Percolation in a Class of Band Structured Random Matrices

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We define a class of random matrix ensembles that pertain to random looped polymers. Such random looped polymers are a possible model for bio-polymers such as chromatin in the cell nucleus. It is shown that the distribution of the largest eigenvalue $\lambda_{\max}$ depends on a percolation transition in the entries of the random matrices. Below the percolation threshold the distribution is multi-peaked and changes above the threshold to the Tracy-Widom distribution. We also show that the distribution of the eigenvalues is neither of the Wigner form nor gaussian.

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Statistical properties of complex systems can be described by random matrix ensembles [1]. Most of the work has been concentrated on describing physical systems where the resulting random matrix elements all are independent and identically distributed (iid) or ensembles of matrices where the probability distribution is invariant with respect to orthogonal or unitary transformations. These two possible generalizations of the gaussian unitary (orthogonal) ensemble represent different dependencies of the entries. While the first possibility has arbitrarily distributed entries, the second imposes strong statistical dependence over long distances resulting in different properties of the eigenvalue spectrum [2, 3]. Common to the random matrix ensembles based on the first possibility is the Wigner semicircle [2] distribution for the eigenvalue spectrum and the Tracy-Widom distribution [4] for the largest eigenvalue, even in the case of a band structured matrix [5].

For biological systems it turns out that random matrices are needed where all of the matrix elements are iid except for the main diagonal and first off-diagonal [6], to describe, for example the conformations and three-dimensional organization of chromatin in the cell. In some case it is necessary to eliminate some matrix elements resulting in a band structured random matrix. Band structure random matrices have also been considered for discretized models of solid state physics [7]. Thus, while most entries are independent, the diagonal introduces correlations. It is thus natural to suspect that the resulting eigenvalue spectrum may not belong to either of the two universality classes.

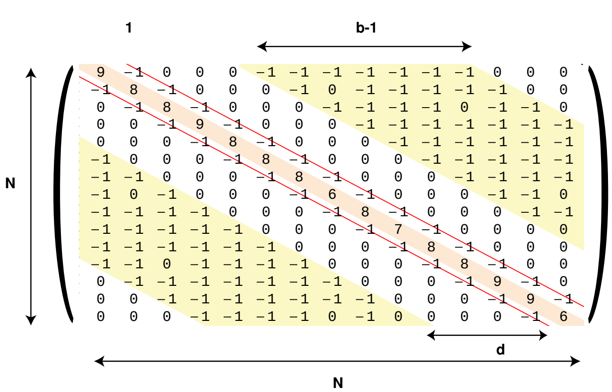

FIG. 1: Shown is the construction and a sample of the random matrices

In this work we define an ensemble of band structured random matrices whose matrix elements can take on two possible values with the main diagonal matrix elements as dependent random variables. We are interested in the resulting eigenvalue spectrum and the distribution of the largest eigenvalue in terms of a percolation transition.

Let b denote the bandwidth of a $N \times N$ matrix with a displacement d from the main diagonal ($N \geq b > 1$) with matrix elements (see Figure 1)

$$H_N(i,j) = N^{-a} h(i,j), \tag{1}$$

where

$$H_N(i,j) = 0 \quad \text{for} \quad \begin{cases} |i-j-d| > b \\ |i-j| < d, i \neq j, j \neq i-1, i+1 \end{cases} \tag{2}$$

and, within the band, we have Bernoulli variables

$$\begin{array}{ll} h(i,j) = -1 & \text{with probability } p \in [0,1] \\ h(i,j) = 0 & \text{with probability } 1-p \end{array} \tag{3}$$

with the additional constraints

$$\begin{array}{ll} h(i-1,i) = h(i,i+1) = -1, & 2 \leq i \leq N-1 \\ h(i,i) = \sum_{|i-j-d| \leq b} |h(i,j)|. & \end{array} \tag{4}$$

N^{-a} is a norming factor for the eigenvalues. Thus the matrices that we consider are real symmetric band structured random matrices. The band consists of random variables that take on the values $-1, 0$ and the band may have been shifted. The main diagonal is the sum of the

