Completing the Picture for the Smallest Eigenvalue of Real Wishart Matrices

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(Received 1 September 2014; published 19 December 2014)

Rectangular real $N \times (N+\nu)$ matrices W with a Gaussian distribution appear very frequently in data analysis, condensed matter physics, and quantum field theory. A central question concerns the correlations encoded in the spectral statistics of WW^T. The extreme eigenvalues of WW^T are of particular interest. We explicitly compute the distribution and the gap probability of the smallest nonzero eigenvalue in this ensemble, both for arbitrary fixed N and ν, and in the universal large N limit with ν fixed. We uncover an integrable Pfaffian structure valid for all even values of $\nu \geq 0$. This extends previous results for odd ν at infinite N and recursive results for finite N and for all ν. Our mathematical results include the computation of expectation values of half-integer powers of characteristic polynomials.

DOI: 10.1103/PhysRevLett.113.250201 PACS numbers: 02.10.Yn, 02.50.-r, 05.45.Mt, 11.15.Ha

Introduction.—To study generic statistical features of spectra, various kinds of random matrices are used. Following Wigner and Dyson [1], Hamiltonians of dynamical systems are modeled by real–symmetric, Hermitian or self-dual matrices in quantum chaos, and many-body and mesoscopic physics. Because of universality, cf. Refs. [2,3] and references therein, Gaussian probability densities suffice, leading to the Gaussian orthogonal ensemble (GOE), the Gaussian unitary ensemble (GUE), and the Gaussian symplectic ensemble (GSE) [4]. This concept was extended to Dirac spectra [5] by imposing chiral symmetry as an additional constraint, resulting in the chiral (ch) ensembles chGOE, chGUE, and chGSE [6]. Wishart [7] put forward random matrices to model spectra of correlation matrices in a quite different context. There are many applications in time series analysis [8–10] (including chaotic dynamics [11]), in a wide range of fields in physics [2,3], biology [12], wireless communication [13], and finance [14]. In the most relevant case, $N \times (N+\nu)$ real matrices W model time series such that WW^T is the random correlation matrix. If it fluctuates around a given average correlation matrix C, the distribution reads

$$\mathbb{P}_{N,\nu}(W|C) \sim \exp[-\mathrm{Tr}WW^T C^{-1}/2]. \tag{1}$$

For $C = \mathbb{1}_N$, this happens to coincide with the chGOE, where W and W^T model the nonzero blocks of the Dirac operator. Closing the circle, one can also extend Wishart's model by using non-Gaussian weights. Here and in the sequel, we focus on Eq. (1) with $C = \mathbb{1}_N$. Since WW^T has positive eigenvalues, the spectrum is bounded from below. Naturally, the distribution of the smallest (nonzero) eigenvalue is of particular importance.

Much interest in the chGOE was sparked by the observation [15] that in the limit $N \to \infty$ its spectral correlators describe the Dirac spectrum in quantum field theories with real fermions and broken chiral symmetry, see Ref. [16] for a review. Based on earlier works for finite N [17,18], the spectral density [15] and all higher density correlation functions [19] were computed in terms of a Pfaffian determinant of a matrix kernel for all ν. These quantities were shown later to be universal [20] for non-Gaussian potentials, and most recently for fixed trace ensembles in the context of quantum entanglement, see Ref. [21] and references therein. Further applications of the chGOE can be found in the recent review [22] on Majorana fermions and topological superconductors.

In an influential paper [23] the condition number of a Wishart random matrix WW^T was investigated, which is the root of the ratio of the largest over the smallest nonzero eigenvalue of WW^T. This quantity is important for a generic matrix as it quantifies the difficulty of computing its inverse. In Ref. [24] the distribution of the smallest eigenvalue was calculated recursively in N for arbitrary rectangular chGOE matrices. Closed expressions were given for quadratic matrices $\nu = 0$ [23] (cf. Ref. [25]) and for $\nu = 1, 2, 3$ [24]. Later Pfaffian expressions were found in Ref. [26] for arbitrary odd ν valid for fixed and asymptotically large N. A more general consideration, including correlations with $C \neq \mathbb{1}_N$, of the smallest eigenvalue for ν odd was given in Ref. [27]. The limiting distributions of the kth smallest eigenvalue were computed in Ref. [28], again for ν odd. These quantities are an efficient tool to test algorithms with exact chiral symmetry in lattice gauge theories [29], distinguishing clearly between different topologies labeled by ν. In Ref. [30] the distributions for higher even $\nu > 0$ were obtained from numerical chGOE simulations. Most recently efficient numerical algorithms have been applied, see, e.g., Ref. [31], in order to compute smallest eigenvalue distributions for arbitrary ν using known analytic Fredholm determinant expressions [32].

