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Level spacing for band random matrices

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Abstract. We examine the spacing distribution of the eigenvalues of tridiagonal real symmetric random matrices, the elements of which are distributed according to a Gaussian law. We show explicitly that for 4×4 matrices the distribution at small spacings behaves as $s \log^2 s$. We surmise that for $N \times N$ matrices the behaviour is $s \log^{N-2} s$ and we present numerical results which support this conjecture.

1. Introduction

The current interest in quantum chaos has rekindled the study of random matrices for their own sake. The spectra of random matrices have been used since the 1950s in order to model the behaviour of the levels of nuclear Hamiltonians [1]. Although it was readily established that the experimentally obtained nearest-neighbour spacing distribution (NNSD) follows closely the predictions based on the Gaussian orthogonal ensemble (GOE) of random matrices [2] there was no convincing explanation of this fact: nuclear Hamiltonians are not random. The study of quantum chaos or, more precisely, of the quantum behaviour of systems which are chaotic at the classical limit, shed some light on the matter. Thus, in [3], it was conjectured that the statistical properties of quantum spectra of classically ergodic Hamiltonians are given by the GOE of random matrices (provided certain symmetry conditions are satisfied). This would explain why the random matrix approach worked well for nuclear Hamiltonians: one can easily assume that their behaviour, if not ergodic, is highly chaotic. This has, of course, merely displaced the problem by one step, as it is now clear that chaotic quantum Hamiltonians are not random [4]. Thus before the ultimate understanding of the question is attained one must explain what is causing the GOE behaviour to appear. Meanwhile the study of quantum Hamiltonians and random matrices progresses along often intersecting paths.

One domain where random matrices have been of considerable help is in the study of the transition from ergodicity to integrability. While the behaviour of the quantum spectra of the two limits is well known [5, 6] and, moreover, universal (i.e. it does not depend on the detailed structure of the system), this is not the case for the transition zone. Here the use of the analogy between random matrices and quantum Hamiltonians has allowed a quantitative study of the sole universal feature of this 'intermediate' behaviour of the system [7]. As soon as integrability is lost the NNSD ceases to be Poisson-like (e^{-s}) and falls linearly to zero at very small spacings [8]. The slope is inversely proportional to the integrability-breaking perturbation [7, 9]. As the system moves towards ergodicity the distribution resembles more and more the GOE one or even simply the Wigner surmise $\frac{1}{2}\pi s e^{-(\pi/4)s^2}$. One thing that was clear from our study [7] (see also [10]) was that one needs banded matrices, i.e. matrices with non-zero elements occurring at or near the diagonal only, in order to describe the transition region. In [7] we considered tridiagonal matrices using a particular statistics which was suitable for our study. So one natural question that arises is what happens to the NNSD when these constraints are raised: what is the level distribution of a band matrix with Gaussian-distributed random matrix elements?

Curiously, very little is known about band random matrices [11], but lately the subject has been the focus of ever increasing interest [12]. The familiar 2×2 model is not of any use here. Only recently has a study of 3×3 matrices made its appearance in the literature [13] and yielded an interesting result. While the full GOE matrix (of any size) has an NNSD which starts linearly at the origin with a slope which goes from $\frac{1}{2}\pi$ for 2×2 to $\frac{1}{6}\pi^2$ for infinite matrices, the 3×3 matrix with the (1, 3) matrix elements equal to zero has a distribution which behaves as $s \log(1/s)$ at the origin. However, the aforementioned study does not go beyond the 3×3 stage. In the present work we will present our findings on an explicit treatment of the 4×4 case and formulate a conjecture for larger matrices.

2. The nearest-neighbour spacing distribution for matrices of dimensions 2, 3 and 4

As stated in the introduction, we deal exclusively with random matrices belonging to the GOE in this paper. This means that the matrices considered are real, symmetric with their elements obtained through a Gaussian distribution characterized by its width σ (we recall that the width for the diagonal matrix elements is $\sqrt{2}$ times that of an off-diagonal one).

