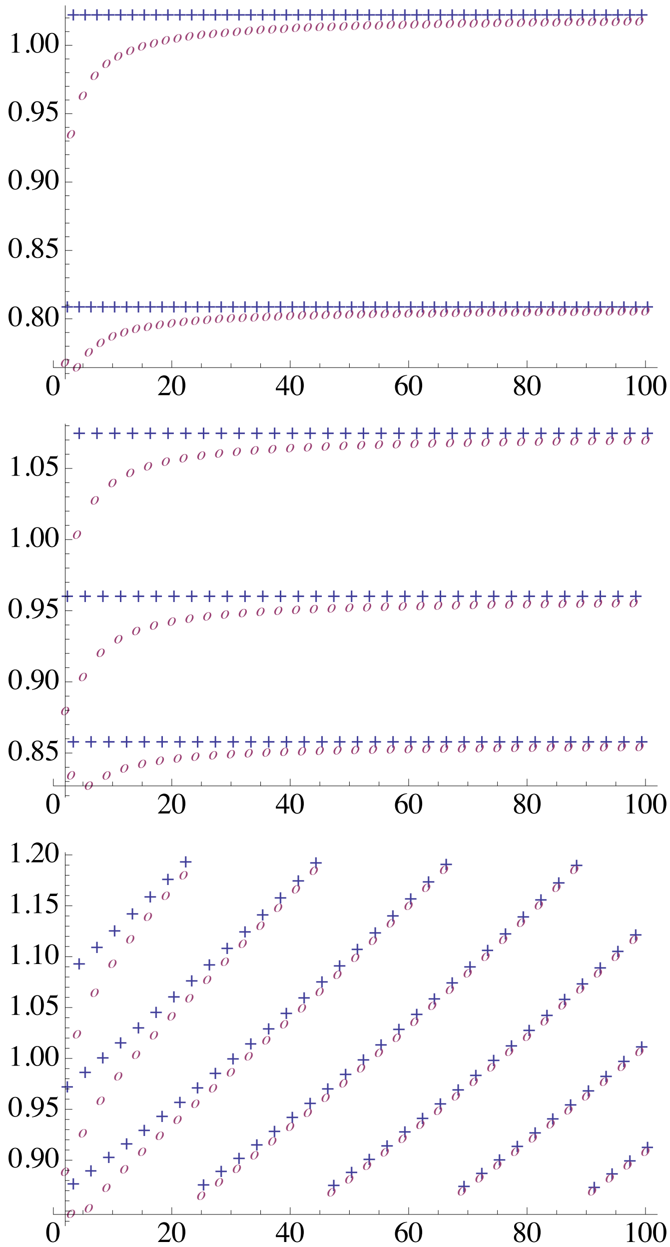

Figure 1. n vs. $D_n(f)/G(f)^n$ for f as in (6). Top: $c = 1/2$; middle: $c = 1/3$; bottom: $c = 1/\pi$. The values of $D_n(f)/G(f)^n$ are marked with circles; the values of $\alpha\beta\gamma^{\{cn\}'}$ are marked with $+$'s. Note that the values of c in the middle and right panels differ by less than 0.0151.