It is our goal to complete the picture for the smallest chGOE eigenvalue distribution and its integral by finding explicit Pfaffian expressions for finite and infinite N valid for all even ν. Together with previous results this completes the integrability of this classical ensemble. A presentation with further results and more mathematical details will be given elsewhere [33].

Smallest eigenvalue and gap probability.—First, we define the quantities of interest and state the problem. In the analytic calculations below we set $C = \mathbb{1}_N$ in Eq. (1), and later we compare our universal large N results to numerical simulations with $C \neq \mathbb{1}_N$. Because we are only interested in correlations of the positive eigenvalues of $WW^T = OXO^T$ contained in $X = \mathrm{diag}(x_1, \ldots, x_N)$, we drop all normalization constants depending on the orthogonal matrix O. Integrating the distribution (1) over all independent matrix elements with respect to flat Lebesgue measure we obtain the partition function expressed in terms of the eigenvalues as

$$\mathcal{Z}_{N,\gamma} = \prod_{i=1}^{N} \int_0^\infty dx_i w_\gamma(x_i) |\Delta_N(X)|, \qquad (2)$$

up to a known constant. Here, we introduce the weight function $w_\gamma(x)$ and Vandermonde determinant $\Delta_N(X)$ stemming from the Jacobian of the diagonalization

$$w_\gamma(x) \equiv x^\gamma \exp[-x/2], \qquad \gamma \equiv (\nu - 1)/2, \qquad (3)$$

$$\Delta_N(X) \equiv \prod_{1\leq i<j\leq N} (x_j - x_i) = \det_{1\leq i,j\leq N}[x_i^{j-1}]. \qquad (4)$$

We note that γ alternates between integer and half-integer values. The expectation value of an observable f only depending on X is defined as

$$\langle f(X)\rangle_{N,\gamma} \equiv \frac{\prod_{i=1}^N \int_0^\infty dx_i w_\gamma(x_i) f(X) |\Delta_N(X)|}{\mathcal{Z}_{N,\gamma}}. \qquad (5)$$

Thus, the gap probability that no eigenvalue occupies the interval $[0, t]$ is given by

$$E_{N,\gamma}(t) \equiv \frac{1}{\mathcal{Z}_{N,\gamma}} \prod_{i=1}^{N} \int_t^\infty dx_i w_\gamma(x_i) |\Delta_N(X)|$$
$$= e^{-Nt/2} \frac{\mathcal{Z}_{N,0}}{\mathcal{Z}_{N,\gamma}} \langle \det{}^\gamma [X + t\mathbb{1}_N]\rangle_{N,0}. \qquad (6)$$

It is expressed as an expectation value of a characteristic polynomial to the power γ with respect to the weight function (3) without the preexponential factor $w_0(x)$. This crucial identity follows from the translation invariance of the Vandermonde determinant (4).

The normalized distribution of the smallest nonzero eigenvalue $P_{N,\gamma}(t)$ is obtained by differentiating Eq. (6)

$$P_{N,\gamma}(t) \equiv -\frac{\partial E_{N,\gamma}(t)}{\partial t}$$
$$= t^\gamma e^{-Nt/2} \frac{N\mathcal{Z}_{N-1,1}}{\mathcal{Z}_{N,\gamma}} \langle \det{}^\gamma [X + t\mathbb{1}_{N-1}]\rangle_{N-1,1}, \qquad (7)$$

where the second line follows along the same steps as in Eq. (6). This relation is well known [26,28], with the difficulty to compute the average (also called massive partition function) for γ half integer, which is our main task.