The NNSD of 2×2 GOE random matrices is the well known Wigner surmise (where the mean level spacing has been normalized to unity)

$$P_2(s) = \frac{1}{2}\pi s \ e^{-(\pi/4)s^2}.$$
 (1)

The essential point here is that the level repulsion behaves linearly for small spacings. In fact, this is a general feature of the GOE, provided we restrict ourselves to full matrices. When the matrices develop a band structure, this is not the case any more. In [13], Molinari and Sokolov computed the small-spacing behaviour of a 3×3 GOE random matrix with a vanishing H_{13} matrix element. They started from the probability measure written as $e^{-(1/4\sigma^2) \operatorname{Tr} H^2} \prod_{i \leq j} dH_{ij}$ which they transformed (following the standard approach [11, 14]) to a new set of variables given by the eigenvalues of the random matrix and the angles of the orthogonal transformation that diagonalizes it.

However, the constraint that $H_{13} = 0$ would destroy the rotational invariance of the 'volume element' $\prod_{i \le j} dH_{ij}$. It is simplest for the subsequent calculations to restore the invariance and introduce the constraint through a δ distribution. We can then rewrite the probability measure as

$$e^{-(1/4\sigma^2)\operatorname{Tr} H^2}\prod_{i\leq j}|E_i-E_j|\prod_i dE_i d\Omega.$$

In the case of 3×3 symmetric matrices the orthogonal transformation needed for diagonalization belongs to SO(3). The rotation angles are simply the Euler angles and

 $d\Omega$ is given by $\sin\beta d\alpha d\beta d\gamma$. The NNSD is obtained from the joint probability distribution of the eigenvalues which is given by

$$P_{3}(E_{1}, E_{2}, E_{3}) = C e^{-(1/4\sigma^{2}) \sum E_{i}^{2}} \prod_{i < j} |E_{i} - E_{j}| \int \delta(H_{13}) d\Omega.$$
(2)

Expressing H_{13} in terms of the eigenvalues and the Euler angles the authors of [13] obtained

$$H_{13} = \sin \beta (B \cos \alpha + A \sin \alpha \cos \beta)$$
(3)

with $A = (E_3 - E_1) \sin^2 \gamma + (E_3 - E_2) \cos^2 \gamma$ and $B = (E_1 - E_2) \sin \gamma \cos \gamma$. Integrating the δ function over the angle α we obtain

$$I = \int \delta(H_{13}) \sin \beta \, d\alpha \, d\beta \, d\gamma = \int d\beta \, d\gamma \left[\frac{1}{A \cos \alpha \cos \beta - B \sin \alpha} \right]_{\tan \alpha = B/A \cos \beta}$$
$$= \int d\gamma \int_0^{\pi} \frac{d\beta}{\sqrt{B^2 + A^2 \cos^2 \beta}}.$$
(4)

The integral over β can be readily expressed in terms of the complete elliptic integral K and we thus have

$$I = \int \frac{2 \,\mathrm{d}\gamma}{\sqrt{A^2 + B^2}} \,K\left(\frac{A}{\sqrt{A^2 + B^2}}\right). \tag{5}$$

In order to investigate the small-spacing behaviour of $P_3(E_1, E_2, E_3)$, we choose one of the differences of eigenvalues, e.g. $E_1 - E_2$ equal to a small quantity s. For small s, B goes to zero, the argument of K goes to unity and K diverges logarithmically [15]. Thus the behaviour of I at small s is $\int 2 d\gamma \log(A/B)/A$.

We can check that the integration over γ does not cancel the coefficient of the logarithmic term. Thus, combining the latter with the factor s from $\prod_{i < j} |E_i - E_j|$, we obtain the small-spacing behaviour of $P_3(s)$ in the form

$$P_3(s) \approx s \log \frac{1}{s}.\tag{6}$$

Next we turn to the 4×4 case, which is our main objective. First we remark that the orthogonal transformation needed for diagonalization belongs here to SO(4) and thus involves six angles. The invariant measure of the rotation group can be written as [16]

$$d\Omega = \sin^2 \theta_6 \sin \theta_5 \sin \theta_2 \prod_{i=1}^6 d\theta_i.$$
⁽⁷⁾

