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Random non-Hermitian tight-binding models

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Abstract. For a one dimensional system tight binding models are described by sparse tridiagonal matrices which describe interactions between nearest neighbors. In this report, we construct open and closed random tight-binding models based in the tridiagonal matrices of the so-called β-ensembles of random matrix theory.

1. Introduction

Tigh-binding models appear in many applications in condensed matter physics [1, 2, 3]. For one dimensional system, they are described by tridiagonal matrices in which diagonal elements represent the sites while the off-diagonal elements describe the interactions between nearest neighbors of relevance to the problem at hand [4]. In the early 2000s and in another context, tridiagonal matrix models were used to provide an extension of certain classical cases of random matrix theory, which became known as the β-ensembles [3, 5, 6]. This ensemble became the basis of recent efforts to provide models which verify the pseudo-Hermitian condition [7], satisfied by PT-symmetric systems [8]. In the present work, we show that the pseudo-Hermitian β-ensemble also constitutes a basis of a random non-Hermitian tight-binding model.

A matrix H is pseudo-Hermitian if it is connected to its adjoint $H^\dagger$ by the relation

$$H^\dagger = \eta H \eta^{-1}, \tag{1}$$

which means that it shares with its adjoint the same set of eigenvalues [7]. As a consequence, eigenvalues of a pseudo-Hermitian are necessarily real or complex conjugate. In particular, real matrices are pseudo-Hermitian and a matrix η, in this case, must exist. On the other hand, if the matrix $\eta^{1/2}$ such that $\eta^{1/2}\eta^{1/2} = \eta$ and its inverse exist, and are Hermitian, then the matrix

$$K = \eta^{1/2} H \eta^{-1/2} = \eta^{-1/2} \eta H \eta^{-1} \eta^{1/2} = K^\dagger \tag{2}$$

is Hermitian and shares with H the same set of eigenvalues. In this case, all the eigenvalues of H are real.

Eqs. (1) and (2) shows that a non-Hermitian matrix can have the same eigenvalues of a Hermitian one. Considering in the opposite direction, Eq. (1) can be used to construct a pseudo-Hermitian matrix out of a Hermitian one. The procedure is simple in the case of tridiagonal matrices aa shown in Ref. [9] where a pseudo-Hermitian β-ensemble was constructed. That procedure is here extended by constructing a family of matrices isospectral to the matrices of