To compute Eqs. (6) and (7) we need to know the normalizing partition functions, which are given for arbitrary real $\nu > -1$ in terms of the Selberg integral, see also Refs. [34,35], and the expectation values. For integer $\gamma = k$ corresponding to odd $\nu = 2k + 1$ closed expressions of Eq. (7) exist [26], given in terms of Laguerre polynomials skew orthogonal with respect to the weight (3). Therefore, we concentrate on the case $\nu = 2k$ even.

Pfaffian structure and finite N results.—To show that the gap probability (6) has a Pfaffian structure when γ is half integer let us define the following parameter dependent weight function

$$w(x; t) \equiv \exp[-\eta x/2]/\sqrt{x + t}. \qquad (8)$$

It absorbs the half-integer part in the expectation value (6) when $\nu = 2k$ is even. We set $\eta = 1$ unless otherwise stated. The monic polynomials $R_k(x; t) = x^k + \cdots$ are defined to be skew orthogonal with respect to the following skew-symmetric scalar product

$$\langle f, g\rangle_t \equiv \int_0^\infty dy \int_0^y dx w(x; t) w(y; t) [f(x)g(y) - f(y)g(x)] \qquad (9)$$

by satisfying for all $i, j = 0, 1, \ldots$ [36] the conditions

$$\langle R_{2j}, R_{2i}\rangle_t = 0 = \langle R_{2j+1}, R_{2i+1}\rangle_t$$
$$\langle R_{2j+1}, R_{2i}\rangle_t = r_j(t)\delta_{ij}. \qquad (10)$$

Their normalizations $r_j(t)$ depend on t. The partition function $\mathcal{Z}_N(t)$ of this new weight (8) is defined by

$$\mathcal{Z}_N(t) \equiv \prod_{i=1}^{N} \int_0^\infty dx_i w(x_i; t) |\Delta_N(X)| = N! \prod_{i=0}^{\frac{N}{2}-1} r_i(t). \qquad (11)$$

The last step holds for N even [4]. Likewise, we define expectation values $\langle f(X)\rangle_N^t$, following Eq. (5). Thus, for even $\nu = 2k$, $k \in \mathbb{N}$, Eq. (6) reduces to

$$E_{N,k-\frac{1}{2}}(t) = e^{-Nt/2} \frac{\mathcal{Z}_N(t)}{\mathcal{Z}_{N,k-\frac{1}{2}}} \langle \det{}^k [X + t\mathbb{1}_N]\rangle_N^t, \qquad (12)$$

given in terms of an integer power of a characteristic polynomial. While the skew-orthogonal polynomials with respect to the weight (3) are know in terms of Laguerre polynomials [26], the difficulty here is to determine the t-dependent polynomials and normalization constants for the nonstandard weight (8). They can be computed following the observation [37]

$$R_{2j}(y,t) = \langle \det[X - y\mathbb{1}_{2j}]\rangle_{2j}^t, \tag{13}$$

$$\begin{aligned} R_{2j+1}(y,t) &= \langle (y + c + \mathrm{Tr}X)\det[X - y\mathbb{1}_{2j}]\rangle_{2j}^t \\ &= (y+c)R_{2j}(y,t) - 2\frac{\partial}{\partial\eta}R_{2j}(y,t)\Big|_{\eta=1}. \end{aligned} \tag{14}$$

The odd polynomials are obtained by differentiation of the weight (8), generating TrX in the average. Note that the $R_{2j+1}(y,t)$ are not unique [37]; we set $c = 0$ in the following. The even polynomials (13) can be calculated by mapping them back to a proper matrix integral over an auxiliary $2j \times (2j+1)$ matrix $\bar{W}$ (corresponding to $\gamma = 0$)

$$R_{2j}(y,t) = C_{2j}(t)\int d\overline{W}\,\frac{\det[\overline{WW^T} - y\mathbb{1}_{2j}]}{\det^{\frac{1}{2}}[\overline{WW^T} + t\mathbb{1}_{2j}]}e^{-(\eta/2)\mathrm{Tr}\overline{WW^T}}, \tag{15}$$