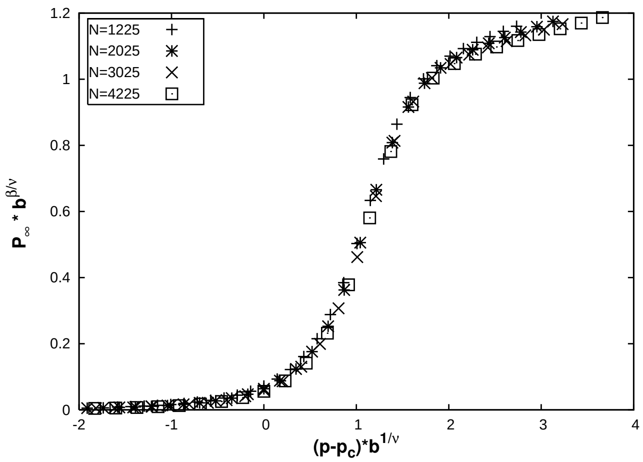

FIG. 2: Finite-size scaling of the percolation probability for the ratio of matrix size N and band width b of $b^2/N = 1$. The exact values of the critical exponents for the two-dimensional site percolation were used. The non-universal value for p_c was determined to be 0.61. Other ratios $b^2/N =$ const also produced good scaling. The data presented in the figure were obtained by averaging over at least 10000 random matrix configurations for each p and matrix size and band width combinations.

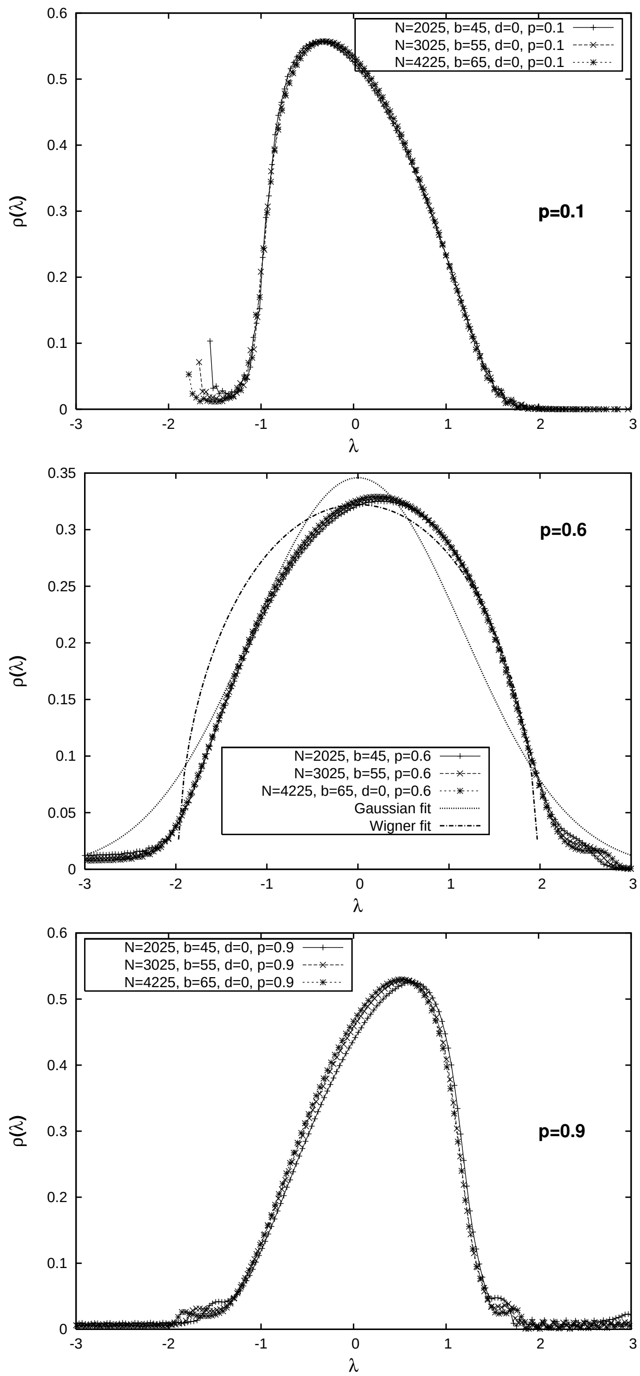

FIG. 3: Shown is the distribution of the eigenvalues. Note that we have shifted the distributions by their mean values. Indicated is also the Wigner distribution and a fit by a Gaussian.

off-diagonal random values with the exception of the first off-diagonal which is never shifted and has always values -1. Thus the matrix is diagonally dominant.

This structure mimics a polymer chain, where the first off-diagonal ensures the integrity of the chain, the diagonal gives the coupling strength and the other off-diagonal elements mimic random loops. Note that the regular polymer case of $b = 1, d = 0$ with gaussian random variables has been solved by Dyson [8].

Before we analyze the eigenvalue spectrum of the above defined random matrix ensemble, we look at the structural properties of the random matrix. Since the elements of the band are variables which can be with -1 or 0 it is tempting to suspect that the geometric distribution of these has an influence on the eigenvalues. If we view the random matrix with the entries -1 or 0 as an adjacency matrix representing an undirected graph (considering only the upper triangular matrix, neglecting the diagonal and the first off-diagonal), then the graph may be a set of unconnected subgraphs or may have a percolation structure. If the graph includes a percolating graph then this introduces a divergent length scale as $N \to \infty$ possibly influencing the eigenvalues through the correlations introduced into the main diagonal.