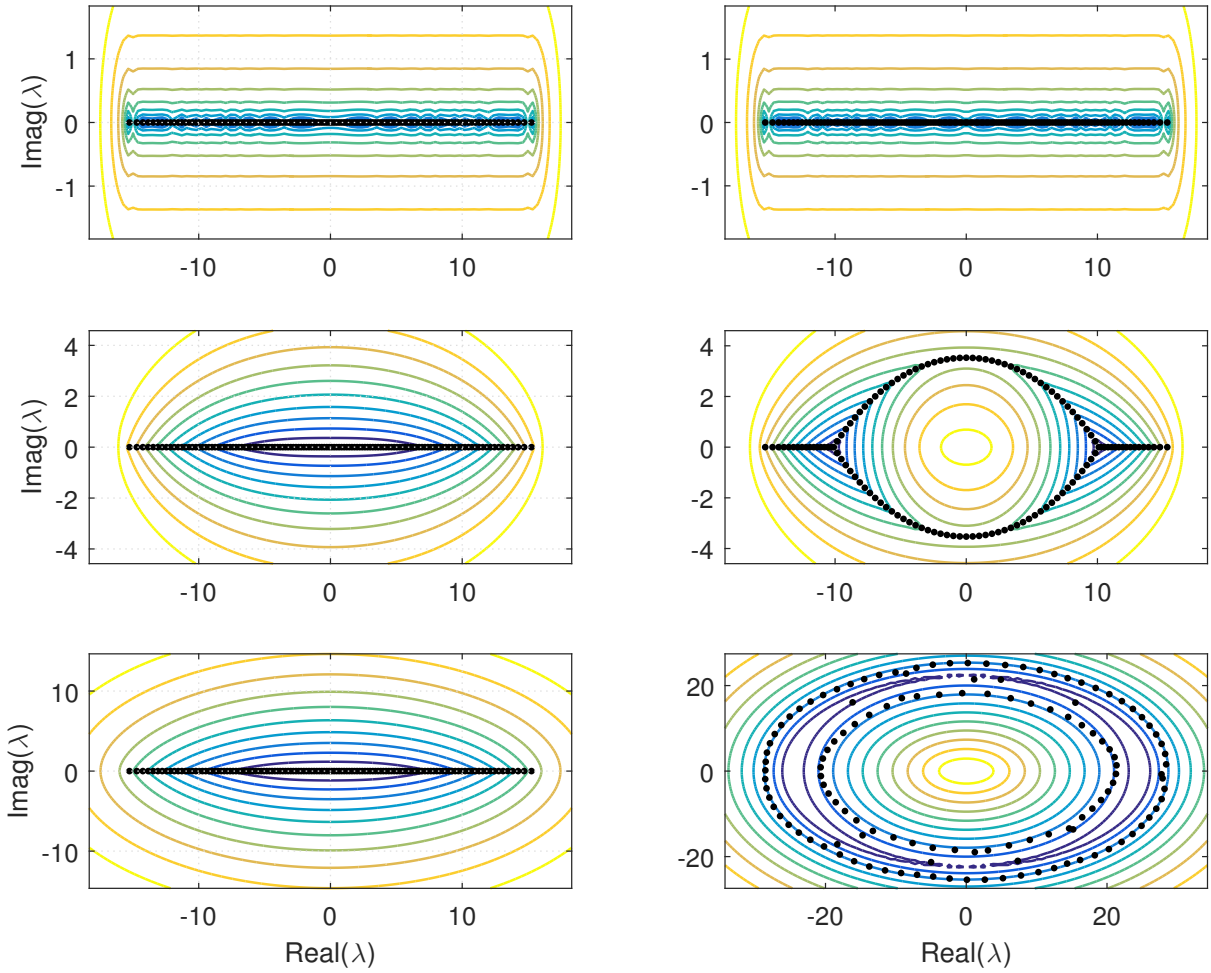

Figure 1. Pseudospectra for the average open chains (left) and closed chains (right) of size $N = 128$ and $\beta = 1$ with $\alpha = 0.0, 0.25, 1.00$ from top to bottom.

the β-ensemble. This family defines an open chain with random hopping in a consistent way the chain is closed and defines a random tight-binding model.

2. The model

Let us start by considering the real matrix

$$H(\alpha) = \begin{pmatrix} a_1 & d_1^{1+\alpha} & & & & d_N^{1-\alpha} \\ d_1^{1-\alpha} & a_2 & d_2^{\alpha+1} & & & \\ & \ddots & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & & & \ddots & \ddots & \ddots \\ & & & d_{N-2}^{1-\alpha} & a_{N-1} & d_{N-1}^{1+\alpha} \\ d_N^{1+\alpha} & & & & d_{N-1}^{1-\alpha} & a_N \end{pmatrix} \tag{3}$$

where α is a real parameter greater or equal to zero. With the presence of elements at the corners the matrix describe a closed chain and, open one, if $d_N = 0$.

2.1. The Open Chain

Starting with the open case, if $\alpha > 0$, the matrix $H(\alpha)$ is non-Hermitian but its eigenvalues are real having the same values of the Hermitian matrix $H(\alpha = 0)$. In other words, the eigenvalues are not affected by the parameter α. This can be proved by constructing the diagonal matrix [10]

$$\eta(\alpha) = \text{diag}\left(1, d_1^{2\alpha}, d_1^{2\alpha} d_2^{2\alpha}, \ldots, \prod_{k=1}^{N-1} d_i^{2\alpha}\right) \tag{4}$$

which possesses a square root $\eta^{1/2}$ such that we can write

$$H(\alpha) = \eta(\alpha)^{1/2} H(0) \eta(\alpha)^{-1/2}. \tag{5}$$

As $H(0)$ is Hermitian $H(\alpha)$ contitutes an isospectral family of matrices. Another way of proving the isospectrality is by considering the recursion relation

$$P_n(x) = [a_n - x]\, P_{n-1}(x) - d_{n-1}^2 P_{n-2}(x) \tag{6}$$

satisfied by its characteristic polynomial in which the parameter α just does not appear.

If now the diagonal elements are taken from the normal distribution $N(0,1)$ and the off-diagonal ones from the χ_ν distribution with $\nu = \beta k$ degrees of freedom, for the k-th row, such that

$$a_k = \{X \quad | \quad f(X) = N(0,1), k = 1, ..., N\} \tag{7}$$

$$d_k = \left\{ \frac{X}{\sqrt{2}} \quad \middle| \quad f(X) = \chi_{\beta k}, k = 1, ..., N-1 \right\} \tag{8}$$

$$d_N = \begin{cases} 0, & \text{open chain} \\ \left\{ \frac{X}{\sqrt{2}} \quad \middle| \quad f(X) = \chi_{\beta N} \right\}, & \text{closed chain} \end{cases} \tag{9}$$

then $H(0)$ is a matrix of the so-called β ensemble whose the joint density distribution of the eigenvalues generalizes the RMT eigenvalues from $\beta = 1, 2, 4$ to any real positive value [6]. For a fixed matrix size and sufficiently small values of β the diagonal is dominant and the eigenvalues become uncorrelated. In the other extreme, that is large values of β the subdiagonal elements dominate and become localized such that fluctuations are suppressed.