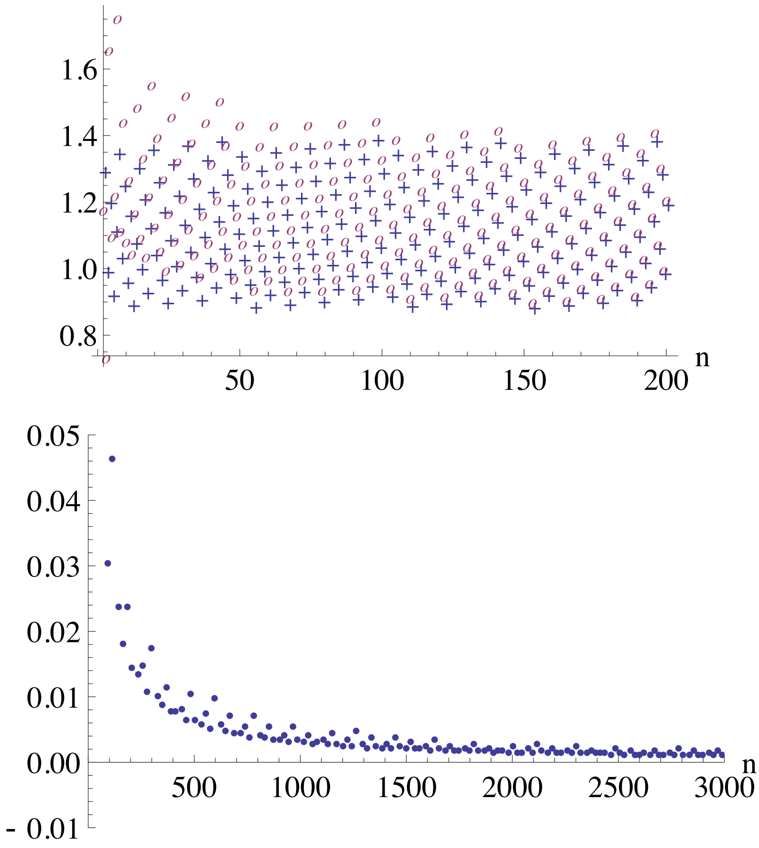

Figure 2. Top: $D_n(f)/G(f)^n$ (circles) and $\alpha\beta\gamma^{\{cn\}}$ (+'s) for f as in (7). Bottom: $D_n(f)/G(f)^n - \alpha\beta\gamma^{\{cn\}}$ in steps of 23.

Moreover, the asymptotic expansion of the complementary error function implies that

$$\int_{n^{1/4}}^{\infty} e^{-\lambda_k t^2}\, dt = \mathcal{O}\Big(\frac{e^{-n^{1/2}}}{n^{1/4}}\Big),$$

and hence

$$\frac{1}{\sqrt{\det A}} = \int_{-n^{1/4}}^{n^{1/4}} \cdots \int_{-n^{1/4}}^{n^{1/4}} \exp[-x^T A x]\, dx_1 dx_2 \cdots dx_n + o(1). \tag{9}$$

This estimate will play a role below when we approximate the above integral. If we apply (8) to $D_n(f)$, we obtain

$$\frac{1}{\sqrt{D_n(f)}} = \frac{1}{(\sqrt{\pi})^n}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\exp\Big[-\sum_{k=1}^{n} f\Big(\frac{k}{n}\Big)x_k^2 + 2\sum_{k=1}^{n-1} x_k x_{k+1}\Big]dx_1\cdots dx_n. \tag{10}$$

To obtain a limit we need to write the integrand as a product of symmetric kernels. To this end, we note

$$\begin{aligned} f\Big(\frac{k}{n}\Big) &= \frac{1}{2}f\Big(\frac{k-1}{n}\Big) + \frac{1}{4n}f'\Big(\frac{k-1}{n}\Big) \\ &\quad + \frac{1}{2}f\Big(\frac{k}{n}\Big) + \frac{1}{4n}f'\Big(\frac{k}{n}\Big) + \mathcal{O}\Big(\frac{1}{n^2}\Big). \end{aligned} \tag{11}$$

Let

$$a_k = f\Big(\frac{k}{n}\Big) + \frac{1}{2n}f'\Big(\frac{k}{n}\Big).$$

Note that $a_k > 2$ for n large enough. Then, by (11), we have

$$\sum_{k=1}^{n} f\Big(\frac{k}{n}\Big)x_k^2 = \frac{1}{2}(a_0x_0^2 + a_nx_n^2) + \frac{1}{2}\sum_{k=1}^{n-1} a_k(x_k^2 + x_{k+1}^2) + \mathcal{O}\Big(\sum_{k=1}^{n}\frac{x_k^2}{n^2}\Big). \tag{12}$$

Thus, if we define the symmetric kernels

$$K\Big(x, y; \frac{k}{n}\Big) = \frac{1}{\sqrt{\pi}}\exp\Big[-\frac{a_k}{2}x^2 + 2xy - \frac{a_k}{2}y^2\Big]$$

then we have

$$\frac{\sqrt{\pi}}{\sqrt{D_n(f)}} = \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} e^{-\frac{a_0}{2}x_1^2}\prod_{k=1}^{n-1} K\Big(x_k, x_{k+1}; \frac{k}{n}\Big)e^{-\frac{a_n}{2}x_n^2}\, e^{\mathcal{O}\left(\frac{\sum_{k=1}^{n} x_k^2}{n^2}\right)}dx_1\cdots dx_n.$$

