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Logarithmic terms in the spectral statistics of band random matrices

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Abstract. We present a detailed analysis of the nearest-neighbour spacing distribution (NNSD) for random matrices on which the non-zero elements are confined to a band around the diagonal. The vanishing of the remaining elements induces non-analytic (logarithmic) behaviour for the NNSD at very small spacings. A conjecture for the precise behaviour of these logarithmic terms is presented and supported by extensive numerical computations.

1. Introduction

Random matrices are frequently introduced in the modelling of quantum systems, in particular whenever one is not interested in the precise spectrum but only in its statistical properties [1, 2]. Introduced initially in the context of nuclear physics [3], random matrices, as a statistical auxiliary, have found applications in the domain of atomic and molecular physics [4], in the description of spin systems [5], solid state physics [6] etc. A more recent extension of their applicability concerns the domain known as 'quantum chaos' [7], i.e. the particular properties of quantum systems the classical counterparts of which behave chaotically. Random matrices have met considerable success in all these domains and while it is clear that the matrix elements of physical Hamiltonians are not *precisely* random [8] the spectral statistics do not deviate substantially from random-matrix predictions.

Quantum chaos is a domain where the use of random matrices has been particularly successful [9]. The main argument here is that the quantal spectral statistics of classically *ergodic* Hamiltonians present a universal behaviour, i.e. they do not depend on the fine details of the system. Thus one can make predictions based on the known results of the theory of random matrices and, in fact, the predictions turn out to be quite accurate. The current literature abounds in examples materializing (for quantum systems) the various classes of level repulsion predicted by Dyson's theory [10]. This universality of the behaviour of ergodic systems is enhanced by the universality of random-matrix level statistics. In fact, as shown in [11], the statistics of level correlations do not depend on the particular ensemble used provided the probability distribution of the matrix elements is smooth. However, when one abandons ergodicity this nice universality disappears. The intermediate region where chaos is of limited extent (in the phase space) while integrability is not yet restored has been the object of numerous studies [12–14] but the question is far from being settled at this point.

Band matrices have recently been the focus of interest because they are well adapted to the description of the transition region from integrability to ergodicity [12, 15]. From a more physical point of view sparse matrices are often encountered in the description of spin systems with finite connectivity [16] or tight-binding models on a disordered lattice [17]. The interest of band random matrices lies in the fact that they mimic the semiclassical structure of the Hamiltonian operator [18]. Several recent works have examined the statistics of diagonal banded matrices which has led to the discovery of a scaling law. In [19] and [20], banded $N \times N$ matrices were considered, in which the non-zero elements are confined in a band of width k around the diagonal. As both works have shown, the only relevant parameter that describes the system when $N \to \infty$ is the ratio k^2/N. The two limits of $k^2/N \to 0$ and $k^2/N \to \infty$ lead to the well-known Poisson and GOE (Wigner-like) statistics for the spectrum. For the intermediate region, the results are not yet conclusive. Still, as far as the nearest-neighbour spacing distribution (NNSD) is concerned, the Brody distribution [21]

$$P_B(s;q) = (q+1)\alpha s^q e^{-\alpha s^{q+1}} \qquad \alpha = \left[\Gamma\left(\frac{q+2}{q+1}\right)\right]^{q+1} \tag{1.1}$$

gives a fair representation. One can obtain equally good results with Izrailev's form [22]

$$P_I(s;q) = A(\pi s/2)^q \exp[-\tfrac{1}{16}q\pi^2 s^2 - (B - \tfrac{1}{4}q\pi)s] \tag{1.2}$$

which is even more suitable than Brody's for $q > 1$, having a more realistic exponential part.

The aim of this paper is to investigate this intermediate region from a slightly different viewpoint. Instead of working with large matrices, fixing k^2/N and letting $N \to \infty$, we consider small matrices and study the appearance in the statistics of deviations from the simple GOE predictions when the size and sparseness of the matrix are varied. This approach has been the object of very few studies until today. In [23], Molinari and Sokolov have studied the NNSD for 3×3 GOE random matrices with the $(1,3)$ element set equal to zero. They have shown that the distribution $P(s)$ of the spacings behaves like $s \log(1/s)$ for $s \to 0$. We have presented the analysis for 4×4 matrices in [24] together with some exploratory numerical results. In this paper, we present a detailed numerical investigation of the problem which supports our conjecture on the behaviour of the logarithmic terms in the spectral statistics. Since we have been able to obtain these high-quality numerical results on GOE matrices, we have attempted a study of GUE band matrices (in particular, for the 3×3 case, where the distribution must behave as $s^2 \log(1/s)$). As we will see in the following sections, despite the s^2 factor, the logarithmic term is also well reproduced here.

