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1992 Europhys. Lett. 17 97

(http://iopscience.iop.org/0295-5075/17/2/002)

EUROPHYSICS LETTERS 7 January 1992

Europhys. Lett., 17 (2), pp. 97-102 (1992) *published in November 1991*

Density of States for Banded and Sparse Random Matrices.

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(received 19 July 1991; accepted 3 October 1991)

PACS. 03.65S – Semiclassical theories and applications.
PACS. 71.20A – Developments in mathematical and computational techniques.

Abstract. – The average density of states for a large class of $N \times N$ banded and sparse random matrices is shown to obey a semi-circle law. The banded matrices belonging to this class are restricted in several ways: 1) they are both real and symmetric, 2) matrix elements are independent random variables with zero average, 3) the variance of the matrix elements, σ_{ij}^2, decays monotonically away from the diagonal, 4) σ_{ij} depends on $|i-j|$ alone and the range over which it significantly varies, δy, satisfies $1 \ll \delta y \ll N$. On the other hand, the sparse matrices for which this results, are obtained by permuting the variance in each of the rows of the banded matrices.

In a multitude of physical situations the microscopic many-body interactions are extremely complex and quite often, only partially known. Accordingly, it is useful to search for properties of such systems which do not depend on the detailed structure of the corresponding Hamiltonian. Following a similar approach to that of statistical mechanics, it has been suggested that the Hamiltonian matrix can be modelled by an ensemble of matrices with random elements [1]. In fact, such models represent a further step of simplification over statistical mechanics as for the latter, the Hamiltonian is precisely known and only the initial conditions are left unspecified. In conceiving the appropriate random matrix model for a particular physical problem one has to compromise between two contradicting requirements. While it is desirable to maintain part of the symmetry and structure of the original problem, the resulting ensemble should be, as much as possible, tractable by analytical tools.

While models of this type have been employed in various fields, in both nuclear [2] and solid-state [3] physics they play an important role. In nuclear physics, the attention was focused on the statistical properties of spectra which therefore lead to ensembles invariant under a change of representation. Only information on symmetry with respect to time-reversal of the original problem appears in the corresponding random matrix model. For example, systems invariant under time-reversal are represented by an ensemble of $N \times N$ real, symmetric matrices. Their elements are independent, normally distributed random variables with zero average and variance σ^2, except for the diagonal where the variance is $2\sigma^2$. This model is known as the Gaussian orthogonal ensemble (GOE). On the other hand, in

tight-binding models for single electrons in disordered lattices, the principal question is directed to the structure of the eigenvectors in the Wannier functions representation. Accordingly, the corresponding random matrix model has significantly more structure than the GOE and only part of the off-diagonal elements, the hopping probabilities, are finite. In particular, for a one-dimensional problem with only nearest-neighbour hopping, the ensemble is composed of tridiagonal matrices. For general types of hopping, one has instead ensembles of banded matrices. These are characterised by off-diagonal matrix elements, h_{ij}, which decay as a function of $|i-j|$ over an interval smaller than the matrix size, N. Translational invariance together with the fact that matrices are symmetric imply that the h_{ij}'s are a function of $|i-j|$ alone.

One of the first properties of random matrices to be studied in details was the average density of states, $\rho(E)$. For the GOE, Wigner [4] has shown that, in the limit of $N \to \infty$, $\rho(E)$ is given by the semi-circle law. Using the notation $\rho(E) = (\sqrt{N/2\sigma^2}) f(E/\sqrt{2N\sigma^2})$, Wigner's result takes the form

$$f(x) = \begin{cases} \frac{1}{\pi}(2-x^2)^{1/2}, & \text{for } x^2 \leqslant 2 \\ 0, & \text{for } x^2 > 2. \end{cases} \tag{1}$$