It also becomes convenient to define an average matrix for this ensemble

$$\langle H(\alpha) \rangle = \eta(\alpha)^{1/2} \langle H(0) \rangle \eta(\alpha)^{-1/2} \tag{10}$$

That may be accomplished by averaging each element independently in (7)-(9), to the mean of the respective distribution. Numerical evidence shows that the spectral behavior of sample matrices displays relatively small fluctuations around that of the average matrix.

For the open chain, that is $d_N = 0$, the eigenvectors of $H(\alpha)$ are obtained from those of $H(0)$ as

$$|\Psi(\alpha)\rangle = \eta^{1/2}(\alpha) |\Psi(0)\rangle \tag{11}$$

where $\eta(\alpha)$ is the similarity transformation of the pseudo-Hermitian condition (1) for a given parameter α.

Therefore, using Appendix A, we can show that besides being isospectral also the localization of the eigenvectors is not affected by the parameter α. The effect of the parameter is to make non-normal the non-Hermitian matrices of the family. This non-normality aspect of the matrices is revealed by investigating the pseudospectra of their eigenvalues. The eigenvectors of the pseudo-Hermitian open chain $H(\alpha)$ are obtained by a gauge transformation of the β-ensembles ones, a transformation which is not expected to produce change in their localization.

In the left column of Fig. 1, we present a comparison of the behavior of the pseudospectra (cf. Appendix B) of open chains of size $n = 64$ and $\beta = 1$ for the parameters $\alpha = 0.0, 0.25$ and 1.00 from top to bottom. The pattern shown in this figure of the pseudospectra is typical of non-normal matrices, and as a consequence indicates that these matrices should display instabilities under small perturbations. It was shown in Ref. [9] that the minimal perturbation for the transition to occur becomes arbitrarily small as the size of the matrix increases.

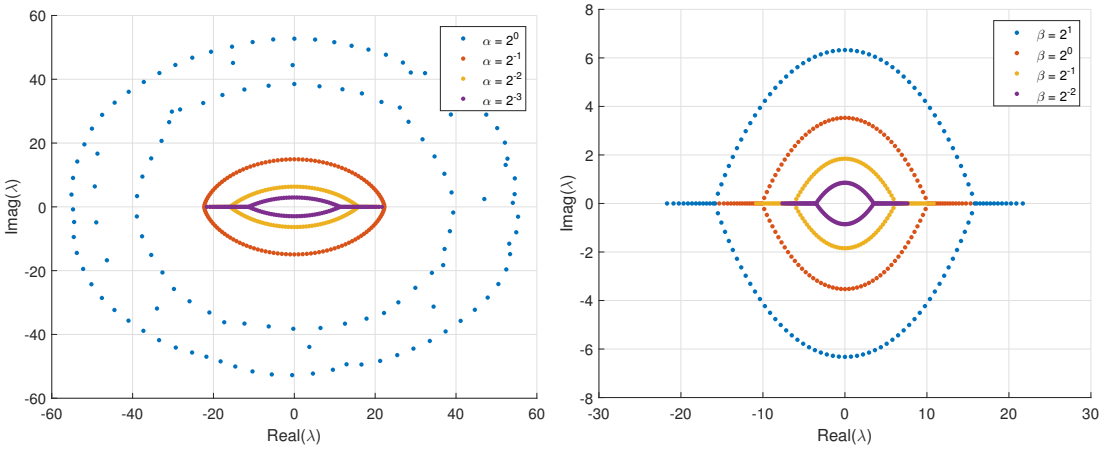

Figure 2. Spectra of the closed chain case for varying α of $N = 128$ and $\beta = 2.0$ average matrices (left) and for varying β of $N = 128$ and $\alpha = 0.25$ average matrices (right).