We define percolation in terms of a site percolation problem with free boundaries except for the left edge entries which are always fixed to -1 (see above). Here, the site percolation probability P_∞ is defined by the mass of the largest cluster divided by the size of the band. Due to the symmetry, we only consider the upper triangular matrix (band). Two matrix elements having both a value of -1 belong to the same cluster if their indices differ at most by 1, i.e., are nearest neighbors in the sense of a simple square lattice [11].

To analyze percolation in the upper band, we use a finite-size scaling ansatz

$$P_\infty = b^{-\beta/\nu}\mathcal{P}((p-p_c)b^{1/\nu}). \quad (5)$$

The finite size scaling of the percolation probability (order parameter) [9, 10] for this staircased slab with aspect ratio $b^2/N = 1$ is shown in Figure 2. The critical value for the percolation threshold p_c for the simple square lattice is $p_c = 0.592746$ [11] and the exact values for the critical exponents are $\alpha = -2/3, \beta = 5/36, \nu = 4/3$ [12]. Assuming universality we use these values for the critical exponents and find a value $p_c = 0.61$ for the percolation threshold that gives the best fit to a scaling function $\mathcal{P}$. Of course, we don't expect p_c to be a universal quantity. Beside possible corrections to the finite-size scaling, the percolation problem posed by the staircased slab geometry is seen to be in the same universality class as the two-dimensional site percolation.

Thus, at p_c we have a correlation length which is diverging as the linear dimension of the matrix goes to infinity. It should be noted that if $b \ll N$, then many percolating clusters in the b direction can occur [13]. In the geometry considered here only one percolating cluster exists [14]. In the following we explore the consequences of this on the eigenvalue spectrum and in particular on the distribution of the largest eigenvalue.

Before we turn our attention on the distribution of the largest eigenvalue, we examine briefly the distribution of the eigenvalues themselves. As suggested by the above percolation analysis we expect the geometric percolation to influence the eigenvalue distribution. The distribution is shown in Figure 3 for three values of p. The data shown in the figures were obtained by averaging over 10000 Monte Carlo samples. Beside the matrix sizes shown, data were also produced for matrices ranging from $N = 196$ up to $N = 4225$ for $b^2/N = 1, 5, 10$ and $d = 0, 10$.

First we note that for different combinations of N and b at fixed ratio $b^2/N = 1$ the data scales, in agreement with other band random matrix ensembles [5]. As a function of p the distribution undergoes a shape transition. The sign of the asymmetry changes and the distribution is nearly symmetric close to the percolation threshold. There we also compare the distribution to the Wigner distribution and to a Gaussian. Neither fits the distribution. Note that for the gaussian unitary ensemble a rapid change has been observed [5, 18], as one increases the band width, from a gaussian to a semicircle distribution.

Let $\lambda_{\max}(H_N)$ denote the largest eigenvalue of the random matrix H_N and

$$F_{N,b,d,p}(\lambda) := P_{N,b,d,p}(\lambda < \lambda_{\max}) \quad (6)$$

the corresponding distribution function. For the non-banded ensembles GUE and GOE, the distribution function is the Tracy-Widom distribution [4]. This distribution is expected to hold for an even broader class of random matrices and the precise characterization of the class is now being investigated [15, 16]. Known is that for symmetric matrices with iid entries of variance $1/N$, such that all moments are finite, the Tracy-Widom distribution holds asymptotically. If the entries decay with a power law then it is expected that the matrices belong to a different universality class [17].

To discover the phase transition in the behavior of the largest eigenvalue we calculate the cumulant of the distribution of the largest eigenvalue and analyze the flow of the cumulant as a function of the matrix size at fixed ratio $b^2/N = 1$ and the probability p with which the matrix elements are set. We define the fourth order cumulant as

$$u(N,p) \sim 1 - \langle\lambda^4\rangle/(3\langle\lambda^2\rangle^2). \quad (7)$$

For a second-order phase transition the cumulant flows to three fix points [10]. Two fix points characterize the values of p below and above p_c and one characterizes the value of p_c.

In Figure 4 is shown the fourth-order cumulant for the distribution of the largest eigenvalue as well as examples of the distribution above and below p_c. While the distribution of the largest eigenvalue below p_c shows multiple peaks, above p_c these are reduced to a single peak. This change is also seen in the flow of the cumulant. For values p well above the percolation transition point p_c the cumulant is almost constant and nearly zero. Below the percolation transition point the cumulant slightly fluctuates in a narrow band. Close to the transition point the flow changes strongly indicating the transition.