The purpose of this paper is to show that this result can be extended to a large class of banded and sparse random matrices. In particular, an ensemble with independent, random matrix elements with distribution functions, $P_{ij}(h)$, is considered [5], such that $\langle h_{ij} \rangle = 0$ and $\mathrm{Var}(h_{ij}) = \sigma(y)^2$, where $\langle \ldots \rangle$ stands for the ensemble average, Var denotes the variance and $y \equiv |i-j|$. Assuming that $\sigma(y)$ is monotonically decreasing and that the range over which it significantly varies, δy, satisfies, $1 \ll \delta y \ll N$, it will be shown that $\rho(E) = (N/\sqrt{2I})\, g(E/\sqrt{2I})$, where $I \equiv \int_0^\infty \sigma(y)^2 \mathrm{d}y$ and [1]

$$g(\tilde{x}) = \begin{cases} \frac{1}{2\pi}(4-\tilde{x}^2)^{1/2}, & \text{for } \tilde{x}^2 \leqslant 4 \\ 0, & \text{for } \tilde{x}^2 > 4. \end{cases} \tag{2}$$

The importance of eq. (2) is greatly enhanced by its being invariant under arbitrary permutations of the matrix elements in each row, as long as the new positions of the $P_{ij}(h)$'s are fixed for an individual ensemble. Such permutations transform a banded random matrix into a sparse one of quite general form.

For a start, eq. (2) will be derived along the same lines as in ref. [4] for the banded case with $\sigma(y) = 1$ for $y < b$ and vanishing otherwise [6]. Notice that here, $I = b$. In order to obtain the density of states, one calculates the moments of $\rho(E)$, M_n,

$$M_n \equiv \int_{-\infty}^{\infty} E^n \rho(E)\, \mathrm{d}E = \left\langle \sum_{i=1}^{N} \lambda_i^n \right\rangle = \langle \mathrm{Tr}\, H^n \rangle . \tag{3}$$

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(1) Since $\delta y \gg 1$, the variable y is interchangeably allowed to be either discrete or continuous. Corrections due to this approximation are of lower order in δy than the leading term and are accordingly neglected. It should be stressed, however, that in fact I is the sum of the variances and the integral form is merely a useful approximation. Notice that the exact I is invariant under permutations of the matrix elements in individual rows. This suggests that the densities of states for the permuted ensembles and the unpermuted ones are exactly equivalent rather than only to lowest order in δy. I have not yet managed to prove this conjecture.

Therefore, this becomes a combinatorial problem of counting sequences of n steps in index space $(i_1, i_2, i_3, \ldots, i_n)$, such that

$$\langle \mathrm{Tr} H^n \rangle = \sum_{i_1, i_2, \ldots, i_n} \langle h_{i_1 i_2} h_{i_2 i_3} \ldots h_{i_n i_1} \rangle . \tag{4}$$

If a particular matrix element appears only once in eq. (4), the corresponding term vanishes due to ensemble averaging. Accordingly, $M_n = 0$ for odd n. For even moments, $n = 2\nu$, a sequence of steps gives a finite contribution only if each step, counted together with its inverse, appears an even number of times. The largest contribution comes from sequences in which all steps appear in groups of exactly two. It is $t_\nu N(2b)^\nu$, where t_ν is the number of ways in which indices in a sequence of n steps can be paired. If instead a group of four indices are paired up together, then there will be two less indices which are free to take any one of the $2b-1$ allowed values. The corresponding contribution will only be $O(N(2b)^{\nu-2})$. On the other hand, since the sequence $(i_1, i_2, \ldots, i_{\nu-1}, i_\nu, i_{\nu-1}, \ldots, i_2, i_1)$ is of leading order, $t_\nu \geq 1$.

In order to calculate t_ν, one defines the number of unpaired steps up to (and including) the i-th step, q_i. Clearly, $q_1 = 1$, $q_n = 0$ and t_ν is given by the number of different q-sequences. Moreover, $t_{\nu-1}$ is equal to the number of q-sequences of length n such that $q_i > 0$ for all $i < n$, t'_ν. In order to obtain this equality, one should delete q_1 and q_n from the latter sequences and replace all the remaining q_i's with $q_i - 1$. In general, sequences of length n can be classified according to the position of the first vanishing q_i, l. Thus, summing over all possible values of l

$$t_\nu = \sum_{l=1}^{\nu} t'_l t_{\nu-l} = \sum_{l=1}^{\nu} t_{l-1} t_{\nu-l} . \tag{5}$$