The $\mathcal{O}$ term plays essentially no role for large n and can therefore be removed. Indeed, it follows from (9)

$$
\begin{aligned}
&\frac{\sqrt{\pi}}{\sqrt{D_n(f)}} \\
&= \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} e^{-\frac{a_0}{2}x_1^2} \prod_{k=1}^{n-1} K\Big(x_k, x_{k+1}; \frac{k}{n}\Big) e^{-\frac{a_n}{2}x_n^2}\, e^{\mathcal{O}\left(\frac{\sum_{k=1}^n x_k^2}{n^2}\right)} dx_1 \cdots dx_n \\
&= \int_{-n^{1/4}}^{n^{1/4}} \cdots \int_{-n^{1/4}}^{n^{1/4}} e^{-\frac{a_0}{2}x_1^2} \prod_{k=1}^{n-1} K\Big(x_k, x_{k+1}; \frac{k}{n}\Big) e^{-\frac{a_n}{2}x_n^2}\, e^{\mathcal{O}\left(\frac{\sum_{k=1}^n x_k^2}{n^2}\right)} dx_1 \cdots dx_n \\
&\quad + o(1) \\
&= \int_{-n^{1/4}}^{n^{1/4}} \cdots \int_{-n^{1/4}}^{n^{1/4}} e^{-\frac{a_0}{2}x_1^2} \prod_{k=1}^{n-1} K\Big(x_k, x_{k+1}; \frac{k}{n}\Big) e^{-\frac{a_n}{2}x_n^2}\, e^{\mathcal{O}\left(n^{-1/2}\right)} dx_1 \cdots dx_n \\
&\quad + o(1) \\
&= \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} e^{-\frac{a_0}{2}x_1^2} \prod_{k=1}^{n-1} K\Big(x_k, x_{k+1}; \frac{k}{n}\Big) e^{-\frac{a_n}{2}x_n^2}\, dx_1 \cdots dx_n + o(1).
\end{aligned}
\tag{13}
$$

Using the self-reciprocity of the Hermite polynomials, one can easily compute the eigenvalues and eigenfunctions of $\frac{1}{\sqrt{\pi}} K(x, y; k/n)$. The eigenvalues are

$$\lambda_j(k/n) = \Big(\frac{a_k + b_k}{2}\Big)^{-j-1/2} \quad (j = 0, 1, 2, \dots)$$

with $b_k = \sqrt{a_k^2 - 4}$, and the corresponding normalized eigenfunctions

$$\phi_j(x; k/n) = \sqrt[4]{\frac{b_k}{\pi}} \frac{1}{2^{j/2}\sqrt{j!}} e^{-\frac{b_k}{2}x^2} H_j(\sqrt{b_k}\, x) \quad (j = 0, 1, 2, \dots)$$

where H_j is the jth Hermite polynomial [1, Cf. Rem. 6.1.1]. Since $b_{k+1} - b_k = \mathcal{O}(n^{-2})$, the normalized eigenfunctions "almost commute" in the following sense:

$$\int_{-\infty}^{\infty} \phi_i\Big(x; \frac{k}{n}\Big)\phi_j\Big(x; \frac{k+1}{n}\Big) dx = \delta_{ij} + \mathcal{O}\Big(\frac{1}{n^2}\Big). \tag{14}$$

For any given k and n, the collection $\{\phi_0(x; k/n), \phi_1(x; k/n), \dots\}$ form a Hilbert basis of $L^2(\mathbb{R})$. Hence, every function $g \in L^2(\mathbb{R})$ can be written as

$$g(x) = \sum_{j=0}^{\infty} \Big(\int_{-\infty}^{\infty} g(y)\phi_j(y; k/n)\, dy\Big)\, \phi_j(x; k/n) \quad (k = 1, \dots, n-1)$$

in the L^2-sense. If we assume furthermore that g is a Schwartz function, then the above series converges pointwise for all x. Therefore, we can apply the dominated convergence theorem to obtain

$$\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty} K\Big(x_{n-1}, x_n; \frac{n-1}{n}\Big) e^{-\frac{a_n}{2}x_n^2}\,dx_n = \sum_{j=0}^{\infty}\lambda_j\Big(\frac{n-1}{n}\Big)\Big[\int_{-\infty}^{\infty}\phi_j\Big(x_n;\frac{n-1}{n}\Big)e^{-\frac{a_n}{2}\,x_n^2}\,dx_n\Big]\,\phi_j\Big(x_{n-1};\frac{n-1}{n}\Big).$$