2. NNSD for band matrices: conjectures and exact results

As already stated, the statistical probe we will use for the analysis of the spectrum of band random matrices is the distribution of spacings between nearest-neighbour levels. The reason for this choice is that the NNSD has been, over the years, the most intensely studied spectral statistical indicator, leading to a wealth of results. Moreover, since this statistical diagnostic requires only the gross features of the spectrum, it shows a universal behaviour, in the sense that it represents with sufficient accuracy the behaviour of systems of various origins. The study of other statistical indicators would also be interesting. However, a caveat is of order here: when one studies the full details of the spectrum, such as distant-level correlations, there is no *a priori* guarantee that the random-matrix results will closely represent the physical situation.

The random matrices we will consider here belong to the Gaussian ensemble. In the major part of the paper we will deal with the orthogonal ensemble (GOE), while in the last part some results from the unitary ensemble (GUE) will be presented as well. GOE matrices are real symmetric with their elements obtained through independent Gaussian distributions characterized by their common variance σ^2 for the diagonal elements, while the variance for the off-diagonal elements is $\sigma^2/2$. (GUE matrices are Hermitian instead of real symmetric.) The reason for the choice of Gaussian ensembles is essentially a question of tradition. The solvability of the Gaussian models has made them particularly popular over the years and, given the remarks of [11] on the universality of the statistical behaviour (i.e. insensitiveness on the precise nature of the ensemble used), they are perfectly suited to our purpose. The NNSD, subject to the constraints

$$\int_0^{+\infty} P(s)\,\mathrm{d}s = 1 \qquad \int_0^{+\infty} sP(s)\,\mathrm{d}s = 1$$

for 2×2 GOE random matrices, can be computed exactly and it is the well-known Wigner surmise

$$P(s) = \tfrac{1}{2}\pi s \mathrm{e}^{-\pi s^2/4}. \tag{2.1}$$

The important point here is that the level repulsion is *linear* at small spacings. This is indeed a generic feature for the GOE: the linear repulsion is present for any dimension of the random matrix, only the slope varies. In fact even this variation is small since for $N \to \infty$ the slope at the origin is $\frac{1}{6}\pi^2$ [25], less than 5% larger than Wigner's slope.

For 3×3 *band* random matrices, i.e. matrices with $a_{13} = 0$, the behaviour of the NNSD near the origin was shown to be of the form $P_3(s) \approx s \log(1/s)$. For 4×4 tridiagonal matrices the calculation has led to a distribution behaving as $P_4(s) \approx s \log^2(1/s)$. Since for 4×4 matrices there is more freedom as to the choice of the zero matrix elements, we have also examined [24] the behaviour of the NNSD when less than three matrix elements are set to zero. If $a_{14} = a_{24} = 0$ then the NNSD behaves as $s \log(1/s)$ at small spacings. When we have only $a_{14} = 0$ the NNSD has non-analytic behaviour of the form $s + \alpha s^2 \log(1/s)$: here the singularity manifests itself in the *second* derivative.

This is about all that exists concerning exact results. From here on, we will continue with the conjectures one can formulate based on these results and the mechanisms of their derivation. From the results on matrices of size 2, 3 and 4 we were led, in [24], to surmise that for $N \times N$ tridiagonal matrices the NNSD at small spacings will be of the form

$$P_N(s) \approx s \log^{N-2}(1/s). \tag{2.2}$$

The rationale behind this surmise was that for an $N \times N$ matrix we transform the probability measure for matrix $\mathbf{A}$ to $\mathrm{e}^{-(1/2\sigma^2)\mathrm{Tr}\,\mathbf{A}^2}\prod_{i<j}|\varepsilon_i - \varepsilon_j|\prod_i \mathrm{d}\varepsilon_i\,\mathrm{d}\Omega$ where ε_i are the N eigenvalues and Ω the $\frac{1}{2}N(N-1)$ angles of the orthogonal transformation that diagonalizes it. The fact that the matrix is tridiagonal is enforced by introducing in the integration one δ-function $\delta(\alpha_{ij})$ for each matrix element that vanishes, i.e. $\frac{1}{2}(N-2)(N-1)$ δ-functions in all. After integration over the δ-functions we are left with $N-1$ angles: $N-2$ of them lead, upon integration, to a power of the logarithm and the remaining one just gives an angular average. Thus the dominant behaviour of the NNSD is just (2.2) but subdominant terms do exist. Since for $N \to \infty$ the NNSD of a tridiagonal matrix should tend to a Poisson distributon, the logarithmic terms must resum in such a way as to compensate the s factor. This can be obtained naturally if, for $s \to 0$, $P(s)/s$ is not just $\log^{N-2}(1/s)$ but the