Notice that if $\nu = 0$, eq. (5) fails and instead, $t_0 = 1$. Since the generating function, $t(x) \equiv \sum_{\nu=0}^{\infty} t_\nu x^\nu$, satisfies

$$t(x) = 1 + x t(x)^2 , \tag{6}$$

one obtains

$$t_\nu = \frac{(2\nu)!}{\nu!(\nu+1)!} . \tag{7}$$

In the notation of eq. (2)

$$\tilde{g}(k) \equiv \int_{-\infty}^{\infty} \exp[ik\tilde{x}]\, g(\tilde{x})\, \mathrm{d}\tilde{x} = \sum_{\nu=0}^{\infty} \frac{(-1)^\nu k^{2\nu}}{\nu!(\nu+1)!} = \frac{1}{k} J_1(2k) , \tag{8}$$

where J_1 is the Bessel function of order 1. Finally, using the relation

$$J_1(z) = \frac{z}{\pi} \int_{-1}^{1} \exp[iz\omega](1-\omega^2)^{1/2}\, \mathrm{d}\omega , \tag{9}$$

one obtains the result stated in eq. (2) for the case of a banded matrix with constant variance.

It is worthwhile to notice that this argument makes no use of the fact that all the finite matrix elements are located in a band around the diagonal. In particular, if a new ensemble is defined by arbitrarily changing the positions of the nonvanishing elements subject to the constraint that there are $2b-1$ in each row, its average density of states will be given by

eq. (2), as well. This is a consequence of the fact that neither the number of values that each index can take, $2b-1$, nor the number of ways in which indices can be paired, t_ν, depend on the actual locations of the elements in the row. While performing different permutations on each row does not affect the behaviour of M_n, it will in general lead to nonsymmetric matrices which, in turn, lie outside the scope of this work.

In the following, it will be shown that the foregoing argument can be generalized to yield eq. (2) also for the case of varying $\sigma(y)$. Consider an ensemble for which $\mathrm{Var}(h_{ij})$ is σ_1^2 when $|i-j|<b_1$, is σ_2^2 for $b_1 \leqslant |i-j|<b_2$ and vanishes otherwise. Moreover, it is assumed that $1 \ll b_1 \ll N$ and $1 \ll (b_1 - b_2) \ll N$. Here, the contributing sequences of indices can be mixed such that m pairs lie in the first strip (the σ_1-strip) and $\nu - m$ pairs in the second one. For each q-sequence, the pairing of indices is completely determined. However, one still has the freedom of choosing which pairs will lie in either strip. If there are m pairs in the first strip, the contribution from each individual q-sequence to $M_{2\nu}$([2]), C_m, is

$$C_m = N \frac{\nu!}{m!(\nu-m)!} (2b_1\sigma_1^2)^{\nu-m} [2(b_2-b_1)\sigma_2^2]^m . \tag{10}$$

Summing over all possible values of m, one obtains

$$\sum_{m=0}^{\nu} C_m = N[2b_1\sigma_1^2 + 2(b_2-b_1)\sigma_2^2]^\nu = N(2I)^\nu . \tag{11}$$

Since the number of q-sequences is the same as before, $\rho(E)$ is once more that of eq. (2). It is straightforward to further generalize eqs. (10) and (11) to the case of l strips of width, Δb_i, such that $\Delta b_i \gg 1$ for all i and also $b_l \ll N$. In this case, eq. (10) becomes the term of a multinomial expansion rather than a binomial one. For large l and if $\sigma_{i+1} \leqslant \sigma_i$, such a sequence of constant σ strips becomes an arbitrarily good approximation to a slowly varying continuous function, $\sigma(y)$.