Iterating this with

$$\frac{1}{\sqrt{\pi}}K\Big(x_{n-2},x_{n-1};\frac{n-2}{n}\Big),\quad \dots,\quad \frac{1}{\sqrt{\pi}}K\Big(x_1,x_2;\frac{1}{n}\Big),$$

and using the almost commuting relations in (14), it follows

$$\frac{\sqrt{\pi}}{\sqrt{D_n(f)}} = \sum_{j=0}^{\infty}\Big[\prod_{k=1}^{n-1}\lambda_j\Big(\frac{k}{n}\Big)\cdot\int_{-\infty}^{\infty}\phi_j\Big(x;\frac{1}{n}\Big)e^{-\frac{a_0}{2}x^2}dx\int_{-\infty}^{\infty}\phi_j\Big(x;\frac{n-1}{n}\Big)e^{-\frac{a_n}{2}x^2}dx\Big] + \mathcal{O}\Big(\frac{1}{n}\Big).$$

From the non-degeneracy of the eigenvalues, the above series is dominated by the leading term ($j=0$) as n gets arbitrary large. Using the facts that $a_n \to f(1)$ and $a_0 \to f(0)$, we conclude

$$\frac{\sqrt{\pi}}{\sqrt{D_n(f)}} = \prod_{k=1}^{n-1}\lambda_0\Big(\frac{k}{n}\Big)\cdot\int_{-\infty}^{\infty}\phi_0(x;0)e^{-\frac{f(0)}{2}x^2}dx\int_{-\infty}^{\infty}\phi_0(x;1)e^{-\frac{f(1)}{2}x^2}dx + o(1). \tag{15}$$

From the expressions for λ_0 and ϕ_0 and after evaluating the integrals in (15), we finally arrive at

$$\lim_{n\to\infty}\frac{D_n(f)}{\prod_{k=1}^{n-1}\Big(\frac{a_k}{2}+\sqrt{\Big(\frac{a_k}{2}\Big)^2-1}\Big)} = \frac{1}{4}\cdot\frac{f(0)+\sqrt{f(0)^2-4}}{\sqrt[4]{f(0)^2-4}}\cdot\frac{f(1)+\sqrt{f(1)^2-4}}{\sqrt[4]{f(1)^2-4}}. \tag{16}$$

Now we need to evaluate the product in the denominator. We write it as the exponential of the sum of logarithms. Expanding

$$\log\left(\frac{a_k}{2}+\sqrt{\left(\frac{a_k}{2}\right)^2-1}\right)$$
$$=\log\left(\frac{f\left(\frac{k}{n}\right)+\sqrt{f^2\left(\frac{k}{n}\right)-4}}{2}\right)+\frac{1}{2n}\frac{f'\left(\frac{k}{n}\right)}{\sqrt{f^2\left(\frac{k}{n}\right)-4}}+\mathcal{O}\left(\frac{1}{n^2}\right).$$

Now, we have the Riemann sum:

$$\sum_{k=1}^{n-1}\frac{1}{2n}\frac{f'\left(\frac{k}{n}\right)}{\sqrt{f^2\left(\frac{k}{n}\right)-4}}=\frac{1}{2}\int_0^1\frac{f'(s)}{\sqrt{f^2(s)-4}}ds+\mathcal{O}\left(\frac{1}{n}\right)$$
$$=\frac{1}{2}\log\left(\frac{f(s)+\sqrt{f^2(s)-4}}{2}\right)\Big|_{s=0}^{s=1}+\mathcal{O}\left(\frac{1}{n}\right). \tag{17}$$