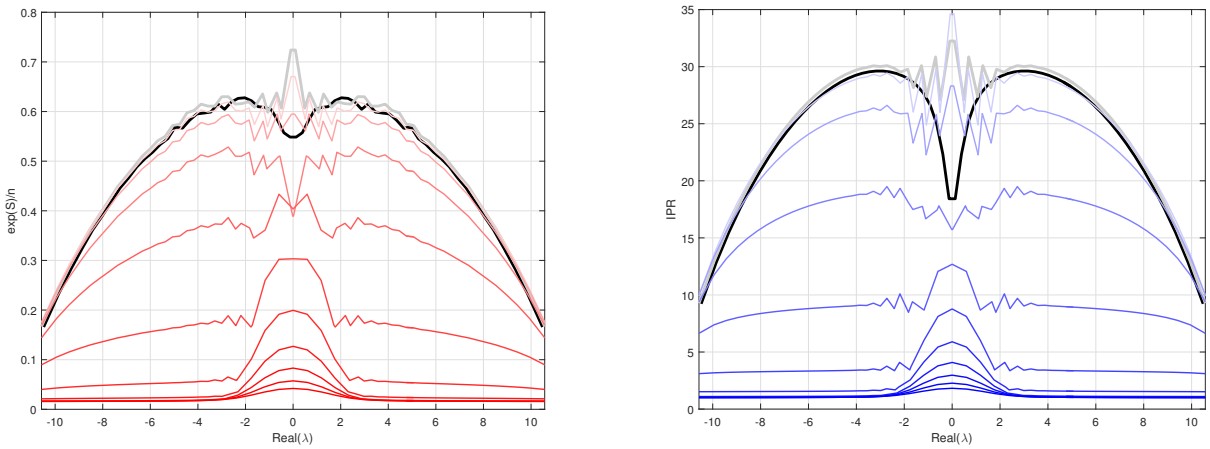

Figure 3. Entropy per lattice point (left) and Inverse Participation Ratio (right) for the open chain (black line), Hermitian closed chain (gray line) and increasing parameter α from 10^{-2} to 10^{-1} (top: red lines, increasing α corresponds to lower lines; bottom: blue lines, increasing α corresponds to lower lines).

2.2. Closed Chain

The analysis using Appendix A does not apply to the closed chain. The right column of Fig. 1 shows the pseudospectra for the average matrices of closed chains for varying α and Fig. 2 presents the eigenvalues of closed chain matrices varying parameters α (left) and β (right).

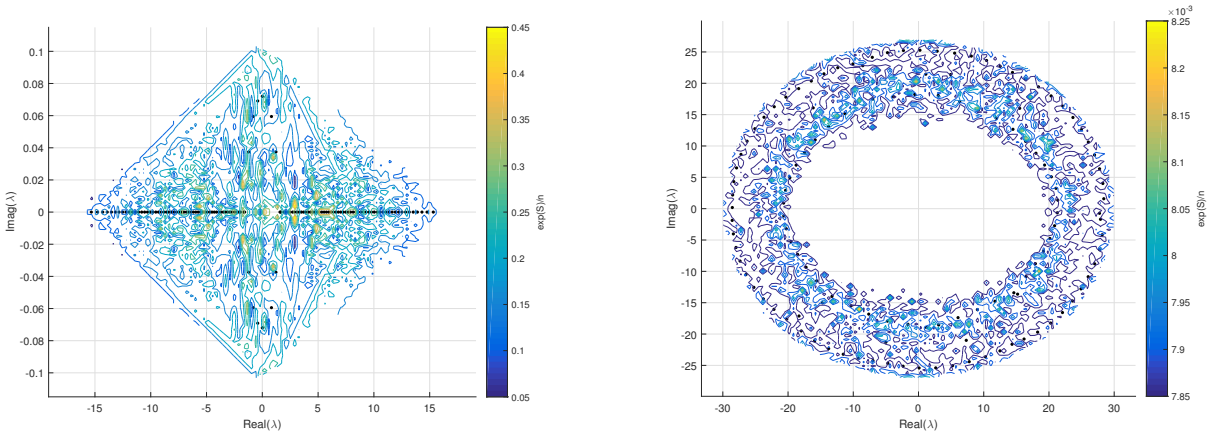

Figure 4. Entropy map for 5000 closed chain matrices of size $n = 128$ and $\beta = 1.0$, with $\alpha = 0.01$ (left) and $\alpha = 1.0$ (right). The black dots denote the eigenvalues of the average matrix.

Although the change in β does not change the characteristic shape of the spectra, the change in α causes dramatic change in the position of the eigenvalues in the complex plane as well as in the pseudospectrum. It is noteworthy that the structure seen in the bottom-right corner of Fig. 1, showing two concentric ellipses, differs from any of the behaviors commonly observed in the literature [4, 9, 11].