cf. Ref. [27]. The known normalization constant $C_{2j}(t)$ follows from the fact that the polynomial is monic. Without giving details Eq. (15) can be computed exactly, representing the determinants by Gaussian integrals over commuting and anticommuting variables and by using standard bosonization techniques [38]. We arrive at

$$R_{2j}^a(y,t) = \frac{(2j)!(U_j(t)L_{2j-a}^{(a+1)}(y) - 2U_j'(t)L_{2j-a}^{(a)}(y))}{(2j-a)!U(\frac{2j+1}{2},\frac{3}{2},\frac{t}{2})} \tag{16}$$

for the ath derivatives of the polynomials $(\partial^a/\partial y^a)R_j(y,t) \equiv R_j^a(y,t)$, $a = 0, 1, \ldots$, needed later. Here, $U_j(t) \equiv U(((2j+1)/2), \frac{1}{2}, (t/2))$ denotes the Tricomi confluent hypergeometric function, satisfying $U'(a,b,t) = -aU(a+1,b+1,t)$ [39]. The derivative in Eq. (16) acts only on the generalized Laguerre polynomials used in monic normalization $L_j^{(a)}(y) = y^j + \cdots$. They satisfy $(\partial^a/\partial y^a)L_n^{(b)}(y) = (n!/(n-a)!)L_{n-a}^{(b+a)}(y)$, where we set $L_n^{(b)}(y) \equiv 0$ for $n < 0$. For the odd polynomials we obtain

$$\begin{aligned} R_{2j+1}^a&(y,t) \\ &= (4j^2 + 4j + y)R_{2j}^a(y,t) + aR_{2j}^{a-1}(y,t) \\ &\quad + \frac{(2j)!/(2j-a)!}{U(\frac{2N+1}{2},\frac{3}{2},\frac{t}{2})}\Big\{4tU_j''(t)L_{2j-a}^{(a)}(y) + 4U_j'(t) \\ &\quad \times \left[aL_{2j-a}^{(a)}(y) + (2j-a)yL_{2j-a-1}^{(a+1)}(y) + \frac{t}{2}L_{2j-a}^{(a+1)}(y)\right] \\ &\quad - 2U_j(t)[aL_{2j-a}^{(a+1)}(y) + (2j-a)yL_{2j-a-1}^{(a+2)}(y)]\Big\}, \end{aligned} \tag{17}$$

and the normalization constants in Eq. (10) read

$$r_j(t) = 2(2j)!(2j+1)!\frac{U(\frac{2j+3}{2},\frac{3}{2},\frac{t}{2})}{U(\frac{2j+1}{2},\frac{3}{2},\frac{t}{2})}. \tag{18}$$

Following Ref. [26] with their Laguerre weight $w_0(x)$ in Eq. (3) replaced by our weight (8), we express the gap probability (12) as a Pfaffian determinant with our kernel consisting of the skew-orthogonal polynomials (16) and (17). In a more general setting averages of characteristic polynomials such as Eq. (12) were considered in Refs. [40,41] for arbitrary but unspecified weights. For finite even N and $\nu = 2k$ with $k = 2m$ even we obtain

$$\begin{aligned} E_{N,k-\frac{1}{2}}(t) &= C_{N,\nu}\sqrt{t}e^{-Nt/2}U\left(\frac{N+2m+1}{2},\frac{3}{2},\frac{t}{2}\right) \\ &\quad \times \mathrm{Pf}\left[\sum_{j=0}^{\frac{N}{2}+m-1}\frac{R_{2j+1}^a(-t,t)R_{2j}^b(-t,t) - (a\leftrightarrow b)}{r_j(t)}\right]_{a,b=0}^{k-1}. \end{aligned} \tag{19}$$

For $k = 2m - 1$ odd the last row (and column) inside the Pfaffian is replaced by $(-)R_{N+k-2}^{b(a)}(-t,t)/r_{N/2+m-1}(t)$, respectively, (for N odd, cf. Ref. [33]). The known t-independent constant $C_{N,\nu}$ is suppressed for simplicity; it ensures $E_{N,k-(1/2)}(t=0) = 1$.