The tridiagonal band matrix is realized through $H_{14} = H_{13} = H_{24} = 0$. The elements to be set to zero are given by expressions analogous to (3) although rather longer. In fact, given the bulk of the computations, all the calculations involved were performed using the REDUCE algebraic manipulation language [17]. The integration over the three δ functions was performed over the angles θ_6 , θ_2 and θ_5 , substituting at each step. The end result is an expression of the form

$$I = \int F(E_2 - E_1, E_3 - E_1, E_4 - E_1, \theta_1, \theta_3, \theta_4) \, \mathrm{d}\theta_1 \, \mathrm{d}\theta_3 \, \mathrm{d}\theta_4.$$
(8)

The function F has a very complicated expression, which we will not reproduce here. The interesting point is that when two of the eigenvalues are very close to each other, say $|E_3 - E_1| = s \ll 1$, one can show that I behaves as $\log^2(1/s)$. (We recall at this point that in order to obtain the spacing distribution $P_4(s)$ one must multiply the angular integral I by $\prod_{i < j} |E_i - E_j|$ which contains one s factor.) In the small-s limit the function F can be written as

$$\Theta(Bs+C\cos^2\theta_3-|\cos\theta_1\cos\theta_3|) \times \frac{A(s/\cos^2\theta_3, E_2-E_1, E_4-E_1, \theta_1, \theta_4)+\mathcal{O}(s, \cos^2\theta_3)}{\sqrt{s^2+\cos^2\theta_3(s+\cos^2\theta_1)}}$$

where B and C have the same behaviour as the numerator of the fraction.

All three functions A, B and C are finite and, moreover, are bounded away from zero for generic values of $E_2 - E_1$, $E_4 - E_1$, θ_1 and θ_4 , even for $\cos^2 \theta_1 \ll 1$. Note that, at lowest order, the dependence on s is through the first argument. The presence of the Heaviside function Θ is due to the integration over θ_2 : one gets a contribution only if the δ function has a zero for $|\cos \theta_2| < 1$. In the domain $s \ll \cos^2 \theta_3 \ll 1$, A goes to a finite limit \tilde{A} . Thus

$$I = \int d\theta_4 \tilde{A} \int d\theta_3 \int \frac{d\theta_1 \Theta(Bs + C \cos^2 \theta_3 - |\cos \theta_1 \cos \theta_3|)}{\sqrt{s^2 + \cos^2 \theta_3 (s + \cos^2 \theta_1)}}.$$
 (9)

Integration over θ_1 for $0 < \cos^2 \theta_1 < C^2 \cos^2 \theta_3$ gives a contribution of the order of

$$\frac{1}{\cos\theta_3}\log\left(1+\frac{\cos^2\theta_3}{s}\right).$$
 (10)

Integration over θ_3 in the domain $s \ll \cos^2 \theta_3 \ll 1$ gives the contribution of order $\log^2(1/s)$. (Note that for $\cos^2 \theta_3 \ll s$, expression (10) does not hold and there is no divergence as $\cos \theta_3 \rightarrow 0$.) The final integration over θ_4 does not cancel the coefficient of $\log^2(1/s)$ which is thus the leading behaviour of I as $s \rightarrow 0$. Thus, the NNSD $P_4(s)$ behaves as $s \log^2(1/s)$ for vanishingly small s.

One question that arises naturally at this point is what happens when less than three matrix elements are set to zero. The calculations are still quite lengthy and we will limit ourselves to a mere presentation of the results. When two matrix elements, say H_{14} and H_{24} , are set to zero, we find that the corresponding integral I behaves as log(1/s) and thus, at small spacings, the NNSD behaves as s log(1/s). The case of only one vanishing matrix element H_{14} is even more interesting. Here the corresponding integral I remains bounded as $s \rightarrow 0$, but has a non-analytic behaviour of the form k+s log(1/s). Thus the NNSD still vanishes linearly at the origin, but the singularity manifests itself on the second derivative.