As was already pointed out before, the actual ordering in the row of the matrix elements with particular value of σ does not affect the result of eq. (2). For example, one can reorder an l-strip matrix with $s = \Delta b_i = \Delta b_j$ for all i, j into a block matrix with $s \times s$ blocks. In this form, eq. (2) represents a generalization of a result by Wegner for an s-band d-dimensional tight-binding model with long-range hopping and $s \to \infty$ [7]. For $d=1$, Wegner's model takes the form of a matrix of $s \times s$ blocks such that the variance of the elements in each block is constant and depends only on the difference in the block indices with respect to the primary matrix. Block random matrices of this type were also used to study the spectral properties of Hamiltonian systems with mixed classical dynamics (chaotic and regular) [8].

The behaviour of the average density of states was checked numerically for both the banded case with constant variance (fig. 1) and for a Gaussian profile (fig. 2), $\sigma(y) = \exp[-y^2/2B^2]$. For $I=20$ and $N=400$, excellent agreement between numerical experiment and eq. (2) is found. At large energies, $|E|$, deviations from theory appear in the form of band tails and are due to violating the $\Delta b_i \gg 1$ assumption. Close to the centre of the band (small $|E|$), the value of the numerical maximum tends to be slightly higher than the theoretical prediction. In the case of fig. 2, this is a consequence of $\sigma(y)$ varying too fast. Violating the $b_l \ll N$ assumption leads to the same sort of effect.

In summary, it was shown that the average density of states obeys the semi-circle law for a large class of structured random matrices. It seems that using similar methods, one could

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([2]) One has to count the number of ways in which the m pairs can be chosen out of the total of ν pairs.

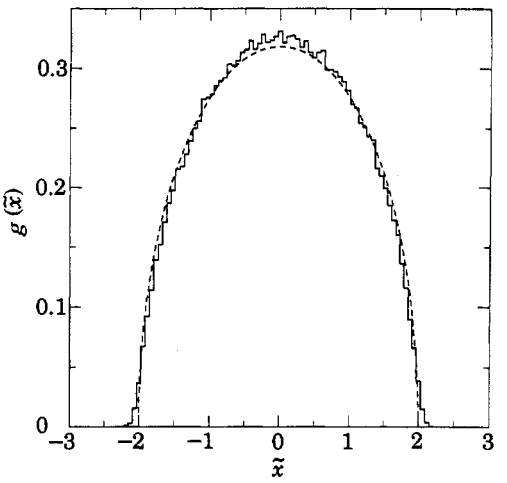

Fig. 1.

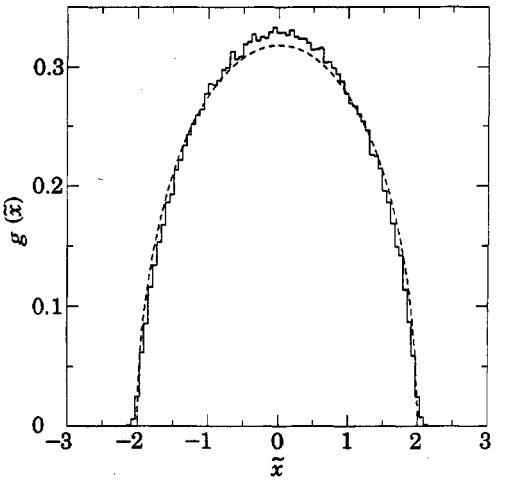

Fig. 2.

Fig. 1. – The form of $g(\tilde{x})$ as obtained from numerically averaging over 250 matrices of size $N = 400$ with $\sigma(y) = 1$ for $y < 20$ and vanishing otherwise (histogram) is compared with the prediction of eq. (2) (dashed).

Fig. 2. – Same as in fig. 1 only that here $\sigma(y)$ is a Gaussian with $I = 20$ and $\sigma(0) = 1$.

approach both the case of small b and that of $\langle h_{ij} \rangle \neq 0$ which are in turn interesting in the context of more realistic tight-binding models.

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The author is grateful to R. GRANEK for many discussions and to M. WILKINSON for both reading the manuscript and many important suggestions. After the completion of this work we were informed that Casati *et al.* have independently obtained numerical evidence for eq. (2) in the case of constant $\sigma(y)$ [9]. Moreover, using methods different than ours, eq. (2) was independently derived by both Kus *et al.* [10] and Casati and Girko [11].

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