Next we use the Euler–Maclaurin formula

$$\sum_{k=1}^{n-1}g\left(\frac{k}{n}\right)=n\int_0^1 g(s)\,ds-\frac{g(0)+g(1)}{2}+\mathcal{O}\left(\frac{1}{n}\right) \tag{18}$$

with

$$g(x)=\log\left(\frac{f(x)+\sqrt{f^2(x)-4}}{2}\right)$$

to get

$$\sum_{k=1}^{n-1}\log\left(\frac{f\left(\frac{k}{n}\right)+\sqrt{f^2\left(\frac{k}{n}\right)-4}}{2}\right)$$
$$=n\int_0^1\log\left(\frac{f(s)+\sqrt{f^2(s)-4}}{2}\right)ds-\frac{g(0)+g(1)}{2}+\mathcal{O}\left(\frac{1}{n}\right). \tag{19}$$

Combining (17) and (19) gives us

$$\sum_{k=1}^{n-1}\log\left(\frac{a_k}{2}+\sqrt{\left(\frac{a_k}{2}\right)^2-1}\right)$$
$$=n\int_0^1\log\left(\frac{f(s)+\sqrt{f^2(s)-4}}{2}\right)ds-\log\left(\frac{f(0)+\sqrt{f^2(0)-4}}{2}\right)$$
$$+\mathcal{O}\left(\frac{1}{n}\right).$$

Thus, the product in the denominator of (16) is

$$\prod_{k=1}^{n-1}\left(\frac{a_k}{2}+\sqrt{\left(\frac{a_k}{2}\right)^2-1}\right)=G(f)^n\left\{\left(\frac{f(0)+\sqrt{f^2(0)-4}}{2}\right)^{-1}+o(1)\right\}.$$

Combining this with (16) gives us (3). □

Remark 8. In the above proof, it is sufficient for $f \in C^{1+\alpha}([0,1])$ for some $\alpha > 0$. For the approximation of the integral (10) in terms of symmetric kernels, it is enough for the error in (11) to be $\mathcal{O}\left(n^{-1-\alpha}\right)$ for some $\alpha > 0$. $f \in C^{1+\alpha}$ guarantees this condition. For the remainder of the proof, one has to keep track of the error and introduce a modest generalization of the Euler–Maclaurin formula.

For the proof of Theorem 2, we need the following lemma.

Lemma 1. *Let g be twice differentiable with a bounded second derivative on an open interval I containing* $[0,1]$. *Fix $\varepsilon \in \mathbb{R}$. Then*

$$\sum_{k=1}^{n-1} g\left(\frac{k-1+\varepsilon}{n}\right) = n\int_0^1 g(x)dx + \left(\varepsilon-\frac{3}{2}\right)g(1)+\left(\frac{1}{2}-\varepsilon\right)g(0)+\mathcal{O}\left(\frac{1}{n}\right). \tag{20}$$

Proof. Let n be large enough so that $\left[\frac{\varepsilon-1}{n},\frac{n-2+\varepsilon}{n}\right]\subset I$. Then, by the Euler–Maclaurin formula

$$\begin{aligned}
&\sum_{k=1}^{n-1} g\left(\frac{k-1+\varepsilon}{n}\right)\\
&= n\int_{\frac{\varepsilon-1}{n}}^{\frac{n-2+\varepsilon}{n}} g(x)dx+\frac{1}{2}(g(1)-g(0))+\mathcal{O}\left(\frac{1}{n}\right)\\
&= n\int_0^1 g(x)dx + n\int_1^{\frac{n-2+\varepsilon}{n}} g(x)dx + n\int_{\frac{\varepsilon-1}{n}}^0 g(x)dx+\frac{1}{2}(g(1)-g(0))+\mathcal{O}\left(\frac{1}{n}\right)\\
&= n\int_0^1 g(x)dx+(\varepsilon-2)g(1)+(1-\varepsilon)g(0)+\frac{1}{2}(g(1)-g(0))+\mathcal{O}\left(\frac{1}{n}\right)
\end{aligned}$$

from which the result follows. □

Proof of Theorem 2. The proof of Theorem 1 carries through almost without change as long as we let n be large enough so that $\left[\frac{\varepsilon-1}{n}, \frac{n-2+\varepsilon}{n}\right] \subset I$, replace $f(k/n)$ with $f((k-1+\varepsilon)/n)$, and let

$$a_k = f\Big(\frac{k-1+\varepsilon}{n}\Big) + \frac{1}{2n} f'\Big(\frac{k-1+\varepsilon}{n}\Big).$$