Equation (19) is our first main result. A similar answer can be obtained for $P_{N,\gamma}(t)$ for even ν, given in terms of skew-orthogonal polynomials with respect to the weight $xw(x;t)$. This provides an explicit integrable Pfaffian structure for both $E_{N,\gamma}(t)$ and $P_{N,\gamma}(t)$. It extends the odd ν result for $P_{N,\gamma}(t)$ in Ref. [26], which is given by a Pfaffian determinant as well, but with a different kernel.

For illustration we give two examples. For $\nu = 0$ the Pfaffian in Eq. (19) is absent, and

$$E_{N,-\frac{1}{2}}(t) = \frac{(N-1)!\sqrt{t}e^{-Nt/2}}{2^{N-1/2}\Gamma(N/2)}U\left(\frac{N+1}{2},\frac{3}{2},\frac{t}{2}\right), \tag{20}$$

whereas for $\nu = 2$ the kernel is absent, and only the polynomial (16) with $a = 0$ contributes:

$$\begin{aligned} E_{N,+\frac{1}{2}}(t) &= \frac{\Gamma(\frac{N+1}{2})\sqrt{t}e^{-Nt/2}}{(-1)^N\sqrt{2\pi}N!} \\ &\quad \times [U_N(t)L_N^{(1)}(-t) - 2U_N'(t)L_N^{(0)}(-t)]. \end{aligned} \tag{21}$$

Equations (20) and (21) are compared to numerical simulations in Fig. 1. They can be matched with the finite N results of Ref. [24] for $\nu = 0, 2$, after differentiating them and using identities for the Tricomi function [39].

Microscopic large N limit.—We turn to the large N limit keeping ν fixed, referred to as the hard edge limit. It is particularly important as the limiting density correlation functions are universal for non-Gaussian weight functions for any integer ν [20]. Because the gap probability can be expressed in terms of the limiting universal kernel [32] [see Eq. (30) for the corresponding density], its universality

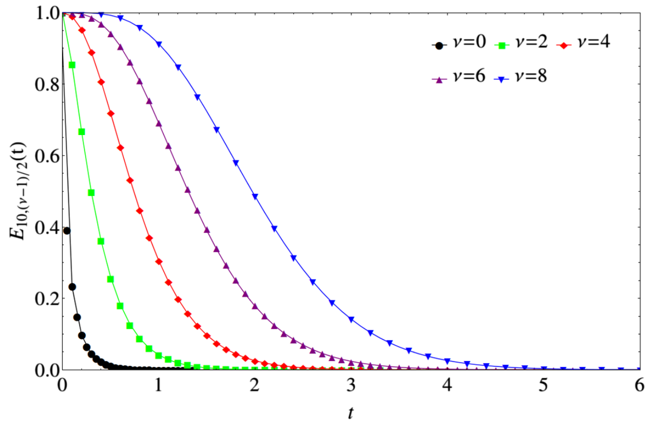

FIG. 1 (color online). The gap probability $E_{N,(\nu-1)/2}(t)$ (straight lines) for finite $N=10$ and $\nu=0,2,4,6,8$ (from left to right) versus numerical simulations (symbols) of 40000 realizations of Wishart matrices, with $C=\mathbb{1}_N$.

carries over to the distribution of the smallest eigenvalue. Moreover, in Ref. [27] it was shown for both ν even and odd, without explicitly calculating the distributions, that the presence of a nontrivial correlation matrix in Eq. (1) does not change the limiting smallest eigenvalue distribution when the spectrum of C has a finite distance to the origin.