truncation, at order $N-2$, of the Taylor series of $e^{\lambda x}$ (in terms of $x = \log(1/s)$) and where $\lambda \to 1$ as $N \to \infty$. Our analysis of small tridiagonal matrices does not allow us to have a more precise estimation of λ. Still, some meaning can be assigned to this parameter if we consider the resummation of $e^{\lambda \log(1/s)}$ to all orders with $\lambda \neq 1$.This results, in the spacing distribution, to a prefactor $s^{1-\lambda}$ which is reminiscent of Brody's or Izrailev's s^q factor. As we will see in the next section, such an approximation can be quite accurate except for very small spacings. In the same spirit, for large but finite N, $P_N(s)$ will be close to a Poisson distribution, except in a very small region around the origin.

3. Numerical results

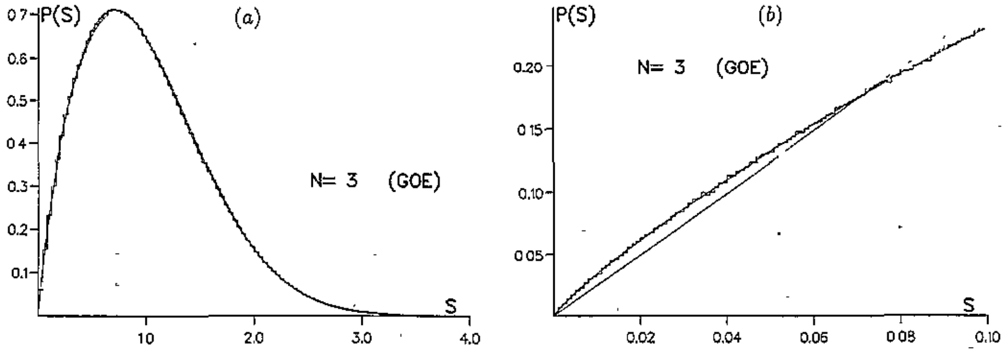
In [24] we have already presented results based on the diagonalization of a large number of random matrices (typically 10^6–10^7 levels were obtained there). This study has convincingly shown that departures from pure Wigner-like statistics for band random matrices exist. However, extracting the logarithmic terms was a much more ambitious enterprise necessitating the equivalent of 10^9–10^{10} levels. It was clear that unless every step of the computation were to be optimized the time needed might well be prohibitively long. The choice of Gaussian-distributed matrix elements is performed using the well known Box–Muller algorithm [26]. For the major part of our calculations we are dealing with tridiagonal symmetric matrices. Thus we can use specific diagonalization routines that are efficiently optimized. Since the statistical properties we are looking at are translation-invariant one can work with traceless random matrices. This means that, provided the variance and correlations of the diagonal elements are appropriately taken, one can eliminate one random variable.

One way to improve the statistics is to focus on the region of interest ($s \to 0$). This is precisely what we have done for small matrices, in particular for the 3×3 and 4×4 cases. First we locate (in the parameter space of the a_{ij}s) the hypersurface representing the condition of degeneracy. Discretizing the parameter space we can define a volume that contains this hypersurface and around which s is sufficiently small (but not *too* small so as not to introduce an undesirable bias). Having determined elementary (hyper)-cubes in this parameter space we choose the matrix elements randomly according to a Gaussian distribution. In order to do this we must invert an error function: a very efficient way to do this is to discretize the interval [0, 1] with a very fine step and to establish (once and for all) an inversion table. For larger matrices the whole procedure of locating the degeneracy hypersurface becomes so time-consuming that the direct approach of choosing the random matrix elements without *a priori* constraints becomes competitive (in terms of CPU time).