Let us now summarize our findings. For 2×2 matrices the NNSD behaves linearly at the origin: $P_2(s) \approx s$. For 3×3 matrices only one matrix element must be put to zero and we have $P_3(s) \approx s \log(1/s)$. For 4×4 tridiagonal matrices we have $P_4(s) \approx$ $s \log^2(1/s)$. We can already see the pattern emerging: as the dimension of the band matrix increases by one so does the power of the leading log. Thus for an $N \times N$ tridiagonal matrix we surmise that the NNSD at small spacings will be of the form

$$P_N(s) \approx s \log^{N-2}(1/s).$$
 (11)

In fact, for an $N \times N$ matrix we have N(N-1)/2 integration angles. After integrating over the (N-1)(N-2)/2 δ functions we are left with N-1 angles: N-2 of them

would lead (upon integration) to one power of log each, and the remaining would just give an angular averaging. One must bear in mind that expressions like (11) concern only the dominant term. Subdominant terms exist as well and their relative coefficient with respect to (11) will depend on the matrix size. In fact, one can offer an even bolder conjecture than (11). If we consider large matrices then we believe that, for $s \rightarrow 0$, the behaviour of $P_N(s)$ will be roughly s multiplied by the truncation, at order N-2, of the Taylor series of $e^{\lambda x}$ in terms of $x = \log(1/s)$ and where $\lambda \rightarrow 1$ as $N \rightarrow \infty$. Therefore $P_N(s)$ will be close to a Poisson distribution except in a very small region around the origin. As we will see in the next section these arguments will be further strengthened by the results of numerical computations.

3. Numerical results and conclusion

In order to illustrate (and confirm) the predictions of the previous section we have performed extensive numerical computations, diagonalizing millions of random matrices and computing the NNSD. In all the examples presented below our statistics are based on more than 10^7 levels. In a first set of figures (figure 1(a)-(d)) we present the global distribution as a function of spacing for matrices of dimensions 3, 4, 5 and 8. It is clear that already at N = 3 the NNSD does not follow the Wigner distribution while for increasing N the tail becomes more and more an exponential Poisson-like one. What is remarkable is that an excellent overall fit can be obtained with the Brody [18] distribution:

$$P_B(s) = \alpha (q+1) s^q e^{-\alpha s^{q+1}} \qquad \alpha = \{ \Gamma[(q+2)/(q+1)] \}^{q+1}.$$
(12)

As can be clearly seen, from (12), this expression is intermediate between Poisson and Wigner, two limits that it attains for q = 0 and q = 1 respectively. On the other hand, for every non-zero value of q, it vanishes at s = 0 but with an infinite derivative (unless q = 1). This vertical slope is a first, rough explanation of the success of the Brody ansatz in describing the NNSD of tridiagonal matrices. From our calculations we were able to extract the N dependence of q: it turned out that 1/q is a linear function of N, i.e. $1/q = \mu N + \nu$. Still at small spacings, there are substantial deviations due to the presence of logarithms. This is clearly illustrated in figure 2(a)-(d) where we present the (very) small-spacing behaviour of P(s) for N = 3, 4, 5 and 8. The Brody distribution cannot reproduce this small-scale structure precisely. On the contrary a (single global parameter) fit based on the truncated expansion of e^x at order N - 2 with $x = \log(1/s)$ (taking $\lambda = 1$) is excellent. In fact what we have done is to perform a χ^2 fit for various orders of the truncation and then minimize with respect to the order. In each case the optimal order of the leading log turned out to be exactly N - 2, in perfect agreement with our results (up to N = 4) or with our conjecture (for N > 4).

Rewriting (12) as

$$P_B(s) = \alpha (q+1) s e^{(1-q) \log(1/s)} e^{-\alpha s^{q+1}}$$
(13)

we remark that the term $e^{(1-q)\log(1/s)}$ is exactly the summation to infinite order of the truncated expansion we introduced in our conjecture at the end of section 2. This would explain the success of the Brody distribution even though the behaviour for very small s of the real distribution is not a power law. In fact, except for a very small region which is expected to shrink exponentially (which is in agreement with our numerical results) the truncated series is well represented by its resummation to all orders, namely $e^{(1-q)\log(1/s)}$.





Thus the detailed numerical results we have obtained confirm the prediction of the authors of [13] for 3×3 matrices, and the one presented above for matrices of dimension 4. Moreover, they support the conjecture we formulated for matrices of higher dimensions. It would be interesting to try to prove this conjecture. However, this would necessitate a novel approach as the (brute force) method we used for 4×4 matrices is limited to matrices of small dimensions. If such an approach is found then it could also be used for the study of the spectra of matrices which are not tridiagonal but have only some vanishing elements. Another interesting problem would be study of the spectral statistics of banded matrices belonging to the other two Gaussian ensembles [14] of random matrices, namely unitary and symplectic.

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