The limiting gap probability and smallest eigenvalue distribution are defined as

$$\mathcal{E}_\gamma(u)\equiv\lim_{N\to\infty}E_{N,\gamma}\left(t=\frac{u}{4N}\right),\quad \frac{\partial}{\partial u}\mathcal{E}_\gamma(u)=-\mathcal{P}_\gamma(u). \tag{22}$$

In view of Eq. (19) we need the following asymptotic limit of the hypergeometric function

$$U\left(aN+c,b,\frac{u}{8N}\right)\approx\frac{2(N^2 8a/u)^{(b-1)/2}}{\Gamma(aN+c)}K_{b-1}\left(\sqrt{\frac{au}{4}3}\right). \tag{23}$$

For a half-integer index the modified Bessel function of second kind simplifies, e.g., for $b=1/2,3/2,5/2$

$$K_{\pm\frac{1}{2}}(z)=\sqrt{\frac{\pi}{2z}}e^{-z},\qquad K_{\frac{3}{2}}(z)=(1-z^{-1})K_{\frac{1}{2}}(z). \tag{24}$$

Inside the Pfaffian (19) the sum is replaced by an integral, $\sum_j\to(N/2)\int_0^1 dx$, with $j=Nx/2$. The limiting skew-orthogonal polynomials follow from Eq. (23) together with the standard Laguerre asymptotic in terms of modified Bessel functions of the first kind, see, e.g., Ref. [39]. This leads to the following limiting kernel inside the Pfaffian (19), independently of N being even or odd,

$$\begin{aligned}\kappa_{ab}(u)\equiv\int_0^u\frac{dz}{u}&[2(b-a)I_a(\sqrt{z})I_b(\sqrt{z})\\&+(2b+1)I_{a+1}(\sqrt{z})I_b(\sqrt{z})\\&-(2a+1)I_{b+1}(\sqrt{z})I_a(\sqrt{z})].\end{aligned} \tag{25}$$

The final answer for the limiting gap probability reads

$$\mathcal{E}_{k-1/2}(u)=C_e e^{-\sqrt{u}/2-u/8}\mathrm{Pf}[\kappa_{ab}(u)]_{a,b=0}^{k-1} \tag{26}$$

for $\nu=2k$ with $k=2m$ even and

$$\begin{aligned}\mathcal{E}_{k-1/2}(u)=&\,C_o e^{-\sqrt{u}/2-u/8}\\&\times\mathrm{Pf}\begin{bmatrix}\kappa_{ab}(u) & -u^{a/2}[I_{a+1}(\sqrt{u})+I_a(\sqrt{u})]\\ u^{b/2}[I_{b+1}(\sqrt{u})+I_b(\sqrt{u})] & 0\end{bmatrix}_{a,b=0}^{k-2}\end{aligned} \tag{27}$$

for $k=2m-1$ odd. We suppress the known u-independent normalization constants $C_{e/o}$. The corresponding limiting result for the smallest eigenvalue distribution is

$$\mathcal{P}_{k-1/2}(u)=\hat{C}_e u^k(1+2/\sqrt{u})e^{-\sqrt{u}/2-u/8}\mathrm{Pf}[\hat{\kappa}_{ab}(u)]_{a,b=0}^{k-1} \tag{28}$$

for $\nu=2k$ with $k=2m$ even, and

$$\begin{aligned}\mathcal{P}_{k-1/2}(u)&\\=&\,\hat{C}_o u^k(1+2/\sqrt{u})e^{-\sqrt{u}/2-u/8}\\&\times\mathrm{Pf}\begin{bmatrix}\hat{\kappa}_{ab}(u) & -\frac{I_{a+2}(\sqrt{u})+\frac{\sqrt{u}}{2+\sqrt{u}}I_{a+3}(\sqrt{u})}{u^{(a+2)/2}}\\ \frac{I_{b+2}(\sqrt{u})+\frac{\sqrt{u}}{2+\sqrt{u}}I_{b+3}(\sqrt{u})}{u^{(b+2)/2}} & 0\end{bmatrix}_{a,b=0}^{k-2}\end{aligned} \tag{29}$$

for $k=2m-1$ odd, suppressing again the u-independent normalization constants $\hat{C}_{e/o}$. Here, $\hat{\kappa}_{ab}(u)$ is the limiting kernel for the skew-orthogonal polynomials with respect to $xw(x;t)$, which is of a similar structure as Eq. (25). For $\nu=0,2$ the results (28) and (29) were known from Refs. [25] and [21], respectively.