In Figure 4 is also shown a fit of the Tracy-Widom distribution to the data above p_c at 0.9. The fit is very good indicating that in this ensemble above p_c the Tracy-Widom result holds. So far, for symmetric $N \times N$ matrices with iid entries of variance $1/N$, the Tracy-Widom distribution has been shown to hold [15], while if the entries fall off with a power law, the matrices fall in a in different universality class [19]. Thus it is quite surprising that for the class of random matrices defined here we do get a Tracy-Widom distribution.

The geometric structure of a random matrix determines the eigenvalues of a matrix to a large extend. In this paper we have introduced a class of band structure random matrices that pertain to the description of polymers and may be capable to describe the observed three-dimensional organization of chromatin. Due to the Bernoulli type of its off-diagonal matrix elements we are able to define a percolation problem and link the change in the eigenvalues to the occurrence of a percolation transition. The change is most noticeable in the density distribution of the largest eigenvalue. The multiple peak distribution gives way to a single peak at the percolation transition. But also the eigenvalue density shows a change in skew at the transition point. Unclear is yet the type of distribution for the eigenvalues as well as for the largest eigenvalue below the transition.

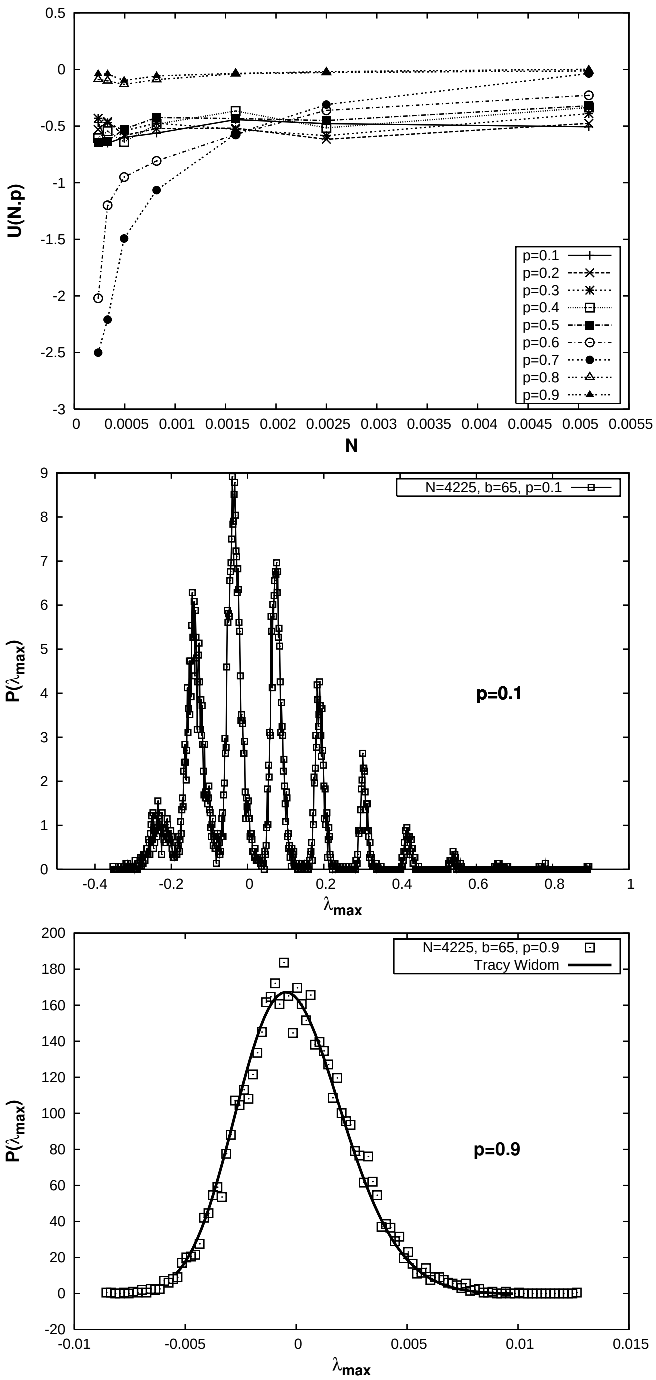

FIG. 4: Shown is the cumulant for the probability distribution of the largest eigenvalue. The figure shows the cumulant $u_{N,p} = 1 - \langle(\lambda - \langle\lambda\rangle)^4\rangle / \langle(\lambda - \langle\lambda\rangle)^2\rangle^2$ keeping the ratio b^2/N fixed to 1. Above the percolation transition at p_c (roughly at 0.61) the flow changes and for higher values of p is almost constant and zero. For values below p_c the cumulant is fluctuating in a narrow band for the matrix sizes considered in this work. Also shown is the distribution at $p = 0.1$ and at $p = 0.9$. While below p_c the distribution is multi-peaked we find a transition to a Tracy-Widom distribution above p_c.

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