We come now to the results we have obtained numerically and we start with the 3×3 case. Figure 1(*a*) presents the global NNSD $P(s)$ as a function of s together with three fits corresponding to the Brody and Izrailev distributions and also to an ansatz of ours:

$$P(s) = AK\left(\frac{1}{1+\beta^2 s^2}\right) s e^{-\alpha^2 s^2} \qquad (3.1)$$

where K is the complete elliptic integral and β is a free parameter to be fixed by χ^2-fit. This ansatz is suggested by our results in [24] where the elliptic integral appears in the derivation of the banded 3×3 NNSD and gives rise to logarithmic behaviour. Here this ansatz is used as a convenient way to regularize the logarithmic term. As we remark from the figure, all three ansätze are in excellent agreement with the numerical results. Next we



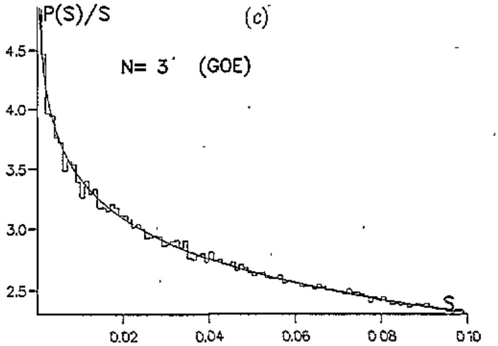
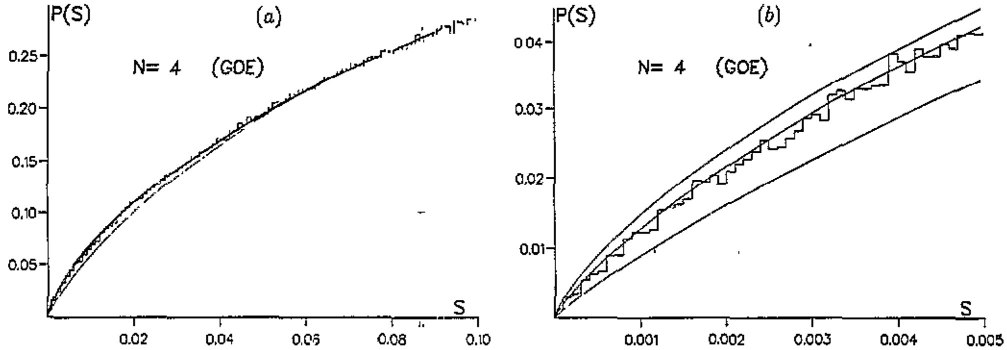


Figure 1. (a) NNSD for 3×3 band random GOE matrices together with the three empirical fits: Brody, Izrailev and 3.1 (lowest curve); (b) blow-up of the NNSD at small spacings together with a straight-line and a logarithmic fit; and (c) extraction of the logarithmic term from $P(s)/s$ together with the best-log fit.

blow up part of figure 1(a) for $0 \leqslant s \leqslant 0.1$ and present, in figure 1(b), the histogram for $P(s)$ together with a linear and logarithmic fit. The deviation from the linear behaviour is perfectly clear and this is made even more explicit in figure 1(c), where we plot $P(s)/s$: the histogram reproduces the behaviour of $\log(1/s)$ even down to the first bin!

In the case of 4×4 matrices we do not show the global NNSD: it suffices to say that its agreement with the Brody and Izrailev distributions is excellent. From our results in [24], we expect the behaviour of NNSD for small spacings to be quadratic in the logarithm. In order to verify this numerically we have proceeded as follows. First we choose a region near the origin (here $0 \leqslant s \leqslant 0.1$) and fit the numerical results with logarithmic terms (in fact, the truncation of the Taylor series of $e^{\lambda \log(1/s)}$) up to order n with $n = 1, 2, 3$ (figure 2(a)). Next we blow-up a region closer to the origin, $0 \leqslant s \leqslant 0.005$, and look closer to the results of the (fixed) fit. Clearly, $n = 2$ gives the best agreement, as expected. In figure 2(c) we present $P(s)/s$ and compare it with the predicted logarithmic dependence which, again, reproduces the numerical data in quite a satisfactory way.