This suggests the possibility of changes in the properties also of the eigenvectors. This is illustrated in Figs. 3 and 4. In Fig. 3 the localization as measured through entropy and IPR are presented. There is a noticeable decrease in the fraction of occupied states as the parameter α increases. In Fig. 4, we can see a mapping for two particular values of α are presented. In the first case, $\alpha = 0.01$, the entropies display a low degree of localization, such that the eigenstates occupy a large fraction of the basis states for most of the matrices' eigenvalues. For the latter case, $\alpha = 1.00$, the states have become highly localized in the complex plane's vicinity to the average matrix's eigenvalues, having fractional occupancy of the basis states.

3. Conclusion

We have constructed a closed chain ensemble of random matrices, derived from the β-ensemble of random matrix theory. Numerical evidence was presented to illustrate the behavior of said matrices. In the tight-binding models of Refs. [4, 11], a spectra of oval shape with trailing real segments was seen. This was again seen in Refs. [9, 16]. The most noteworthy difference the present model has in regard to those previouly present in the literature is the presence, of a second elliptical structure in the spectrum, corroborated by the pseudospectral evidence, which appears spontaneously as the parameter α is increased.

Appendix A. The eigenvector delocalization

In order to study the localization of the eigenvectors, let us consider the Shannon entropy of a given state $\Psi(\alpha)$

$$S_{\eta(\alpha);N}[\Psi(\alpha)] = -\sum_{i=1}^{N} p_i[\Psi(\alpha)] \log\left(p_i[\Psi(\alpha)]\right) \tag{A.1}$$

of an eigenvector normalized in the inner product $\langle\phi|\,\psi\rangle_{\eta(\alpha)} \equiv \langle\phi|\,\eta(\alpha)\,|\psi\rangle$ [12], in which the probabilities of occupation of a given state $|i\rangle$ are given by

$$p_i = \langle\Psi(\alpha)|\,\eta(\alpha)\,|i\rangle\,\langle i|\,\Psi(\alpha)\rangle\,. \tag{A.2}$$

By taking exponential $N_c = \exp[S_{\eta(\alpha);N}(\Psi(\alpha))]$ we have a measure of the occupation of number of eigenstates of the basis. Assuming the scaling $N_c \sim N^D$, if $N_c \to 1$ when $N \to \infty$ the state is localized. For $0 < D < 1$ the eigenvector spreads over a fixed fraction of the states.

As long as the matrix $\eta^{1/2}|\eta = \eta^{1/2}\eta^{1/2}$ may be define, the eigenvectors $\Psi(\alpha)$ of matrices of the pseudo-Hermitian ensemble are expressed in terms of those $\Psi(0)$ of the Hermitian β-ensemble as

$$|\Psi(\alpha)\rangle = \eta(\alpha)^{1/2}\,|\Psi(0)\rangle\,. \tag{A.3}$$

For the case of the open chain, this relation implies that eigenvector localization independent of α as can easily be shown from Eqs. (A.2) and (A.3).

Additionally, the Inverse Participation Ratio

$$\mathrm{IPR} = \frac{1}{\sum\limits_{k=1}^{N} p_i^2} \tag{A.4}$$

is another way to measure the localization [13] of normalized vectors.

Appendix B. Pseudospectra

The pseudospectrum of a linear operator has been shown to be useful in analyzing operators for which there is no eigenvector basis (see *e.g.* [14, 15] and references therein). There are multiple equivalent ways by which the pseudospectrum of a linear operator can be defined. Here we use instead another definition that uses the resolvent of the matrix A, where the set z satisfies

$$|(z - A)|^{-1} < \frac{1}{\epsilon}, \tag{B.1}$$

with ϵ being positive and very small. The $||.||_2$ pseudospectrum may be related to the smallest singular value of the operator, that is for an operator H, the pseudospectrum is given by

$$\Sigma_\epsilon(H) = \{w \in \mathbb{C} : \sigma_{\min}(wI - H) \leq \epsilon\}\,. \tag{B.2}$$

For a normal matrix A, that is one for which $AA^\dagger = A^\dagger A$, the pseudospectra yields circles in the complex plane centered in the eigenvalues. On the other hand, for non-normal matrices, the pseudospectra present behaviors not regularly distributed close to the eigenvalues.

Acknowledgements

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[12] The notation $\langle\phi|\ \psi\rangle = \sum_{i=1}^{N} \phi_i^* \psi_i$ denotes the usual inner product in $\mathbb{C}^N$ space. The fact that generally for a pseudo-Hermitian matrix, the right eigenvectors $|\psi\rangle$ are not pairwise orthogonal requires us to normalize with respect to the left eigenvectors $\langle\phi|$. Instead they are connected as $|\phi\rangle = \eta\,|\psi\rangle$, which can be readily shown using (1).
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