The only difference is equation (19). There we will get

$$\sum_{k=1}^{n-1} g\Big(\frac{k-1+\varepsilon}{n}\Big)$$

for

$$g(x) = \log\Big(\frac{f(x)+\sqrt{f^2(x)-4}}{2}\Big).$$

Then we apply Lemma 1 in this sum, so that

$$\sum_{k=1}^{n-1} \log\Big(\frac{a_k}{2} + \sqrt{\Big(\frac{a_k}{2}\Big)^2 - 1}\,\Big) = n\int_0^1 \log\Big(\frac{f(s)+\sqrt{f^2(s)-4}}{2}\Big) ds + (\varepsilon-1)g(1) - \varepsilon g(0) + \mathcal{O}\Big(\frac{1}{2}\Big).$$

Thus, the product in the denominator of (16) becomes

$$\prod_{k=1}^{n-1} \Big(\frac{a_k}{2} + \sqrt{\Big(\frac{a_k}{2}\Big)^2 - 1}\Big) = G(f)^n \Big\{\Big(\frac{f(0)+\sqrt{f^2(0)-4}}{2}\Big)^{-\varepsilon} \Big(\frac{f(1)+\sqrt{f^2(1)-4}}{2}\Big)^{\varepsilon-1} + o(1)\Big\}$$

Combining this with (16) gives us (4). □

To prove Theorem 3, we need the following generalization of the Euler–Maclaurin formula.

Lemma 2. (i) *Suppose g is twice differentiable with a bounded second derivative except for $r < \infty$ jump discontinuities at $0 < c_1 < c_2 < \cdots < c_r < 1$. Assume that both sided limits exist and are finite, and that g is left-continuous at these points. Then*

$$\sum_{k=1}^{n-1} g\Big(\frac{k}{n}\Big) = n\int_0^1 g(x)\,dx - \frac{g(0)+g(1)}{2} + \sum_{j=1}^{r} \Big(\{nc_j\} - \frac{1}{2}\Big)[g(c_j+) - g(c_j-)] + \mathcal{O}\Big(\frac{1}{n}\Big). \tag{21}$$

(ii) *If g is right-continuous at c_j, then the formula* (21) *holds with $\{nc_j\}$ replaced by $\{nc_j\}'$.*

Proof. (i) Suppose g has a single jump discontinuity at $c \in (0,1)$ and is left-continuous at c. Apply the Euler–Maclaurin formula (18) for twice differentiable functions to each of the following sums:

$$\begin{aligned}\sum_{k=1}^{n-1} g\Big(\frac{k}{n}\Big) &= \sum_{k=1}^{\lfloor nc\rfloor} g\Big(\frac{k}{n}\Big) + \sum_{k=\lfloor nc\rfloor+1}^{n-1} g\Big(\frac{k}{n}\Big)\\ &= n\int_0^{\lfloor nc\rfloor/n} g(x)\,dx + \frac{1}{2}\Big[g\Big(\frac{\lfloor nc\rfloor}{n}\Big) - g(0)\Big]\\ &\quad + n\int_{(\lfloor nc\rfloor+1)/n}^{1} g(x)\,dx + \frac{1}{2}\Big[-f(1) + g\Big(\frac{\lfloor nc\rfloor+1}{n}\Big)\Big] + \mathcal{O}\Big(\frac{1}{n}\Big)\\ &= n\int_0^1 g(x)\,dx + \frac{1}{2}\Big[-g(1) - g(0) + g\Big(\frac{\lfloor nc\rfloor}{n}\Big) + g\Big(\frac{\lfloor nc\rfloor+1}{n}\Big)\Big]\\ &\quad - n\int_{\lfloor nc\rfloor/n}^{(\lfloor nc\rfloor+1)/n} g(x)\,dx + \mathcal{O}\Big(\frac{1}{n}\Big).\end{aligned} \tag{22}$$