Equations (26)–(29) constitute our second main result and are universal. In Fig. 2 they are compared to the universal microscopic density [15,42] valid for all ν values

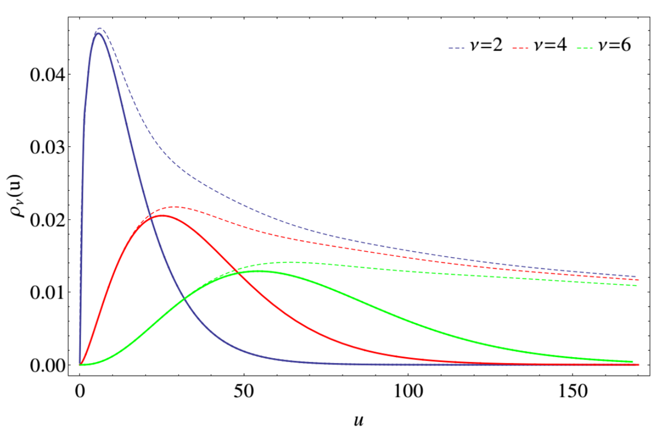

FIG. 2 (color online). The microscopic density $\rho(u)$ (30) (dashed lines) versus the corresponding smallest eigenvalue distribution $\mathcal{P}_{(\nu-1)/2}(u)$ (straight lines) for $\nu=2,4,6$ (from left to right). The smallest eigenvalue nicely follows the density for all ν.

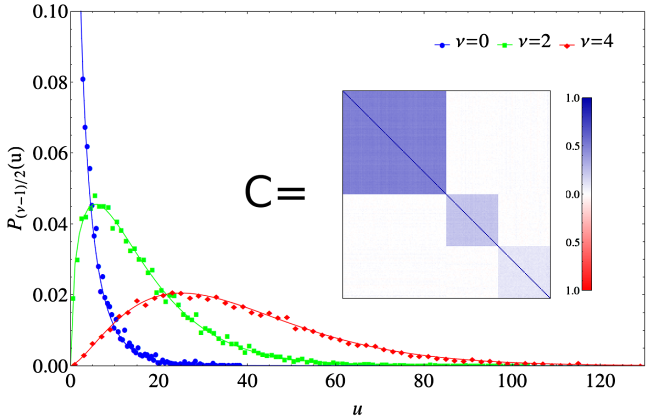

FIG. 3 (color online). The microscopic smallest eigenvalue distribution $\mathcal{P}_{(\nu-1)/2}(u)$ (straight lines) for $\nu = 0, 2, 4$ (from left to right) versus numerical simulations (symbols) of 10000 realizations of matrices with $N = 200$ and correlation matrix $C \neq \mathbb{1}_N$ as indicated in the inset.

$$\rho_\nu(u) = \frac{1}{4}[J_\nu(\sqrt{u})^2 - J_{\nu-1}(\sqrt{u})J_{\nu+1}(\sqrt{u})] + \frac{1}{4\sqrt{u}}J_\nu(\sqrt{u})\left(1 - \int_0^{\sqrt{u}} ds J_\nu(s)\right). \quad (30)$$

We further illustrate the universality of our results by comparing to numerical simulations with a nontrivial correlation matrix C for large N, see Fig. 3.

Conclusions and outlook.—We have computed closed expressions for the distribution of the smallest nonzero eigenvalue and its integral, the gap probability, for rectangular $N \times (N + \nu)$ real Wishart matrices with ν even, both for finite N and in the universal microscopic large N limit. They only depend on a single kernel instead of three different ones for the density correlation functions and are thus much simpler than these known results. We confirm our findings by numerical simulations, even including a nontrivial correlation matrix C. This completes the calculation of all eigenvalue correlation functions in this classical ensemble of random matrices and shows its integrable structure. Furthermore, our finite N results allow us to analyze deviations from the universal large N limit, as was very recently proposed in Ref. [43] for the chGUE.

We thank the Sonderforschungsbereich TR12 (G. A., T. G., and T. W.) and the Alexander von Humboldt-Foundation (M. K.) for support.

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