For the 8×8 matrix case we show first the global NNSD (figure 3(a)). We remark that both the Brody and Izrailev distributions represent the numerical results fairly accurately. The fit of the logarithmic term has been performed in the same way as for the 4×4 case, starting from the region $0 \leqslant s \leqslant 0.02$ and going down to $0 \leqslant s \leqslant 0.0002$. We present only this final blow-up (figure 3(b)) where the five lower curves correspond to the truncation of the Taylor series of $e^{\lambda \log(1/s)}$ up to order n with $n = 4, 5, 6, 7, 8$. The agreement of the histogram with $n = 6$ is clear. The topmost curve in 3(b) represents $se^{\lambda \log(1/s)}$ without truncation, i.e. $s^{1-\lambda}$. We remark that even close to the origin this simple power fit is still a fair approximation. This is precisely one of the reasons why the Brody or Izrailev ansatz works well (see also [27]): except for a very small region around the origin the single-power ansatz is sufficient and, moreover, it improves with increasing N. One can think of



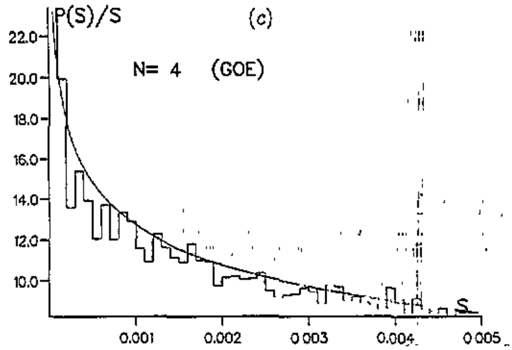


Figure 2. (*a*) Blow-up of the NNSD at small spacings together with logarithmic fits: expansions up to $n = 1, 2, 3$; (*b*) blow-up of the previous at very small spacings; and (*c*) extraction of the logarithmic term from $P(s)/s$ together with the best-log fit ($n = 2$).

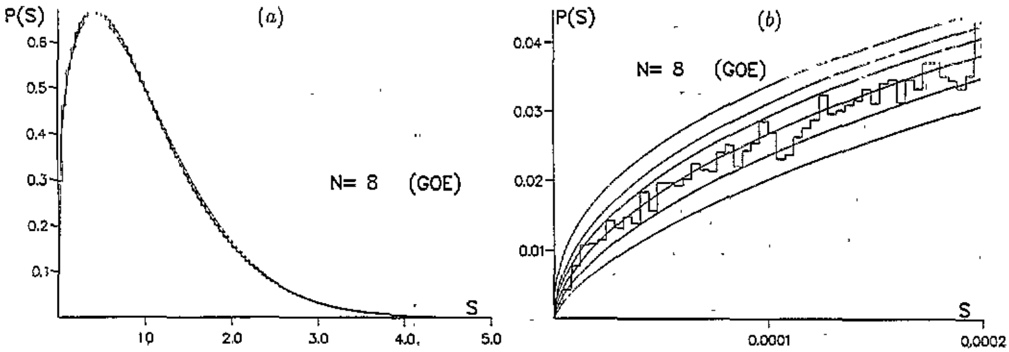


Figure 3. (*a*) NNSD for 8×8 band random GOE matrices together with the two empirical fits: Brody (upper curve) and Izrailev (lower curve); (*b*) blow-up of the NNSD at very small spacings together with logarithmic fits: expansions up to $n = 4, 5, 6, 7, 8$ and full resummation.

it as a particular 'naïve' regularization of the logarithmic terms that is suitable for global fits. As we have explained in the previous section, we do not have any *a priori* estimate of λ and its dependence on N. We can even wonder whether it does indeed tend to 1 as $N \to \infty$. In order to examine this we have studied the dependence of the parameter q from the Brody and Izrailev expressions in terms of N, since we expect λ and q to be related through $q = 1 - \lambda$. Fitting a Brody or Izrailev ansatz to the global distribution for matrices of various size (up to 32) we have found a relation $1/q \approx 0.430 + 0.285N$ that fairly approximates the data in the region $2 \leqslant N \leqslant 32$ while having the correct behaviour as $N = 2$ and $N \to \infty$. The values of λ in the same region are much more difficult to obtain numerically. Contrary to Brody's q, which can be assessed through a global fit, λ needs a detailed study of very small spacings. Moreover the truncated $e^{\lambda \log(1/s)}$ is not very sensitive to the precise value of λ over a range of values. Typically, the use of the value $\lambda = 1 - q$ leads to the same conclusions concerning the order of the truncation ($n = 2$ in figure 2(b) and $n = 6$ in figure 3(b)) as the individually optimized λ.

Finally, a much more stringent test of our calculations is presented by the study of GUE band random matrices. The analysis that led to a logarithmic dependence in the GOE case can be repeated along the same lines here leading to a behaviour of the NNSD at small spacings of the form $s^2 \log(1/s)$. Figure 4(a) gives the global histogram together with the Wigner-like ansatz $(32/\pi^2)s^2 e^{-4s^2/\pi}$ and a fit using Izrailev's form. A blow-up of the region near the origin (figure 4(b)) clearly shows the deviations from a pure s^2 dependence. They become even more explicit when one represents $P(s)/s^2$ as in figure 4(c) where the logarithmic term is apparent.