Now,

$$\begin{aligned}\int_{\lfloor nc\rfloor/n}^{(\lfloor nc\rfloor+1)/n} g(x)\,dx &= \Big(c - \frac{\lfloor nc\rfloor}{n}\Big)g(c-) + \Big(\frac{\lfloor nc\rfloor+1}{n} - c\Big)g(c+) + \mathcal{O}\Big(\frac{1}{n^2}\Big)\\ &= \frac{1}{n}\Big\{\{nc\}[g(c-) - g(c+)] + g(c+) + \mathcal{O}\Big(\frac{1}{n}\Big)\Big\}.\end{aligned}$$

Combining this with (22), and using

$$g\Big(\frac{\lfloor nc\rfloor}{n}\Big) = g(c-) + \mathcal{O}\Big(\frac{1}{n}\Big), \quad \text{and} \quad g\Big(\frac{\lfloor nc\rfloor+1}{n}\Big) = g(c+) + \mathcal{O}\Big(\frac{1}{n}\Big),$$

establishes the result for a single jump discontinuity.

When there are $r > 1$ jump discontinuities, we break the sum into $r+1$ parts:

$$\sum_{k=1}^{n-1} g\Big(\frac{k}{n}\Big) = \Big(\sum_{k=1}^{\lfloor nc_1\rfloor} + \sum_{k=\lfloor nc_1\rfloor+1}^{\lfloor nc_2\rfloor} + \cdots + \sum_{k=\lfloor nc_r\rfloor+1}^{n-1}\Big) g\Big(\frac{k}{n}\Big).$$

We then apply the Euler–Maclaurin formula to each of the sums. The proof for each of the sums is identical to that when there is a single jump discontinuity.

(ii) If f is right-continuous at c, then we have to break the sum into

$$\sum_{k=1}^{n-1} g\Big(\frac{k}{n}\Big) = \sum_{k=1}^{\lceil nc\rceil-1} g\Big(\frac{k}{n}\Big) + \sum_{k=\lceil nc\rceil}^{n-1} g\Big(\frac{k}{n}\Big).$$

The rest of the proof proceeds as in case (i), *mutatis mutandis*. □

With the above lemma, we can now proceed to the proof of Theorem 3 by making the necessary changes to the proof of Theorem 1.

Proof of Theorem 3. (i) Suppose f has a single jump discontinuity at $c \in (0,1)$, and is left-continuous at c. Extend the restriction of f on $(c,1]$ to a C^2 function $\tilde{f}(s)$ on $[0,1]$, and let m be the index such that

$$\frac{m}{n} \le c < \frac{m+1}{n}$$

Then $f(k/n)$ are as in (11) for all k except $k = m+1$, where we have

$$\begin{aligned} f\Big(\frac{m+1}{n}\Big) &= \frac{1}{2}\tilde{f}\Big(\frac{m}{n}\Big) + \frac{1}{4n}\tilde{f}'\Big(\frac{m}{n}\Big) + \frac{1}{2}f\Big(\frac{m+1}{n}\Big) + \frac{1}{4n}f'\Big(\frac{m+1}{n}\Big) \\ &\quad + \mathcal{O}\Big(\frac{1}{n^2}\Big) \\ &= \frac{1}{2}\tilde{a}_m + \frac{1}{2}a_{m+1} + \mathcal{O}\Big(\frac{1}{n^2}\Big), \end{aligned}$$

where

$$\tilde{a}_m = \tilde{f}\Big(\frac{m}{n}\Big) + \frac{1}{2n}\tilde{f}'\Big(\frac{m}{n}\Big).$$

Then the sum (12) has to be modified by adding to it the term

$$\frac{1}{2}(\tilde{a}_m - a_m)x_{m+1}^2.$$

(Note that $\tilde{a}_m \to f(c+)$ and $a_m \to f(c-)$ as $n \to \infty$.) This modifies (13) to

$$\begin{aligned} &\frac{\sqrt{\pi}}{\sqrt{D_n(f)}} \\ &= \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} e^{-\frac{a_1}{2}x_1^2}\prod_{k=1}^{n-1}K\Big(x_k,x_{k+1};\frac{k}{n}\Big)e^{-\frac{1}{2}(\tilde{a}_m-a_m)x_{m+1}^2}e^{-\frac{a_n}{2}x_n^2}\,dx_1\cdots dx_n \\ &\quad + o(1) \end{aligned}$$