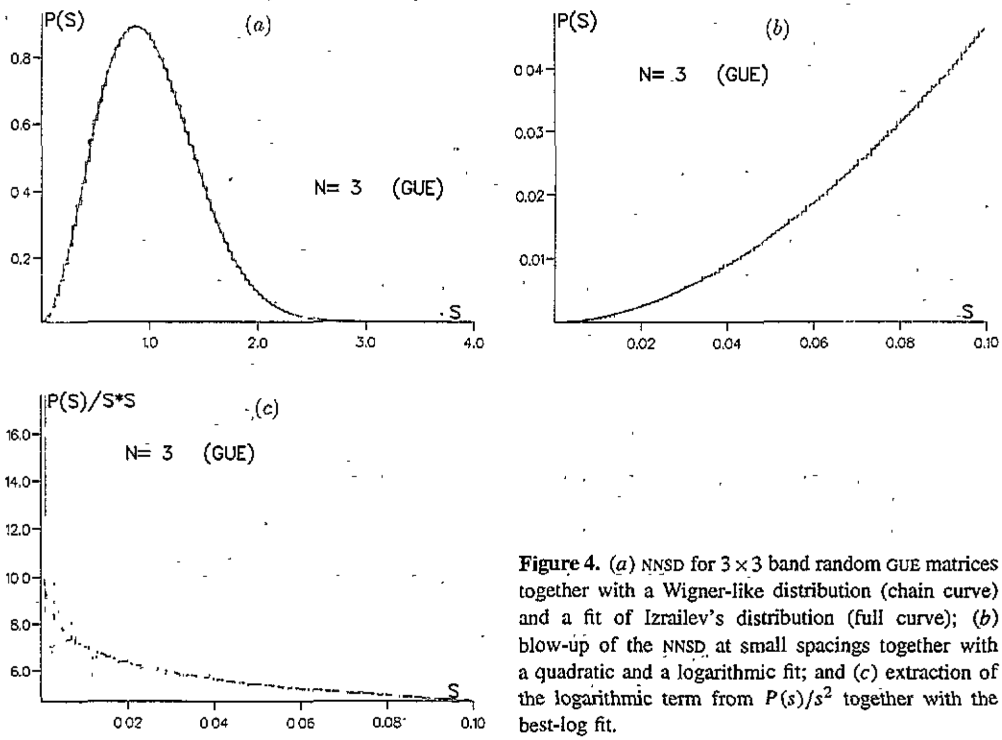


Figure 4. (a) NNSD for 3×3 band random GUE matrices together with a Wigner-like distribution (chain curve) and a fit of Izrailev's distribution (full curve); (b) blow-up of the NNSD at small spacings together with a quadratic and a logarithmic fit; and (c) extraction of the logarithmic term from $P(s)/s^2$ together with the best-log fit.

4. Conclusion

Random matrices have provided a most useful guide in the evaluation of the statistical properties of various physical systems and most recently in the domain of quantum chaos. Band matrices are of particular interest because they reproduce the structure of the (quantal) Hamiltonian operator and, as far as quantum chaos is concerned, they can model the mechanism of the transition from ergodicity to integrability [12, 28]. Our results have shown that this transition from a Wigner-like to a Poisson NNSD is mediated by logarithmic terms. These logarithmic terms, when adequately resummed, may lead to a power s^q behaviour of the NNSD at small spacings, akin to the one encountered in Brody's or Izrailev's ansätze. This explains the success of these two empirical distributions in the description of the transition region. Still, one must bear in mind that neither of these distributions is entirely satisfactory: Brody's expression is definitely inadequate for $q > 1$, while Izrailev's is plagued by a Gaussian fast-decreasing factor that can never (apart from the pure Poisson limit) be made to disappear.

Several problems remain open in the domain of band random matrices. Our surmise (2.2) concerning matrices of size larger than 4 is still a conjecture. Moreover, our results on 4×4 matrices suggest a whole line of research on sparse matrices where the zeros do not occupy lines parallel to the diagonal but can occur in any position, perhaps in a random distribution. One should thus study the spectral properties of such matrices for given distributions of the matrix sparseness [16]. The scaling law discovered in [18] and [19] cannot find a simple interpretation in the framework of our approach and a more refined analysis is needed in this case. Clearly random matrices are with us to stay.

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