Expanding again in eigenfunctions, eq. (15) holds as long as we multiply the RHS by

$$\begin{aligned} &\int_{-\infty}^{\infty} e^{-\frac{1}{2}(\tilde{a}_m-a_m)x^2}\phi_0\Big(x;\frac{m}{n}\Big)\phi_0\Big(x;\frac{m+1}{n}\Big)dx \\ &\quad = \frac{\sqrt{2}[(f(c-)^2-4)(f(c+)^2-4)]^{1/8}}{\sqrt{f(c-)-f(c+)+\sqrt{f(c-)^2-4}+\sqrt{f(c+)^2-4}}} + o(1). \end{aligned} \tag{23}$$

Thus (16) holds as long as we multiply the RHS by the -2 power of the above expression.

Next we apply Lemma 2 in the calculation of the product in the denominator of the LHS of (16). With

$$g(x) = \log\Big(\frac{f(x) + \sqrt{f^2(x) - 4}}{2}\Big),$$

we have

$$\begin{aligned}
&\sum_{k=1}^{n-1} \log\Big(\frac{a_k}{2} + \sqrt{\Big(\frac{a_k}{2}\Big)^2 - 1}\,\Big) \\
&\quad = \sum_{k=1}^{n-1} g\Big(\frac{k}{n}\Big) + \frac{1}{2}[g(1) - g(0)] - \frac{1}{2}[g(c+) - g(c-)] + o(1) \\
&\quad = n\int_0^1 g(x)dx - \frac{1}{2}[g(1) + g(0)] + \Big(\{nc\} - \frac{1}{2}\Big)[g(c+) - g(c-)] \\
&\qquad + \frac{1}{2}[g(1) - g(0)] - \frac{1}{2}[g(c+) - g(c-)] + o(1) \\
&\quad = n\int_0^1 g(x)dx - g(0) + (\{nc\} - 1)\,[g(c+) - g(c-)] + o(1)
\end{aligned}$$

Taking exponentials, we obtain

$$\begin{aligned}
&\prod_{k=1}^{n-1} \Big(\frac{a_k}{2} + \sqrt{\Big(\frac{a_k}{2}\Big)^2 - 1}\Big) \\
&\quad = G(f)^n \Big\{\Big(\frac{f(0) + \sqrt{f^2(0) - 4}}{2}\Big)^{-1} \Big[\frac{f(c+) + \sqrt{f(c+)^2 - 4}}{f(c-) + \sqrt{f(c-)^2 - 4}}\Big]^{\{nc\}-1} + o(1)\Big\}.
\end{aligned} \tag{24}$$

Now, taking (16), multiplying the RHS by the -2 power of (23), and combining this with (24) gives us (5) when there is a single left-continuous jump discontinuity. When there are r such discontinuities, we simply apply the same reasoning to each of them.

(ii) The case when f is right-continuous is similar. We only have to change the index m to be such that

$$\frac{m}{n} < c \le \frac{m+1}{n}$$

The calculation of the extra term on the RHS of (16) is then identical. The calculation of the denominator on the LHS of (16) proceeds in the same way, by using the other part of Lemma 2. □

References

[1] G. E. Andrews, R. Askey, and R. Roy, *Special functions.* Encyclopedia of Mathematics and its Applications, 71. Cambridge University Press, Cambridge, 1999. MR 1688958 Zbl 0920.33001

[2] M. Kac, W. L. Murdock, and G. Szegő, On the eigenvalues of certain Hermitian forms. *J. Rational Mech. Anal.* **2** (1953), 767–800. MR 0059482

[3] M. Kac, Asymptotic behaviour of a class of determinants. *Enseignement Math.* (2) **15** (1969), 177–183. MR 0249911 Zbl 0183.04801

[4] L. C. Mejlbo and P. F. Schmidt, On the eigenvalues of generalized Toeplitz matrices. *Math. Scand.* **10** (1962), 5–16. MR 0141949 Zbl 0117.32901

[5] B. Simon, *Szegő's theorem and its descendants.* Spectral theory for L^2 perturbations of orthogonal polynomials. M. B. Porter Lectures. Princeton University Press, Princeton, N.J., 2011. MR 2743058 Zbl 1230.33001

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